GEOS-Chem Reference 2. Core Modules

GEOS-CHEM SUPPORT TEAM

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1 GEOS-Chem header modules

Here follows a list modules that are used to define various global parameters and variables used by GEOS-Chem. These were formerly COMMON-block include files (*.h), but were converted to Fortran-90 modules as part of the GEOS-Chem HP (high-performance) project.

1.1 Fortran: Module Interface CMN_DIAG_mod.F

Module CMN_DIAG_mod contains size parameters and global variables for the GEOS-Chem diagnostic arrays. This is mostly historical baggage.

INTERFACE:

```
MODULE CMN_DIAG_MOD
```

USES:

```
USE CMN_SIZE_MOD
USE CMN_FJX_MOD, ONLY : W_
USE PRECISION_MOD, ONLY : fpp => fp    ! For GEOS-Chem Precision (fp)
IMPLICIT NONE
PUBLIC
```

DEFINED PARAMETERS:

```
INTEGER, PARAMETER :: PD05=14
      INTEGER, PARAMETER :: PD06=NDSTBIN
      ! +3 for SEAC4RS SOA tracers (jaf, 6/25/13)
      INTEGER, PARAMETER :: PD07=15
      INTEGER, PARAMETER :: PD08=4
      INTEGER, PARAMETER :: PD09=6
      INTEGER, PARAMETER :: PD10=20
      INTEGER, PARAMETER :: PD11=5
      INTEGER, PARAMETER :: PD16=2
      INTEGER, PARAMETER :: PD17=8
      INTEGER, PARAMETER :: PD18=8
      INTEGER, PARAMETER :: PD21=5+(NRHAER+NDUST)*3+(NRHAER*2)+
                                 (NSTRATAER*3)
      INTEGER, PARAMETER :: PD22=28
      INTEGER, PARAMETER :: PD40=4
      INTEGER, PARAMETER :: PD43=7
      INTEGER, PARAMETER :: PD55=3
      ! Potential temperature diagnostic (hotp 7/31/09)
      INTEGER, PARAMETER :: PD57=1
      INTEGER, PARAMETER :: PD58=12
#if
      defined( TOMAS )
      ! Special settings for TOMAS aerosol microphysics (win, bmy, 1/22/10)
      INTEGER, PARAMETER :: PD59=TOMASBIN*TOMASSPEC
      INTEGER, PARAMETER :: PD60=TOMASBIN*TOMASSPEC
```

```
INTEGER, PARAMETER :: PD61=2
#else
     ! Normal settings for non-TOMAS simulations
     INTEGER, PARAMETER :: PD59=0
     INTEGER, PARAMETER :: PD60=1
     INTEGER, PARAMETER :: PD61=0
#endif
     INTEGER, PARAMETER :: PD64=W_
     INTEGER
                    :: PD65
     INTEGER, PARAMETER :: PD66=6
     INTEGER, PARAMETER :: PD67=23 ! (Lin, 31/03/09)
     INTEGER, PARAMETER :: PD68=8
     INTEGER, PARAMETER :: PD69=1
     !number of rad flux and optics output types
     !8 flux and 3*3=9 optics
     INTEGER, PARAMETER :: PD72R=17
     !total number of possible rad outputs (types*specs)
     !there are 11 possible flux output 'species' but
     !only 8 possible optics output 'species'
     !for simplicity we take the largest and put up with
     !some redundancy (should be 88+72=160)
     INTEGER, PARAMETER :: PD72=187 ! Radiation (Ridley 10/2012)
     !-----
     ! Variables for printing out selected tracers in diagnostic output
     #if
     defined( RRTMG )
     INTEGER, PARAMETER :: MAX_DIAG = 187
#else
     ! SDE 2013-11-17: Increased to 80 for UCX
     INTEGER, PARAMETER :: MAX_DIAG
#endif
#if
     defined( TOMAS )
     INTEGER, PARAMETER :: MAX_TRACER = NNPAR+1 ! For TOMAS (win, 1/25/10)
#else
     INTEGER, PARAMETER :: MAX_TRACER = NNPAR+6 ! For non-TOMAS simulations
#endif
PUBLIC DATA MEMBERS:
     ! Diagnostic counters & time variables
     |-----
     INTEGER :: KDA48, NJDAY(366)
     |-----
     ! Variables for the number of levels in multi-level diagnostics
```

```
! Removed LD03 -- this is now in diag03_mod.f (bmy, 1/21/05)
     ! Added LD09 (bmy, 6/27/05)
     ! Added LD54 (phs, 9/22/06)
     ! Added LD10 (phs, 9/18/07)
     ! Added LD31 (bmy, 5/8/07)
     ! Added LD52 (jaegle, 02/26/09)
     ! Added LD59, LD60, LD61 (bmy, 1/22/10)
     ! Added LD57 (hotp 7/31/09)
     !-----
     INTEGER :: LD12, LD13, LD14, LD15, LD16, LD17, LD18, LD21, LD22
     INTEGER :: LD24, LD25, LD26, LD37, LD38, LD39, LD43, LD45, LD47
     INTEGER :: LD54, LD64, LD65, LD66, LD68, LD01, LD02, LD05, LD07
     INTEGER :: LD09, LD10, LD31, LD52, LD19, LD57, LD58, LD59, LD60
     INTEGER :: LD61, LD62
     ! NDxx diagnostic flags
     INTEGER :: ND01, ND02, ND05, ND06, ND07, ND08, ND09, ND10, ND11
     INTEGER :: ND12, ND13, ND14, ND15, ND16, ND17, ND18, ND19, ND20
     INTEGER :: ND21, ND22, ND23, ND24, ND25, ND26, ND27, ND28, ND29
     INTEGER :: ND30, ND31, ND32, ND33, ND34, ND35, ND36, ND37, ND38
     INTEGER :: ND39, ND40, ND43, ND44, ND45, ND46, ND47, ND48, ND49
     INTEGER :: ND50, ND51, ND52, ND54, ND55, ND57, ND58, ND59
     INTEGER :: ND60, ND61, ND62, ND63, ND64, ND65, ND66, ND67, ND68
     INTEGER :: ND69, ND70, ND71, ND72, ND73, ND74, ND75
     ! Variables for printing out selected tracers in diagnostic output
     !-----
     INTEGER :: TINDEX(MAX_DIAG,MAX_TRACER)
     INTEGER :: TCOUNT(MAX_DIAG)
     INTEGER :: TMAX(MAX_DIAG)
     ! OH, J-Value, and 2-PM diagnostic arrays (bmy, 9/25/98)
     ! Move this here for now (bmy, 7/20/04)
     ! Removed HR1_NO and HR2_NO (mpayer, 11/8/13)
     REAL(fpp) :: HR1_JV, HR2_JV
     REAL(fpp) :: HR1_OH, HR2_OH, HR1_OTH, HR2_OTH
REMARKS:
   %%% NOTE: THIS MODULE IS DEPRECATED. MANY OF THE QUANTITIES STORED
   %%% in CMN_DIAG_MOD ARE NOW INCLUDED IN THE INPUT OPTIONS OBJECT,
                                                            %%%
   %%% BASED ON THE DERIVED TYPE IN Headers/input_opt_mod.F90.
                                                            %%%
   %%% (bmy, 11/19/12)
                                                            %%%
```

%%%		%%%
%%%	ALSO NOTE: IN GEOS-CHEM v11-01, WE WILL BE RETIRING THE BPCH	%%%
%%%	DIAGNOSTICS. MANY OF THESE PARAMETERS CAN THEN BE REMOVED.	%%%
%%%	(bmy, 6/24/16)	%%%
%%%%	o, o	/ %%%%

REVISION HISTORY:

- (1) Changed RCS ID tag comment character from "C" to "!" to allow freeform compilation. Also added & continuation characters in column 73 to allow header files to be included in F90 freeform files. Also converted PARAMETER statements to F90 syntax. (bmy, 6/25/02)
- (2) Add LD05 for sulfate prod/loss (rjp, bdf, bmy, 9/20/02)
- (3) Removed obsolete variables NTAUO, IDAYO, JDATEO, JYEARO, KDACC, KDADYN, KDACONV, KDASRCE, KDACHEM, KDA3FLDS, KDA6FLDS, KDKZZFLDS (bmy, 2/11/03)
- (4) Fix for LINUX remove & from column 73 (bmy, 6/27/03)
- (5) Added LDO3 for Kr85 Prod/loss diagnostic (bmy, 8/20/03)
- (6) Removed obsolete arrays (bmy, 1/21/05)
- (7) Rename MAXDIAG to MAX_DIAG and MAXTRACER to MAX_TRACER in order to avoid name conflicts with "gamap_mod.f" (bmy, 5/3/05)
- (8) Remove reference to TRCOFFSET (bmy, 5/16/06)
- (9) Added multi level LD54 to common CDIAG1 (phs, 9/22/06)
- (10) Added multi level LD10 to common CDIAG1. Set PD10 to 20. Set PD66 to 6. (phs, 9/18/07)
- (11) Added LD52 to common CDIAG1 (jaegle, 02/26/09)
- (12) Add GLYX, MGLY, SOAG, SOAM, and a few other tracers to AD17, AD18 for archiving rainout and washout fraction. (tmf, 1/7/09)
- (13) Add GLYX, MGLY J value archive. (tmf, 1/7/09)
- (14) Add GLYX, MGLY, SOAG, SOAM, and a few other tracers to AD37, AD38, AD39 $\,$
 - for archiving rainout and washout flux. (tmf, 1/7/09)
- (15) Add GLYX, MGLY, GLYC, 6 PANs, SOAG, SOAM dry dep, PD44 = 41.(tmf, 1/7/09)
- (16) Add biogenic C2H4 emission, PD46 = 6. (tmf, 1/20/09)
- (17) Add one met field to ND67 (EFLUX). (ccc, 5/14/09)
- (18) Add declarations for PD58 and PD60, LD19, LD58. (kjw,8/18/09)
- (19) Redimension PD59, PD60, PD61 for TOMAS microphysics. Added LD59, LD60, LD61 to common block. Reset MAX_TRACER to NNPAR+1 for TOMAS. (win, bmy, 1/22/10)
- (20) Add LD57 and PD57 (potential temperature) (hotp, 3/15/10)
- 03 Aug 2010 R. Yantosca Added ProTeX headers
- 03 Aug 2010 P. Kasibhatla & R. Yantosca Now set MAX_TRACER to NNPAR+6 to match ND09 diagnostic
- 09 Mar 2011 R. Yantosca Updated MAX_TRACER for APM (G. Luo)
- 03 Aug 2011 M. Long Converted from Header file to Module
- 08 Nov 2013 M. Sulprizio- Remove HR1_NO and HR2_NO. They are no longer needed for ND43 because NO, NO2, and NO3 are now tracers.

```
O2 Dec 2014 - M. Yannetti - Added PRECISION_MOD

15 Dec 2014 - M. Sulprizio- Moved radiation diagnostic from ND72 to ND72 to avoid conflicts with hourly max ppbv diagnostic.

23 Jun 2016 - R. Yantosca - Remove references to APM code; it is no longer compatible with the FlexChem implementation

21 Jul 2016 - R. Yantosca - Remove instances of NNPAR & obsolete parameters
```

1.1.1 Init_Cmn_Diag

Subroutine INIT_CMN_DIAG initializes quantities based on the grid-independent size parameters.

INTERFACE:

```
SUBROUTINE Init_CMN_DIAG( am_I_Root, RC )
```

USES:

USE ErrCode_Mod

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC     ! Success or failure?
```

REVISION HISTORY:

```
19 Nov 2012 - R. Yantosca - Added ProTeX headers
```

1.2 Fortran: Module Interface CMN_FJX_mod.F

Module CMN_FJX_MOD contains parameters and global variables used to interface between Harvard chemistry and UC-Irvine photolysis programs (Fast-J/Fast-JX), along with all Fast-J(X) global variables and some physical constants for the GEOS-Chem chemistry code.

INTERFACE:

MODULE CMN_FJX_MOD

USES:

```
USE CMN_SIZE_MOD, ONLY: IIPAR, JJPAR, LLPAR, LLCHEM
USE CMN_SIZE_MOD, ONLY: NDUST, NAER, NRHAER, NSTRATAER, NRH

USE PRECISION_MOD! For GEOS-Chem Precision (fp)

IMPLICIT NONE
PUBLIC
```

DEFINED PARAMETERS:

```
! New (SDE 03/28/13)
     ! Index in RAA & QAA of 999 nm wavelength
     INTEGER, PARAMETER :: IND999 = 5
     ! Required size of aerosol arrays
     INTEGER
                                      ! Number of CTM layers
                      :: L_
     INTEGER
                    :: L1_ ! Number of CTM layer edges
     INTEGER
                      :: L2_
                                      ! Number of levels in FJX grid that
                                      ! inc. both edges and mid-points
                                      ! Vertical levels for J-values
     INTEGER
                      :: JVL_
     INTEGER, PARAMETER :: JVN_ = 121     ! Max number of J-values
#if defined( UCX )
     INTEGER, PARAMETER :: AN_ = 37    ! Including PSCs
#else
     INTEGER, PARAMETER :: AN_ = 35     ! # of separate aerosols per layer
#endif
     ! Variables used to interface GEOS-Chem and Fast-JX at runtime
     ! Branches for photolysis species
     INTEGER
                      :: BRANCH(JVN_)
     ! Names of photolysis species
     CHARACTER (LEN=10) :: RNAMES(JVN_)
     ! Mapping array from Harvard species names to UCI species names
                      :: RINDEX(JVN )
     INTEGER
     ! Output J values
     REAL(fp), ALLOCATABLE :: ZPJ(:,:,:)
     !-----
     ! variables used to map fast-JX J's onto CTM J's
     I-----
     ! Multiplication factor for fast-JX calculated J
     REAL(fp)
                       :: JFACTA(JVN_)
     ! Index arrays that map Jvalue(j) onto rates
                      :: JIND(JVN_)
     ! Mumber of Photolysis reactions in CTM chemistry, derived here NRATJ
```

```
! must be .le. JVN_
     INTEGER
                 :: NRATJ
     ! Label of J-value used in the main chem model
     CHARACTER*50 :: JLABEL(JVN_)
     ! JXL_: vertical(levels) dim for J-values computed within fast-JX
                       :: JXL_
     INTEGER
     INTEGER
                      :: JXL1_
     ! JXL2_: 2*JXL_ + 2 = mx no. levels in the basic Fast-JX grid (mid-level)
     INTEGER
                     :: JXL2_
     ! WX_ = dim = no. of wavelengths in input file
     INTEGER, PARAMETER :: WX_ = 18
     ! X_ = dim = max no. of X-section data sets (input data)
     INTEGER, PARAMETER :: X_{-} = 72
     ! A_ = dim = no. of Aerosol/cloud Mie sets (input data)
     INTEGER, PARAMETER :: A_
                               = 56
     ! W_ = dim = no. of Wavelength bins: =18 std, =12 trop only
#if defined( UCX )
     INTEGER, PARAMETER :: W_{-} = 18
#else
     INTEGER, PARAMETER :: W_{-} = 12
#endif
     ! N_{-} = no. of levels in Mie scattering arrays
           = 2*NC+1 = 4*(L_+1) + 1 + 2*sum(JADDLV)
     INTEGER, PARAMETER :: N_{-} = 601
     ! M_ = no. of Gauss points used, must = 4 in fast_JX (no option)
     INTEGER, PARAMETER :: M_
                                = 4
     ! M2_ = 2*M_ = 8, replaces MFIT
     INTEGER, PARAMETER :: M2_ = 2*M_
     I-----
     ! 4 Gauss pts = 8-stream
     REAL(fp), DIMENSION(M_), PARAMETER ::
                 EMU = [.06943184420297e+0_fp, .33000947820757e+0_fp,
                        .66999052179243e+0_fp, .93056815579703e+0_fp]
     REAL(fp), DIMENSION(M_), PARAMETER ::
                 WT = [.17392742256873e+0_fp, .32607257743127e+0_fp,
                        .32607257743127e+0_fp, .17392742256873e+0_fp]
```

```
! ZZHT: scale height (cm)
REAL(fp), PARAMETER :: ZZHT = 5.e+5_fp
! RAD: Radius of Earth (cm)
REAL(fp), PARAMETER :: RAD = 6375.e+5_fp
! ATAU: heating rate (factor increase from one layer to the next)
REAL(fp), PARAMETER :: ATAU = 1.120e+0_fp
! ATAUO: minimum heating rate
REAL(fp), PARAMETER :: ATAU0 = 0.010e+0_{fp}
! JTAUMX = maximum number of divisions (i.e., may not get to ATAUMN)
INTEGER
               :: JTAUMX
! Physical constants
REAL(fp), PARAMETER :: UVXPLANCK = 6.62606957e-34
REAL(fp), PARAMETER :: UVXCCONST = 2.99792458e8
! Conversion factors from photons/cm2s to W/m2
REAL(fp), DIMENSION(WX_) :: UVXFACTOR
!-----
! Variables in file 'FJX_spec.dat' (RD_XXX)
T-----
! WBIN: Boundaries of wavelength bins
REAL(fp)
             :: WBIN(WX_+1)
! WL: Centres of wavelength bins - 'effective wavelength'
REAL(fp)
                  :: WL(WX_)
! FL: Solar flux incident on top of atmosphere (cm-2.s-1)
REAL(fp)
                 :: FL(WX_)
          :: Q02(WX_,3) ! Q02: 02 cross-sections
:: Q03(WX_,3) ! Q03: 03 cross-sections
REAL(fp)
REAL(fp)
REAL(fp) :: Q1D(WX_,3) ! Q1D: 03 => O(1D) quantum yield
! QQQ: Supplied cross sections in each wavelength bin (cm2)
REAL(fp) :: QQQ(WX_,3,X_)
! QRAYL: Rayleigh parameters (effective cross-section) (cm2)
           :: QRAYL(WX_+1)
REAL(fp)
! TQQ: Temperature for supplied cross sections
REAL(fp) :: TQQ(3,X_{-})
```

```
! LQQ = 1, 2, or 3 to determine interpolation with T or P
TNTEGER.
               :: LQQ(X_)
! TITLEJX: Title for supplied cross sections, from 'FJX_spec.dat'
CHARACTER*6
            :: TITLEJX(X_)
! SQQ: Flag for supplied cross sections, from 'FJX_spec.dat'
              :: SQQ(X_)
CHARACTER*1
!-----
! Variables in file 'jv_spec_mie.dat' (RD_MIE)
1-----
! QAA: Aerosol scattering phase functions
REAL(fp)
                :: QAA(5,A_)
! WAA: 5 Wavelengths for the supplied phase functions
REAL(fp)
           :: WAA(5,A_)
! PAA: Phase function: first 8 terms of expansion
REAL(fp)
         :: PAA(8,5,A_{-})
! RAA: Effective radius associated with aerosol type
REAL(fp) :: RAA(5,A_{-})
! SAA: Single scattering albedo
REAL(fp) :: SAA(5,A_{-})
! NAA: Number of categories for scattering phase functions
INTEGER
               :: NAA
!-----
! Variables in file 'jv_spec_aod.dat' (RD_AOD)
! QAA_AOD: Aerosol scattering phase functions
                :: QAA_AOD(A_)
REAL(fp)
! WAA: 5 Wavelengths for the supplied phase functions
REAL(fp)
                :: WAA_AOD(A_)
! PAA: Phase function: first 8 terms of expansion
                :: PAA_AOD(8,A_)
REAL(fp)
! RAA: Effective radius associated with aerosol type
REAL(fp)
          :: RAA_AOD(A_)
```

```
! SAA: Single scattering albedo
     REAL(fp)
                      :: SAA_AOD(A_)
     1-----
     ! Variables in file 'atmos_std.dat' (RD_PROF)
     I-----
     ! T and O3 reference profiles
     REAL(fp), DIMENSION(51,18,12) :: TREF, OREF
     ! Interfacing indices for GC and FJX aerosols
     INTEGER, DIMENSION(AN_) :: MIEDX
     ! TITLEAA: Title for scattering data
     CHARACTER*20, DIMENSION(A_) :: TITLEAA
     ! Dust and aerosol optical depths
     REAL(fp), ALLOCATABLE :: ODMDUST(:,:,:,:)
     REAL(fp), ALLOCATABLE :: ODAER(:,:,:,:)
     INTEGER NJX, NW1, NW2
     I-----
     ! Variables added for RRTMG (dar, mps, 12/5/14)
     T-----
     INTEGER, PARAMETER :: NWVAA = 41 !number of wavelengths in LUT INTEGER, PARAMETER :: NWVAAO = 11 !number of non-RRTMG wavelengths
     INTEGER, PARAMETER :: NWVAART = NWVAA-NWVAAO !number of RRTMG wvs
     INTEGER, PARAMETER :: NRAA = 7 !number of aer sizes in LUT
#if defined( UCX )
     INTEGER, PARAMETER :: NSPAA = 8 !number of species in LUT
     INTEGER, PARAMETER :: NASPECRAD = 16  !aerosol species in RT
     INTEGER, PARAMETER :: NSPECRAD = 18 !aerosol+gas species in RT
     INTEGER, PARAMETER :: NSPECRADMENU = 11!number of choices for RT flux
#else
     INTEGER, PARAMETER :: NSPAA = 6 !number of species in LUT
     INTEGER, PARAMETER :: NASPECRAD = 14 !aerosol species in RT
     INTEGER, PARAMETER :: NSPECRAD = 16 !aerosol+gas species in RT
     INTEGER, PARAMETER :: NSPECRADMENU = 10!number of choices for RT flux
#endif
     INTEGER, PARAMETER :: NALBD = 2
     INTEGER, PARAMETER :: NEMISS = 16
     ! New optical arrays
     REAL*8 :: WVAA(NWVAA, NSPAA)
     REAL*8 :: RHAA(NRAA, NSPAA)
     REAL*8 :: NRLAA(NWVAA, NRAA, NSPAA)
```

EOC

```
REAL*8 :: NCMAA(NWVAA, NRAA, NSPAA)
      REAL*8 :: RDAA(NRAA,NSPAA)
     REAL*8 :: RWAA(NRAA, NSPAA)
     REAL*8 :: SGAA(NRAA, NSPAA)
     REAL*8 :: QQAA(NWVAA, NRAA, NSPAA)
     REAL*8 :: ALPHAA(NWVAA, NRAA, NSPAA)
     REAL*8 :: REAA(NRAA, NSPAA)
     REAL*8 :: SSAA(NWVAA, NRAA, NSPAA)
     REAL*8 :: ASYMAA(NWVAA, NRAA, NSPAA)
     REAL*8 :: PHAA(NWVAA, NRAA, NSPAA, 8)
     REAL*8 :: WVSELECT(3) !wavelengths requested by user
      INTEGER :: IWVSELECT(2,3) !index of requested wavelengths
      INTEGER :: IRTWVSELECT(2,3) !index of requested RT wavelengths
      ! max of 3 but need 2 per wavelength if interpolating
      INTEGER :: NWVSELECT !number of selected AOD output wavelengths
                           !(max=3)
      INTEGER :: NWVREQUIRED !number of wvs required for interpolation
      INTEGER :: IWVREQUIRED(6) !index of wavelengths for interpo.
      INTEGER :: NRTWVREQUIRED !number of wvs required for RT interpolation
      INTEGER :: IRTWVREQUIRED(6) !index of wavelengths for RT interpo.
      ! list of required wavelengths, up to max of 3 x 2
      INTEGER :: IWV1000 !Store the wavelength index for 1000nm for Fast-J
      !coefficients for interpolation of wavelength (and for RT too)
                :: ACOEF_WV(3),BCOEF_WV(3),CCOEF_WV(3)
      REAL*8
      REAL*8
                :: ACOEF_RTWV(3),BCOEF_RTWV(3),CCOEF_RTWV(3)
      CHARACTER*5 :: STRWVSELECT(3) !String array of requested wavelengths
                :: LSPECRADMENU(NSPECRADMENU) !indices for number of species on input menu
      INTEGER
      INTEGER
                 :: SPECMASK(NSPECRAD) !list of binary switches for different
                                    !species flux output
      ! RH indices
      INTEGER, ALLOCATABLE :: IRHARR(:,:,:)
#if defined( RRTMG )
      !to pass to RT code
      !one for each hydrophilic/hydrophobic aerosol and optical dust bin
      !and also sulfate, nitrate and ammonia are separate too
      REAL*8, ALLOCATABLE :: RTODAER(:,:,:,:)
      REAL*8, ALLOCATABLE :: RTSSAER(:,:,:,:)
     REAL*8, ALLOCATABLE :: RTASYMAER(:,:,:,:)
#endif
      CONTAINS
```

```
GEOS-Chem Global Chemical Transport Model
\mbox{}\hrulefill\
 \subsubsection [Init\_Cmn\_Fjx] {Init\_Cmn\_Fjx}
 Routine INIT\_CMN\_FJX initializes quantities based on
   the grid-independent size parameters.
 //
 \\{\bf INTERFACE:}
\begin{verbatim}
      SUBROUTINE Init_CMN_FJX( am_I_Root, RC )
USES:
      USE ErrCode_Mod
INPUT PARAMETERS:
      LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
OUTPUT PARAMETERS:
      INTEGER, INTENT(OUT) :: RC     ! Success or failure?
REVISION HISTORY:
   21 Feb 2014 - M. Sulprizio- Renamed from Set_CMN_FJX_MOD to Init_CMN_FJX.
                             We now set several variables here that depend on
                            LLPAR, since LLPAR is no longer a parameter and
                             can't be used to define a parameter.
1.2.1 Cleanup_Cmn_Fjx
Subroutine CLEANUP_CMN_FJX deallocates all module arrays.
INTERFACE:
      SUBROUTINE Cleanup_CMN_FJX( am_I_Root, RC )
USES:
      USE ErrCode_Mod
INPUT PARAMETERS:
      LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC     ! Success or failure?
```

REVISION HISTORY:

```
21 Feb 2014 - M. Sulprizio- Initial version
```

1.3 Fortran: Module Interface CMN_O3_mod.F

Common blocks for anthro emissions (via SMVGEAR!)

INTERFACE:

MODULE CMN_03_MOD

USES:

```
USE CMN_SIZE_MOD, ONLY : IIPAR, JJPAR, LLPAR
USE PRECISION_MOD

IMPLICIT NONE
PUBLIC
```

PUBLIC DATA MEMBERS:

REMARKS:

```
NOTE: Now NEMPARA = max no. of anthropogenic emissions
NEMPARB = max no. of biogenic emissions
```

REVISION HISTORY:

```
23 Aug 2011 - M. Long - Converted to Module from Header file
29 Mar 2013 - M. Payer - Removed FRACO3, FRACNO, FRACNO2, SAVENO, SAVENO2, and SAVENO3. They are no longer needed because 03, NO, NO2, and NO3 are now tracers.

13 Aug 2013 - M. Sulprizio- Increase last dimension of EMISS_BVOC to include sesquiterpenes and add EMISTNAP for SOA + semivolatile POA simulation (H. Pye)

21 Feb 2014 - M. Sulprizio- Added SAVEO1D and SAVEO3P for UCX (S.D. Eastham)

03 Dec 2014 - M. Yannetti - Added PRECISION_MOD

22 May 2015 - R. Yantosca - Remove arrays made obsolete by HEMCO
```

1.3.1 Init_Cmn_O3

Subroutine INIT_CMN_O3 allocates all module arrays.

INTERFACE:

```
SUBROUTINE Init_CMN_O3( am_I_Root, RC )
```

USES:

USE ErrCode_Mod

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

```
19 Nov 2012 - R. Yantosca - Added ProTeX headers
01 Feb 2013 - R. Yantosca - Now allocate EMISS_BVOC to 19 emission species
29 Mar 2013 - M. Payer - Removed FRACO3, FRACNO, FRACNO2, SAVENO, SAVENO2, and SAVENO3. They are no longer needed because
03, NO, NO2, and NO3 are now tracers.

13 Aug 2013 - M. Sulprizio- Increase last dimension of EMISS_BVOC to include sesquiterpenes and add EMISTNAP for SOA + semivolatile POA simulation (H. Pye)
22 May 2015 - R. Yantosca - Remove arrays made obsolete by HEMCO
```

1.3.2 Cleanup_Cmn_O3

Subroutine CLEANUP_CMN_O3 allocates all module arrays.

INTERFACE:

```
SUBROUTINE Cleanup_CMN_03( am_I_Root, RC )
```

USES:

USE ErrCode_Mod

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

```
19 Nov 2012 - R. Yantosca - Added ProTeX headers
29 Mar 2013 - M. Payer - Removed FRACO3, FRACNO, FRACNO2, SAVENO, SAVENO2, and SAVENO3. They are no longer needed because 03, NO, NO2, and NO3 are now tracers.
22 May 2015 - R. Yantosca - Remove arrays made obsolete by HEMCO
```

1.4 Fortran: Module Interface CMN_SIZE_mod.F

CMN_SIZE contains size parameters for GEOS-Chem arrays.

INTERFACE:

MODULE CMN_SIZE_MOD

USES:

```
USE PRECISION_MOD, ONLY : fpp => fp    ! For GEOS-Chem Precision (fpp)
IMPLICIT NONE
PUBLIC
```

DEFINED PARAMETERS:

```
REAL(fpp), PARAMETER :: DJSIZE = 4.0e+0_fpp
#elif defined( GRID2x25 )
     REAL(fpp), PARAMETER :: DISIZE = 2.5e+0_fpp
     REAL(fpp), PARAMETER :: DJSIZE = 2.0e+0_fpp
#elif defined( GRID1x125 )
     REAL(fpp), PARAMETER :: DISIZE = 1.25e+0_fpp
     REAL(fpp), PARAMETER :: DJSIZE = 1.0e+0_fpp
#elif defined( GRID1x1 )
     REAL(fpp), PARAMETER :: DISIZE = 1.0e+0_fpp
     REAL(fpp), PARAMETER :: DJSIZE = 1.0e+0_fpp
#elif defined( GRID05x0666 )
     REAL(fpp), PARAMETER :: DISIZE = 2e+0_fpp/3e+0_fpp
     REAL(fpp), PARAMETER :: DJSIZE = 0.5e+0_fpp
#elif defined( GRID05x0625 )
     REAL(fpp), PARAMETER :: DISIZE = 0.625e+0_fpp
     REAL(fpp), PARAMETER :: DJSIZE = 0.5e+0_fpp
#elif defined( GRID025x03125)
     REAL(fpp), PARAMETER :: DISIZE = 0.3125e+0_fpp
     REAL(fpp), PARAMETER :: DJSIZE = 0.25e+0_fpp
#elif defined( EXTERNAL_GRID )
     REAL(fpp)
                       :: DISIZE
     REAL(fpp) :: DJSIZE
#endif
     |-----
     ! GRID SETTINGS #1: Necessary for the grid-independent GEOS-Chem
     1-----
     INTEGER
                         :: I_LO
                                       ! Minimum lon index on this CPU
                                    ! Minimum lat index on this CPU
                          :: J_LO
     INTEGER
                                       ! Maximum lon index on this CPU
                         :: I_HI
     INTEGER
                                       ! Maximum lat index on this CPU
     INTEGER
                         :: J_HI
                         :: IM_WORLD ! # of lons in the global grid
:: JM_WORLD ! # of lats in the global grid
     INTEGER
     INTEGER
                         :: LM_WORLD
     INTEGER
                                       ! # of levs in the global grid
     REAL(fpp), ALLOCATABLE :: DLON(:,:,:) ! Array of delta-lon [degrees]
     REAL(fpp), ALLOCATABLE :: DLAT(:,:,:) ! Array of delta-lat [degrees]
     ! GRID SETTINGS #2: Mostly historical declarations (keep for now)
     ! IGLOB
                 = global longitude dimension
     ! JGLOB
               = global latitude dimension
     ! LGLOB
               = max number of sigma levels
     ! IIPAR
               = window longitude dimension
     ! JJPAR
               = window latitude dimension
     ! LLPAR
               = window vertical dimension
     ! LLTROP
               = maximum number of tropospheric levels for variable
                  tropopause
     ! LLTROP_FIX = number of tropospheric levels for offline simulations
```

```
! LLSTRAT = maximum number of levels below stratopause
    ! LLCHEM = maximum number of levels included in chemistry grid
    ! LLCHEM_FIX = number of chemgrid levels for offline simulations
             = model top pressure (mb)
    ! Most of the time, GEOS-CHEM is used for global simulations.
    ! In this case, then IIPAR=IGLOB, JJPAR=JGLOB, LLPAR=LGLOB.
    ! For nested grids, then IIPAR<IGLOB, JJPAR<JGLOB, LLPAR<LGLOB.
    ! IIPAR and JJPAR are always set at runtime
    ! for both GEOS-Chem HP and GEOS-Chem Classic
    INTEGER
                     :: IIPAR
    INTEGER
                    :: JJPAR
#if defined ( EXTERNAL_GRID ) || defined( EXTERNAL_FORCING ) || defined( ESMF_ )
    I-----
            %%%%%% GEOS-Chem HP (with ESMF & MPI) %%%%%%%
    ! We need to make all of these be variables rather than
    ! parameters, so that they can be defined directly from the
    ! ESMF interface. (bmy, 10/11/12)
                    :: IGLOB
    INTEGER
    INTEGER
                    :: JGLOB
    INTEGER
                    :: LGLOB
    INTEGER
                    :: LLPAR
                    :: LLTROP_FIX
    INTEGER
    INTEGER
                    :: LLTROP
                 :: LLSTRAT
    INTEGER
    REAL*8, PARAMETER :: PTOP = 0.01d0
#else
    !-----
            %%%%%% GEOS-Chem CLASSIC (with OpenMP) %%%%%%%
    ! For GEOS-Chem "Classic", we can preset the values of IGLOB,
    ! JGLOB, LGLOB, LLTROP, LLTROP_FIX, LLSTRAT, (bmy, 5/22/15)
    1-----
#if
    defined(GCAP) && defined(GRID4x5)
    !-----
    ! GCAP: 4 x 5
    I-----
                              = 72
    INTEGER
                    :: IGLOB
    INTEGER
                    :: JGLOB
                              = 45
                    :: LGLOB
    INTEGER
                               = 23
                  :: LLPAR
    INTEGER
    INTEGER, PARAMETER :: LLTROP = 12
    INTEGER, PARAMETER :: LLTROP_FIX = LLTROP
```

```
INTEGER,
              PARAMETER :: LLSTRAT
    REAL(fpp), PARAMETER :: PTOP = 0.002e+0_fpp
#elif defined( GEOS_4 ) && defined( GRID4x5 )
    1-----
    ! GEOS-4: 4 x 5
    1-----
                     :: IGLOB
                               = 72
    INTEGER
    INTEGER
                     :: JGLOB
                               = 46
                     :: LGLOB = 55
    INTEGER
    defined( GRIDREDUCED )
#if
    INTEGER :: LLPAR = 30 ! Reduced vertical grid INTEGER, PARAMETER :: LLTROP = 22 ! -- 30 levels
    INTEGER, PARAMETER :: LLSTRAT = 27
#else
    INTEGER
                     :: LLPAR
                                          ! Full vertical grid
    INTEGER, PARAMETER :: LLTROP = 23
                                       ! -- 55 levels
    INTEGER, PARAMETER :: LLSTRAT = 42
#endif
    INTEGER, PARAMETER :: LLTROP_FIX = 17
    REAL(fpp), PARAMETER :: PTOP = 0.01e+0_fpp
#elif defined( GEOS_4 ) && defined( GRID2x25 )
    ! GEOS-4: 2 x 2.5
    1-----
                               = 144
    INTEGER
                     :: IGLOB
                    :: JGLOB
    INTEGER
                                = 91
                     :: LGLOB
    INTEGER
                                = 55
#if
    defined( GRIDREDUCED )
    INTEGER :: LLPAR = 30 ! Reduced vertical grid INTEGER, PARAMETER :: LLTROP = 22 ! -- 30 levels
    INTEGER, PARAMETER :: LLSTRAT = 27
#else
    INTEGER
                    :: LLPAR
                                         ! Full vertical grid
    INTEGER, PARAMETER :: LLTROP
                               = 23
                                         ! -- 55 levels
    INTEGER, PARAMETER :: LLSTRAT = 42
#endif
    INTEGER, PARAMETER :: LLTROP_FIX = 17
    REAL(fpp), PARAMETER :: PTOP = 0.01e+0_fpp
#elif defined( GEOS_4 ) && defined( GRID1x125 )
    !-----
    ! GEOS-4: 1 x 1.2.5
```

```
= 288
     INTEGER
                      :: IGLOB
     INTEGER
                      :: JGLOB
                                 = 181
                      :: LGLOB
     INTEGER
                                  = 55
#if
    defined( GRIDREDUCED )
     INTEGER :: LLPAR = 30 ! Reduced vertical grid
     INTEGER, PARAMETER :: LLTROP
                                 = 22
                                            ! -- 30 levels
     INTEGER, PARAMETER :: LLSTRAT = 27
#else
     INTEGER
                      :: LLPAR
                                             ! Full vertical grid
     INTEGER, PARAMETER :: LLTROP = 23
                                            ! -- 55 levels
     INTEGER, PARAMETER :: LLSTRAT = 42
#endif
     INTEGER, PARAMETER :: LLTROP_FIX = 17
     REAL(fpp), PARAMETER :: PTOP = 0.01e+0_fpp
#elif defined( GEOS_5 ) && defined( GRID4x5 )
     !-----
     ! GEOS-5: 4 x 5
                                 = 72
     INTEGER
                      :: IGLOB
     INTEGER
                                 = 46
                      :: JGLOB
     INTEGER
                      :: LGLOB
                                 = 72
     defined( GRIDREDUCED )
#if
                                          ! Reduced vertical grid
     INTEGER :: LLPAR = 47
     INTEGER, PARAMETER :: LLTROP_FIX = 38
                                            ! -- 47 levels
     INTEGER, PARAMETER :: LLTROP = 38
     INTEGER, PARAMETER :: LLSTRAT = 44
#else
                      :: LLPAR
     INTEGER
                                            ! Full vertical grid
     INTEGER, PARAMETER :: LLTROP_FIX = 40
                                            ! -- 72 levels
     INTEGER, PARAMETER :: LLTROP = 40
     INTEGER, PARAMETER :: LLSTRAT = 59
#endif
    REAL(fpp), PARAMETER :: PTOP = 0.01e+0_fpp
#elif defined( GEOS_5 ) && defined( GRID2x25 )
     ! GEOS-5: 2 x 2.5
                      :: IGLOB = 144
     INTEGER
                      :: JGLOB
                                 = 91
     INTEGER
     INTEGER
                      :: LGLOB
                                 = 72
     defined( GRIDREDUCED )
#if
     INTEGER :: LLPAR = 47 ! Reduced vertical grid INTEGER, PARAMETER :: LLTROP_FIX = 38 ! -- 47 levels
                :: LLPAR = 47
     INTEGER, PARAMETER :: LLTROP = 38
```

```
PARAMETER :: LLSTRAT = 44
    INTEGER,
#else
    INTEGER
                    :: LLPAR
                                       ! Full vertical grid
    INTEGER, PARAMETER :: LLTROP_FIX = 40
                                       ! -- 72 levels
    INTEGER, PARAMETER :: LLTROP = 40
    INTEGER, PARAMETER :: LLSTRAT = 59
#endif
    REAL(fpp), PARAMETER :: PTOP = 0.01e+0_fpp
#elif defined( GEOS_5 ) && defined( GRID1x125 )
    !-----
    ! GEOS-5: 1 x 1.25
    1-----
                   :: IGLOB = 288
:: JGLOB = 181
    INTEGER
    INTEGER
                   :: LGLOB
                              = 72
    INTEGER
#if
    defined( GRIDREDUCED )
              :: LLPAR = 47
                                     ! Reduced vertical grid
! -- 47 levels
    INTEGER
    INTEGER, PARAMETER :: LLTROP_FIX = 38
    INTEGER, PARAMETER :: LLTROP = 38
    INTEGER, PARAMETER :: LLSTRAT = 44
#else
    INTEGER
                    :: LLPAR
                                       ! Full vertical grid
    INTEGER, PARAMETER :: LLTROP_FIX = 40
                                       ! -- 72 levels
    INTEGER, PARAMETER :: LLTROP = 40
    INTEGER, PARAMETER :: LLSTRAT = 59
#endif
    REAL(fpp), PARAMETER :: PTOP = 0.01e+0_fpp
#elif defined( GEOS_5 ) && defined( GRIDO5x0666 )
    !-----
    ! GEOS-5: 0.5 x 0.666
    !-----
#if
    defined( NESTED_CH )
    INTEGER
                   :: IGLOB = 121 ! NESTED CH 0.5x0.666
                   :: JGLOB
    INTEGER
                              = 133
                   :: LGLOB
    INTEGER
                              = 72
#elif defined( NESTED_NA )
                   :: IGLOB = 151 ! NESTED NA 0.5x0.666
    INTEGER
    INTEGER
                   :: JGLOB
                              = 121
                              = 72
                   :: LGLOB
    INTEGER
#elif defined( NESTED_EU )
    INTEGER
                   :: IGLOB = 121 ! NESTED EU 0.5x0.666
                   :: JGLOB
                              = 81
    INTEGER
                   :: LGLOB = 72
    INTEGER
#endif
#if defined( GRIDREDUCED )
```

```
INTEGER
                     :: LLPAR = 47
                                          ! Reduced vertical grid
    INTEGER, PARAMETER :: LLTROP_FIX = 38
                                         ! -- 47 levels
    INTEGER, PARAMETER :: LLTROP = 38
    INTEGER, PARAMETER :: LLSTRAT = 44
#else
    INTEGER
                     :: LLPAR
                                          ! Full vertical grid
    INTEGER, PARAMETER :: LLTROP_FIX = 40
                                         ! -- 72 levels
    INTEGER, PARAMETER :: LLTROP = 40
    INTEGER, PARAMETER :: LLSTRAT
                               = 59
#endif
    REAL(fpp), PARAMETER :: PTOP = 0.01e+0_fpp
#elif defined( MERRA ) && defined( GRID2x25 )
    I-----
    ! MERRA: 2 x 2.5
    INTEGER
                     :: IGLOB
                               = 144
    INTEGER
                    :: JGLOB
                               = 91
                    :: LGLOB
                               = 72
    INTEGER
#if
    defined( GRIDREDUCED )
                                       ! Reduced vertical grid
    INTEGER :: LLPAR = 47
    INTEGER, PARAMETER :: LLTROP_FIX = 38
                                         ! -- 47 levels
    INTEGER, PARAMETER :: LLTROP = 38
    INTEGER, PARAMETER :: LLSTRAT = 44
#else
    INTEGER
                    :: LLPAR
                                         ! Full vertical grid
    INTEGER, PARAMETER :: LLTROP_FIX = 40
                                        ! -- 72 levels
    INTEGER, PARAMETER :: LLTROP
                               = 40
    INTEGER, PARAMETER :: LLSTRAT
                               = 59
#endif
    REAL(fpp), PARAMETER :: PTOP = 0.01e+0_fpp
#elif defined( MERRA ) && defined( GRID4x5 )
    1-----
    ! MERRA: 4 x 5
    !-----
    INTEGER
                    :: IGLOB = 72
                               = 46
                    :: JGLOB
    INTEGER
    INTEGER
                    :: LGLOB
                               = 72
    defined( GRIDREDUCED )
#if
                    :: LLPAR = 47
                                       ! Reduced vertical grid
! -- 47 levels
    INTEGER
    INTEGER, PARAMETER :: LLTROP_FIX = 38
    INTEGER, PARAMETER :: LLTROP
                               = 38
    INTEGER, PARAMETER :: LLSTRAT = 44
#else
    INTEGER
                    :: LLPAR
                                         ! Full vertical grid
```

```
PARAMETER :: LLTROP_FIX = 40 ! -- 72 levels
    INTEGER,
    INTEGER, PARAMETER :: LLTROP = 40
    INTEGER, PARAMETER :: LLSTRAT = 59
#endif
    REAL(fpp), PARAMETER :: PTOP = 0.01e+0_fpp
#elif defined( GEOS_FP ) && defined( GRIDO25x03125 ) && defined( NESTED_CH )
    !-----
    ! GEOS-FP: Nested China Grid
                     :: IGLOB
                               = 225
    INTEGER
                    :: JGLOB
    INTEGER
                               = 161
                    :: LGLOB = 72
    INTEGER
    defined( GRIDREDUCED )
#if
    INTEGER :: LLPAR = 47 ! Reduced vertical grid
                                        ! -- 47 levels
    INTEGER, PARAMETER :: LLTROP_FIX = 38
    INTEGER, PARAMETER :: LLTROP = 38
    INTEGER, PARAMETER :: LLSTRAT = 44
#else
    INTEGER
                    :: LLPAR
                                         ! Full vertical grid
    INTEGER, PARAMETER :: LLTROP_FIX = 40 ! -- 72 levels
    INTEGER, PARAMETER :: LLTROP = 40
    INTEGER, PARAMETER :: LLSTRAT = 59
#endif
    REAL(fpp), PARAMETER :: PTOP = 0.01e+0_fpp
#elif defined( GEOS_FP ) && defined( GRID025x03125 ) && defined( NESTED_NA)
    I-----
    ! GEOS-FP Nested NA Grid
    !-----
                    :: IGLOB = 225
    INTEGER
    INTEGER
                    :: JGLOB
                               = 202
    INTEGER
                    :: LGLOB = 72
#if
    defined( GRIDREDUCED )
                    :: LLPAR = 47 ! Reduced vertical grid
    INTEGER
    INTEGER, PARAMETER :: LLTROP_FIX = 38
                                        ! -- 47 levels
    INTEGER, PARAMETER :: LLTROP = 38
    INTEGER, PARAMETER :: LLSTRAT = 44
#else
    INTEGER
                    :: LLPAR
                                         ! Full vertical grid
    INTEGER, PARAMETER :: LLTROP_FIX = 40
                                      ! -- 72 levels
    INTEGER, PARAMETER :: LLTROP = 40
    INTEGER, PARAMETER :: LLSTRAT = 59
#endif
    REAL(fpp), PARAMETER :: PTOP = 0.01e+0_fpp
```

!Anna Prot added the following sizes for nesting EU, 7 May 2015

#elif defined(GEOS_FP) && defined(GRID025x03125) && defined(NESTED_EU) 1-----! GEOS-FP Nested EU Grid :: IGLOB = 177 INTEGER = 115 INTEGER :: JGLOB :: LGLOB INTEGER = 72 #if defined(GRIDREDUCED) ! Reduced vertical grid :: LLPAR = 47INTEGER INTEGER, PARAMETER :: LLTROP_FIX = 38 ! -- 47 levels INTEGER, PARAMETER :: LLTROP = 38 INTEGER, PARAMETER :: LLSTRAT = 44 #else :: LLPAR ! Full vertical grid INTEGER INTEGER, PARAMETER :: LLTROP_FIX = 40 ! -- 72 levels INTEGER, PARAMETER :: LLTROP = 40 INTEGER, PARAMETER :: LLSTRAT = 59 #endif REAL(fpp), PARAMETER :: PTOP = 0.01e+0_fpp #elif defined(GEOS_FP) && defined(GRID2x25) I-----! GEOS-FP: 2 x 2.5 !-----INTEGER :: IGLOB = 144 = 91 :: JGLOB INTEGER :: LGLOB INTEGER = 72 #if defined(GRIDREDUCED) ! Reduced vertical grid ! -- 47 levels :: LLPAR = 47INTEGER INTEGER, PARAMETER :: LLTROP_FIX = 38 INTEGER, PARAMETER :: LLTROP = 38 INTEGER, PARAMETER :: LLSTRAT = 44 #else INTEGER :: LLPAR ! Full vertical grid INTEGER, PARAMETER :: LLTROP_FIX = 40 ! -- 72 levels INTEGER, PARAMETER :: LLTROP = 40 INTEGER, PARAMETER :: LLSTRAT = 59 #endif REAL(fpp), PARAMETER :: PTOP = 0.01e+0_fpp #elif defined(GEOS_FP) && defined(GRID4x5) !-----! GEOS-FP: 4 x 5

```
:: IGLOB
                                = 72
    INTEGER
    INTEGER
                     :: JGLOB
                                = 46
                     :: LGLOB
    INTEGER
                                = 72
#if
    defined( GRIDREDUCED )
                     :: LLPAR = 47
    INTEGER
                                       ! Reduced vertical grid
    INTEGER, PARAMETER :: LLTROP_FIX = 38
                                         ! -- 47 levels
    INTEGER, PARAMETER :: LLTROP = 38
    INTEGER, PARAMETER :: LLSTRAT = 44
#else
    INTEGER
                     :: LLPAR
                                          ! Full vertical grid
    INTEGER, PARAMETER :: LLTROP_FIX = 40
                                       ! -- 72 levels
    INTEGER, PARAMETER :: LLTROP
                               = 40
    INTEGER, PARAMETER :: LLSTRAT = 59
#endif
    REAL(fpp), PARAMETER :: PTOP = 0.01e+0_fpp
#elif defined( MERRA2 ) && defined( GRIDO5x0625 ) && defined( NESTED_AS )
    ! MERRA2: Nested China Grid
                     :: IGLOB = 145
    INTEGER
    INTEGER
                     :: JGLOB
                                = 133
                     :: LGLOB = 72
    INTEGER
    defined( GRIDREDUCED )
#if
                     :: LLPAR = 47 ! Reduced vertical grid
    INTEGER
    INTEGER, PARAMETER :: LLTROP_FIX = 38
                                         ! -- 47 levels
    INTEGER, PARAMETER :: LLTROP = 38
    INTEGER, PARAMETER :: LLSTRAT = 44
#else
    INTEGER
                     :: LLPAR
                                           ! Full vertical grid
    INTEGER, PARAMETER :: LLTROP_FIX = 40
                                         ! -- 72 levels
    INTEGER, PARAMETER :: LLTROP = 40
    INTEGER, PARAMETER :: LLSTRAT = 59
#endif
    REAL(fpp), PARAMETER :: PTOP = 0.01e+0_fpp
#elif defined( MERRA2 ) && defined( GRIDO5x0625 ) && defined( NESTED_NA)
    I-----
    ! MERRA2: Nested NA Grid
    I-----
    INTEGER
                     :: IGLOB
                                = 161
    INTEGER
                     :: JGLOB
                                = 121
                     :: LGLOB
    INTEGER
                                = 72
    defined( GRIDREDUCED )
#if
                     :: LLPAR = 47 ! Reduced vertical grid
    INTEGER
    INTEGER, PARAMETER :: LLTROP_FIX = 38
                                         ! -- 47 levels
```

```
INTEGER,
             PARAMETER :: LLTROP
                               = 38
    INTEGER, PARAMETER :: LLSTRAT = 44
#else
    INTEGER
                    :: LLPAR
                                         ! Full vertical grid
    INTEGER, PARAMETER :: LLTROP_FIX = 40
                                         ! -- 72 levels
    INTEGER, PARAMETER :: LLTROP = 40
    INTEGER, PARAMETER :: LLSTRAT = 59
#endif
    REAL(fpp), PARAMETER :: PTOP
                               = 0.01e + 0_{fpp}
#elif defined( MERRA2 ) && defined( GRID05x0625 ) && defined( NESTED_EU)
    1-----
    ! MERRA2: Nested EU Grid
    I-----
                     :: IGLOB
                               = 129
    INTEGER
                    :: JGLOB
                               = 81
    INTEGER
                    :: LGLOB = 72
#if
    defined( GRIDREDUCED )
                                        ! Reduced vertical grid
    INTEGER :: LLPAR = 47
    INTEGER, PARAMETER :: LLTROP_FIX = 38
                                         ! -- 47 levels
    INTEGER, PARAMETER :: LLTROP = 38
    INTEGER, PARAMETER :: LLSTRAT = 44
#else
    INTEGER :: LLPAR
INTEGER, PARAMETER :: LLTROP_FIX = 40
                                         ! Full vertical grid
                                      ! -- 72 levels
    INTEGER, PARAMETER :: LLTROP = 40
    INTEGER, PARAMETER :: LLSTRAT = 59
#endif
    REAL(fpp), PARAMETER :: PTOP
                               = 0.01e + 0_{fpp}
#elif defined( MERRA2 ) && defined( GRID2x25 )
    ! MERRA2: 2 x 2.5
    1-----
                    :: IGLOB = 144
    INTEGER
                     :: JGLOB
    INTEGER
                               = 91
    INTEGER
                     :: LGLOB = 72
    defined( GRIDREDUCED )
#if
                    :: LLPAR = 47
    INTEGER
                                        ! Reduced vertical grid
                                         ! -- 47 levels
    INTEGER, PARAMETER :: LLTROP_FIX = 38
    INTEGER, PARAMETER :: LLTROP
                               = 38
    INTEGER, PARAMETER :: LLSTRAT = 44
#else
    INTEGER
                     :: LLPAR
                                         ! Full vertical grid
    INTEGER, PARAMETER :: LLTROP_FIX = 40 ! -- 72 levels
    INTEGER, PARAMETER :: LLTROP = 40
```

```
INTEGER,
             PARAMETER :: LLSTRAT = 59
#endif
    REAL(fpp), PARAMETER :: PTOP = 0.01e+0_fpp
#elif defined( MERRA2 ) && defined( GRID4x5 )
    I-----
    ! MERRA2: 4 x 5
    !-----
    INTEGER
                    :: IGLOB = 72
                    :: JGLOB
    INTEGER
                               = 46
                    :: LGLOB = 72
    INTEGER
    defined( GRIDREDUCED )
#if
                                     ! Reduced vertical grid
! -- 47 levels
                    :: LLPAR = 47
    INTEGER
    INTEGER, PARAMETER :: LLTROP_FIX = 38
    INTEGER, PARAMETER :: LLTROP = 38
    INTEGER, PARAMETER :: LLSTRAT = 44
#else
    INTEGER :: LLPAR
INTEGER, PARAMETER :: LLTROP_FIX = 40
                                        ! Full vertical grid
                                        ! -- 72 levels
    INTEGER, PARAMETER :: LLSTRAT = 59
#endif
    REAL(fpp), PARAMETER :: PTOP = 0.01e+0_fpp
#endif
#endif
    1-----
    ! For stratospheric chemistry
    !-----
    INTEGER
                     :: LLCHEM
    TNTEGER.
                     :: LLCHEM_FIX
    ! TRACER & EMISSION SPECIES PARAMETERS
    ! NNPAR = max number of tracers
    ! NEMPARA = max number of anthropogenic emission species
    ! NEMPARB = max number of biogenic emission species
    !-----
    ! increase NNPAR and NEMPARA an extra amount (hotp 7/31/09)
#if
    defined( TOMAS )
# if defined( TOMAS40 )
             PARAMETER :: NNPAR = 430 ! For TOMAS40 (sfarina 6/11/13)
    INTEGER,
# elif defined( TOMAS15 )
    INTEGER,
            PARAMETER :: NNPAR = 205 ! For TOMAS15 (sfarina 6/11/13)
# elif defined( TOMAS12 )
    INTEGER, PARAMETER :: NNPAR = 178  ! For TOMAS12 (sfarina 6/11/13)
```

```
# else
    INTEGER, PARAMETER :: NNPAR = 340 ! For TOMAS (win, bmy, sfarina 6/11/13)f
# endif
#else
    INTEGER, PARAMETER :: NNPAR = 150 ! For non-TOMAS simulations
#endif
    ! OTHER PARAMETERS
     ! NVEGTYPE - Maximum number of surface types: 74 olson
    ! NTYPE - Maximum number of veg types in a CTM grid box
    ! NPOLY - Number of coefficients for polynomial fits
    INTEGER, PARAMETER :: NVEGTYPE = 74
#if defined( EXTERNAL_GRID ) || defined( EXTERNAL_TYPE )
     I-----
            %%%%%% GEOS-Chem HP (with ESMF & MPI) %%%%%%%
    ! For testing the ESMF interface to GEOS-Chem with a grid that
    ! is smaller than the usual 72x46, increase NTYPE (bmy, 12/4/12)
    .
!-----
    INTEGER, PARAMETER :: NTYPE = 50
#else
    1-----
            %%%%%%% GEOS-Chem CLASSIC (with OpenMP) %%%%%%%
    ! Current practice in the std GEOS-Chem is to set NTYPE to 25,
    ! which is large enough if using the Olson 2001 land map at
    ! 0.25 \times 0.25 resolution. (bmy, 12/4/12)
    INTEGER,
             PARAMETER :: NTYPE = 25
#endif
    INTEGER, PARAMETER :: NPOLY = 20
    ! LLCONVM - Max number of layers for convection
                      :: LLCONVM
    INTEGER
    ! MAXFAM -- Max number of families for prod and loss output
    INTEGER, PARAMETER :: MAXFAM = 40
    ! MAXMEM is maximum number of families of prod and loss
    ! moved from input_mod and diag_pl_mod to here (hotp 7/31/09)
    ! MAXMEM also increased from 10 to 20 by FP
    ! MAXMEM increased from 20 to 22 for bromine (jpp, mpayer, 12/28/11)
    INTEGER, PARAMETER :: MAXMEM = 22
    ! MAXPL increased from 100 to 500 and moved from diag_pl_mod
    ! to here by FP (hotp 7/31/09)
    INTEGER. PARAMETER :: MAXPL = 500
```

%%%

```
! NDUST -- Number of FAST-J aerosol size bins (rvm, bmy, 11/15/01)
      INTEGER. PARAMETER :: NDUST = 7
      ! NRHAER -- Number of aerosols undergoing hygroscopic growth
      INTEGER,
                 PARAMETER :: NRHAER = 5
      ! NSTRATAER -- Number of stratospheric aerosols (SDE 04/17/13)
#if defined( UCX )
      INTEGER, PARAMETER :: NSTRATAER = 2
#else
      INTEGER, PARAMETER :: NSTRATAER = 0
#endif
      ! NAER -- number of other aerosol categories (rvm, bmy, 2/27/02)
      INTEGER, PARAMETER :: NAER = NRHAER + NSTRATAER
      ! NRH -- number of relative humidity bins (rvm, bmy, 2/27/02)
      INTEGER, PARAMETER :: NRH = 5
#if
      defined( TOMAS )
                PARAMETER :: TOMASSPEC = 8
      INTEGER,
# if defined( TOMAS40 )
      INTEGER, PARAMETER :: NDSTBIN = 40
      INTEGER, PARAMETER :: TOMASBIN = 40
# elif defined( TOMAS15 )
      INTEGER, PARAMETER :: NDSTBIN = 15
               PARAMETER :: TOMASBIN = 15
      INTEGER,
# elif defined( TOMAS12 )
      INTEGER, PARAMETER :: NDSTBIN = 12
      INTEGER, PARAMETER :: TOMASBIN = 12
# else
      ! NDSTBIN -- redimensioned for TOMAS (dwest, bmy, 2/1/10)
      INTEGER, PARAMETER :: NDSTBIN
                                     = 30
      INTEGER, PARAMETER :: TOMASBIN = 30 ! Number of TOMAS bins
# endif
#else
      ! NDSTBIN -- number of dust size bins for transport (tdf, bmy, 3/31/04)
      INTEGER, PARAMETER :: NDSTBIN
                                    = 4
#endif
REMARKS:
   %%% NOTE: THIS WAS MADE INTO A MODULE IN ORDER TO REMOVE COMMON BLOCKS
```

%%% WE WILL KEEP THIS FOR NOW. EVENTUALLY WE MIGHT MIGRATE THESE DATA %%%

%%% INTO A DERIVED TYPE OBJECT. (bmy, 12/3/12)

- (1) Now set LLTROP = 20 for GEOS-3 (bmy, 4/12/01)
- (2) Eliminated obsolete commented-out code (bmy, 4/20/01)
- (3) Now set MAXFAM = 12 for more P-L families (bmy, 6/28/01)
- (4) Comment out {IJL}GCMPAR -- these are obosolete (bmy, 9/24/01)
- (5) Also set LLPAR = 30 for GEOS-3, will regrid online (bmy, 9/24/01)
- (6) Removed obsolete code from 9/01 (bmy, 10/23/01)
- (7) Removed NAIR, LAIREMS, these are now defined in "aircraft_nox_mod.f" (bmy, 2/14/02)
- (8) Eliminated commented-out code from 2/14/02. Also added NAER and NRH parameters for aerosols. (rvm, bmy, 2/27/02)
- (9) Removed IM, JM, IMX, JMX to avoid namespace pollution. This is needed to get the new TPCORE to work. Also changed RCS ID tag comment character from "C" to "!" to allow freeform compilation. (bmy, 6/25/02)
- (10) Removed obsolete code from 6/02 (bmy, 8/26/02)
- (11) Added NUMDEP_SULF in a common block for sulfate dry deposition. Also set MAXDEP=31 and NNPAR=31 for coupled fullchem/sulfate simulations. (rjp, bdf, bmy, 11/15/02)
- (12) Removed IO, JO; these are now superseded by "grid_mod.f" (bmy, 2/11/03)
- (13) Added parameters for GEOS-4 (bmy, 6/18/03)
- (14) Now defines both 55 level and 30 level GEOS-4 grids. Also define LLTROP=19 for GEOS-4 grids. Also remove obsolete GEOS-2 grid declarations. (bmy, 10/31/03)
- (15) LLTROP should be 17 for GEOS-4...based on the ND55 diagnostic when computed for 2003 met fields (bmy, 2/18/04)
- (16) Increase NNPAR from 31 to 39 for carbon & dust tracers. Also declare NDSTBIN as # of dust bins. (rvm, tdf, bmy, 4/1/04)
- (17) Increase NNPAR to 41 for seasalt tracers (rjp, bec, bmy, 4/20/04)
- (18) Increase NNPAR to 50 for SOA tracers (rjp, bmy, 7/15/04)
- (19) Now use NESTED_CH and NESTED_NA cpp switches to define parameters for 1x1 nested grids. Also add parameters for the 1 x 1.25 global grid. (bmy, 12/1/04)
- (20) Now add parameters for GCAP and GEOS-5 grids. Remove references to obsolete LGEOSCO and FULLCHEM Cpp switches (bmy, 6/24/05)
- (21) Now add I1x1 and J1x1 parameters for data on the 1x1 GEOS grid. (bmy, 10/24/05)
- (22) Increase NNPAR to 52 (bmy, 12/6/05)
- (23) Increase NNPAR to 54 (dkh, bmy, 5/22/06)
- (24) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (25) Added variable tropopause case (bmy, phs, bdf, 8/21/06)
- (26) Set LLTROP to level of first box entirely above 20 km for GEOS-3 and GEOS-4 (phS, 9/14/06)
- (27) Bug fix: set LLTROP_FIX = LLPAR for GCAP (bmy, 11/29/06)
- (28) Reset vertical coordinates for GEOS-5. Also renamed GRID30LEV

to GRIDREDUCED (bmy, 4/3/07)

- (29) New parameters for GEOS-5 nested grid (yxw, dan, bmy, 11/6/08)
- (30) NEMPARA set to 12 to emit 03 and HNO3 (phs, 4/3/08)
- (31) Add tracers to NNPAR = 73. (tmf, 1/7/09)
- (32) NEMPARA set to 21 to emit new tracers for GLYX chemistry (tmf, ccc, 3/2/09)
- (33) NEMPARB set to 3 to emit MBO, MONX (tmf, ccc, 3/2/09)
- (34) Added EUROPE grid parameters (amv, 10/19/09)
- 18 Dec 2009 Aaron van D Added NESTED_EU grid parameters
- 18 Dec 2009 R. Yantosca Added ProTeX headers
- 25 Jan 2010 R. Yantosca Set NNPAR=320 for TOMAS simulations
- 25 Jan 2010 R. Yantosca Define TOMASBIN and TOMASSPEC for TOMAS sims
- 08 Feb 2010 F. Paulot Increase NNPAR, NEMPARA and NEMPARB
- 08 Feb 2010 F. Paulot Move MAXMEM and MAXPL from diag_pl_mod.
- 30 Nov 2010 R. Yantosca Increase LLTROP (from 38 to 40) for GEOS-5 and MERRA for the full 72-layer grids (i.e. when the Cpp switch GRIDREDUCED is not set).
- 09 Mar 2011 R. Yantosca Updated NNPAR for APM (G. Luo)
- 23 Aug 2011 M. Long Converted to Module from Header file
- 27 Dec 2011 M. Payer Updated NNPAR, NEMPARB, MAXMEM for bromine chemistry (J. Parrella)
- 10 Feb 2012 R. Yantosca Added #if blocks for GEOS-5.7.x nested CH grid
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 27 Mar 2012 R. Yantosca Increase NTYPE from 15 to 25 for Olson 2001 map
- 22 Oct 2012 M. Payer Increase NNPAR to 100 for tagged Hg simulation (E. Corbitt)
- 25 Oct 2012 R. Yantosca Now also set LLPAR, LLTROP, LLTROP_FIX to LGLOB for grid-independent simulation
- 19 Nov 2012 R. Yantosca Renamed to INIT_CMN_SIZE, to better follow adopted GEOS-Chem naming convention
- 27 Nov 2012 R. Yantosca Removed commented out code
- 05 Jun 2013 R. Yantosca Now define GEOS-5 0.25x0.3125 nested NA grid
- 13 Aug 2013 M. Sulprizio- Increase NNPAR & NBIOMAX for updated SOA and SOA + semivolatile POA simulations (H. Pye)
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 26 Sep 2013 R. Yantosca Renamed GEOS_57 Cpp switch to GEOS_FP
- 03 Dec 2014 M. Yannetti Added PRECISION_MOD
- 22 May 2015 R. Yantosca Updated comments, cosmetic changes
- 22 May 2015 R. Yantosca Removed variables made obsolete by HEMCO
- 28 Jan 2016 M. Sulprizio- Remove NBIOMAX made obsolete by HEMCO
- 18 May 2016 M. Sulprizio- Remove MAXIJ made obsolete by FlexChem
- 23 Jun 2016 R. Yantosca Remove references to APM code; it is no longer compatible with the FlexChem implementation

1.4.1 Init_Cmn_Size

Routine INIT_CMN_SIZE initializes the grid dimension values in module CMN_SIZE_mod.F.

INTERFACE:

```
SUBROUTINE Init_CMN_SIZE( am_I_Root,
                                           RC,
                           value_I_LO,
                                           value_J_LO,
&
                           value_I_HI,
                                           value_J_HI,
                           value_IM,
&
                                           value_JM,
&
                           value_LM,
                                           value_IM_WORLD,
                           value_JM_WORLD, value_LM_WORLD,
&
                           value_LLTROP, value_LLSTRAT )
&
```

USES:

USE ErrCode_Mod

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root
                                       ! Are we on the root CPU?
INTEGER, OPTIONAL
                                       ! Lower lon index on this CPU
                    :: value_I_LO
INTEGER, OPTIONAL
                    :: value_J_LO
                                       ! Lower lat index on this CPU
INTEGER, OPTIONAL
                   :: value_I_HI
                                       ! Upper lon index on this CPU
INTEGER, OPTIONAL
                    :: value_J_HI
                                       ! Upper lat index on this CPU
                                       ! # of lons
INTEGER, OPTIONAL
                   :: value_IM
                                                    on this CPU
INTEGER, OPTIONAL
                   :: value_JM
                                      ! # of lats
                                                    on this CPU
INTEGER, OPTIONAL
                    :: value_LM
                                      ! # of levels on this CPU
                    :: value_IM_WORLD
INTEGER, OPTIONAL
                                      ! # of lons in the global grid
INTEGER, OPTIONAL
                                       ! # of lats in the global grid
                    :: value_JM_WORLD
INTEGER, OPTIONAL
                    :: value_LM_WORLD
                                       ! # of levs in the global grid
INTEGER, OPTIONAL
                                       ! # of levs in troposphere
                    :: value_LLTROP
                    :: value_LLSTRAT
                                       ! # of levs in stratosphere
INTEGER, OPTIONAL
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC     ! Success or failure?
```

```
15 Oct 2012 - M. Long - Initial version
15 Oct 2012 - R. Yantosca - Added ProTeX Headers, use F90 format/indents
22 Oct 2012 - R. Yantosca - Renamed to GIGC_Init_Dimensions
03 Dec 2012 - R. Yantosca - Rewritten for clarity. Also pass optional
arguments to carry values from ESMF environment
03 Dec 2012 - R. Yantosca - Now allocate DLON, DLAT arrays here.
04 Aug 2015 - C. Keller - Added value_LLTROP and value_LLSTRAT.
```

1.4.2 Cleanup_Cmn_Size

Subroutine CLEANUP_CMN_SIZE deallocates all module arrays.

INTERFACE:

```
SUBROUTINE Cleanup_CMN_SIZE( am_I_Root, RC )
```

USES:

USE ErrCode_Mod

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC     ! Success or failure?
```

REVISION HISTORY:

```
3 Dec 2012 - R. Yantosca - Initial version
```

1.5 Fortran: Module Interface errcode_mod.F90

Module ERRCODE_MOD contains the error codes (i.e. that report success or failure) returned by GEOS-Chem routines.

INTERFACE:

MODULE ErrCode_Mod

USES:

IMPLICIT NONE PRIVATE

DEFINED PARAMETERS:

```
INTEGER, PUBLIC, PARAMETER :: GC_SUCCESS = 0 ! Routine returns success INTEGER, PUBLIC, PARAMETER :: GC_FAILURE = -1 ! Routine returns failure
```

REMARKS:

The error codes are returned by routines at various levels of the Grid-Independent GEOS-Chem implementation.

```
19 Oct 2012 - R. Yantosca - Initial version
16 Aug 2016 - M. Sulprizio- Rename from gigc_errcode_mod.F90 to
errcode_mod.F90. The "gigc" nomenclature is
no longer used.
```

1.6 Fortran: Module Interface input_opt_mod.F90

Module INPUT_OPT_MOD contains the derived type for GEOS-Chem options and logical switches.

INTERFACE:

```
MODULE Input_Opt_Mod
```

USES:

```
USE PRECISION_MOD ! For GEOS-Chem Precision (fp)
```

IMPLICIT NONE

PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: Set_Input_Opt
PUBLIC :: Cleanup_Input_Opt

PUBLIC DATA MEMBERS:

```
! Derived type for Input Options
TYPE, PUBLIC :: OptInput
 !-----
 ! General Runtime & Distributed Comp Info
                  :: NPES
 INTEGER
                          ! Number of MPI procs
                          ! Local MPI process handle
 INTEGER
                  :: myCpu
                  :: MPICOMM ! MPI Communicator Handle
 INTEGER
 LOGICAL
                  :: HPC ! Is this an HPC (ESMF or otherwise) sim?
 LOGICAL
                  :: RootCPU ! Is this the root cpu?
 1-----
 ! SIZE PARAMETER fields
```

!-----! SIMULATION MENU fields

!-----

INTEGER :: NYMDb INTEGER :: NHMSb

```
INTEGER
                            :: NYMDe
INTEGER
                            :: NHMSe
CHARACTER (LEN=255)
                            :: RUN_DIR
CHARACTER (LEN=255)
                            :: IN_RST_FILE
CHARACTER (LEN=255)
                           :: DATA_DIR
                           :: CHEM_INPUTS_DIR
CHARACTER (LEN=255)
                           :: RES_DIR
CHARACTER (LEN=255)
CHARACTER (LEN=255)
                            :: GCAP_DIR
                           :: GEOS_4_DIR
CHARACTER (LEN=255)
CHARACTER (LEN=255)
                           :: GEOS_5_DIR
                           :: GEOS_FP_DIR
CHARACTER (LEN=255)
                           :: MERRA_DIR
CHARACTER (LEN=255)
CHARACTER (LEN=255)
                           :: MERRA2_DIR
CHARACTER (LEN=255)
                           :: DATA_DIR_1x1
CHARACTER (LEN=255)
                            :: TEMP_DIR
LOGICAL
                            :: LUNZIP
LOGICAL
                            :: LWAIT
LOGICAL
                            :: LVARTROP
                            :: LCAPTROP
LOGICAL
REAL(fp)
                            :: OZONOPAUSE
INTEGER
                            :: NESTED_IO
                            :: NESTED_JO
INTEGER
CHARACTER (LEN=255)
                            :: HcoConfigFile
```

1-----

! ADVECTED SPECIES MENU fields

1-----

:: N_ADVECT INTEGER

CHARACTER(LEN=255), POINTER :: AdvectSpc_Name(:)

:: SIM_TYPE INTEGER CHARACTER (LEN=255) :: SIM_NAME :: LSPLIT LOGICAL

LOGICAL :: ITS_A_RnPbBe_SIM :: ITS_A_CH3I_SIM LOGICAL LOGICAL :: ITS_A_FULLCHEM_SIM LOGICAL :: ITS_A_HCN_SIM :: ITS_A_TAGO3_SIM LOGICAL LOGICAL :: ITS_A_TAGCO_SIM LOGICAL :: ITS_A_C2H6_SIM LOGICAL :: ITS_A_CH4_SIM LOGICAL :: ITS_AN_AEROSOL_SIM :: ITS_A_MERCURY_SIM LOGICAL :: ITS_A_CO2_SIM LOGICAL :: ITS_A_H2HD_SIM LOGICAL :: ITS_A_POPS_SIM LOGICAL LOGICAL :: ITS_A_SPECIALTY_SIM :: ITS_NOT_COPARAM_OR_CH4 LOGICAL

```
1-----
! AEROSOL MENU fields
!-----
LOGICAL
                          :: LSULF
LOGICAL
                          :: LCRYST
LOGICAL
                          :: LCARB
                          :: LBRC
LOGICAL
LOGICAL
                          :: LSOA
LOGICAL
                          :: LMPOA
LOGICAL
                          :: LSVPOA
LOGICAL
                          :: LDUST
                          :: LDEAD
LOGICAL
                          :: LSSALT
LOGICAL
                          :: LDSTUP
LOGICAL
LOGICAL
                          :: LDICARB
                  POINTER :: SALA_REDGE_um(:)
REAL(fp),
REAL(fp),
                  POINTER :: SALC_REDGE_um(:)
LOGICAL
                          :: LGRAVSTRAT
LOGICAL
                          :: LSOLIDPSC
                          :: LHOMNUCNAT
LOGICAL
                          :: T_NAT_SUPERCOOL
REAL(fp)
REAL(fp)
                          :: P_ICE_SUPERSAT
LOGICAL
                          :: LPSCCHEM
LOGICAL
                          :: LSTRATOD
! EMISSIONS MENU fields
I -----
LOGICAL
                          :: LEMIS
                          :: TS_EMIS
INTEGER
INTEGER
                          :: LBIOFUEL
LOGICAL
                          :: LOTDLOC
LOGICAL
                          :: LSOILNOX
LOGICAL
                          :: LWARWICK_VSLS
                          :: LSSABr2
LOGICAL
LOGICAL
                          :: LFIX_PBL_BRO
LOGICAL
                          :: LCH4EMIS
LOGICAL
                          :: LCH4SBC
LOGICAL
                          :: LOCSEMIS
                          :: LCFCEMIS
LOGICAL
LOGICAL
                          :: LCLEMIS
LOGICAL
                          :: LBREMIS
LOGICAL
                          :: LN20EMIS
LOGICAL
                          :: LBASICEMIS
LOGICAL
                          :: LSETH20
LOGICAL
                          :: LSETCH4
LOGICAL
                          :: LSETOCS
LOGICAL
                          :: LSETCFC
```

LOGICAL LOGICAL LOGICAL LOGICAL LOGICAL LOGICAL LOGICAL LOGICAL LOGICAL INTEGER LOGICAL	:: LSETCL :: LBRGCCM :: LSETBR :: LSETBRSTRAT :: LSETNOYSTRAT :: LSETN20 :: LSETH2SO4 :: CFCYEAR :: LFUTURECFC				
! CO2 MENU fields					
LOGICAL	:: LFOSSIL :: LCHEMCO2 :: LBIODIURNAL :: LBIONETCLIM :: LOCEAN :: LSHIP :: LPLANE :: LFFBKGRD :: LFOSSILTAG :: LSHIPTAG :: LSHIPTAG :: LSHIPTAG :: LPLANETAG				
INTEGER CHARACTER(LEN=255)	:: FUTURE_YEAR :: FUTURE_SCEN				
!! CHEMISTRY MENU fields !					
LOGICAL LOGICAL LOGICAL INTEGER REAL(fp) LOGICAL INTEGER, POINTER	:: LCHEM :: LSCHEM :: LSYNOZ :: TS_CHEM :: GAMMA_HO2 :: LUCX :: LCH4CHEM :: LACTIVEH2O :: LO3FJX :: LINITSPEC :: NTLOOPNCS(:)				

!! RADIATION MENU fi	elds		
LOGICAL LOGICAL LOGICAL LOGICAL, POINTER INTEGER		:: :: ::	LRAD LLWRAD LSWRAD LSKYRAD(:) TS_RAD
!! TRANSPORT MENU fi	elds		
LOGICAL LOGICAL LOGICAL LOGICAL LOGICAL INTEGER		::	LTRAN LFILL TPCORE_IORD TPCORE_JORD TPCORE_KORD TS_DYN
! ! CONVECTION MENU f ! LOGICAL LOGICAL LOGICAL INTEGER	ields	::	
!! DEPOSITION MENU f	ields		
LOGICAL LOGICAL REAL(fp) LOGICAL LOGICAL		:: :: ::	LDRYD LWETD WETD_CONV_SCAL USE_OLSON_2001 PBL_DRYDEP
!! GAMAP MENU fields			
CHARACTER (LEN=255) CHARACTER (LEN=255)		::	GAMAP_DIAGINFO GAMAP_TRACERINFO
!! OUTPUT MENU field	s		
·			NJDAY(:)

INTEGER	:: NDO1,	L
INTEGER	:: NDO1,	L
INTEGER	:: ND03,	L
INTEGER	:: ND04,	L
INTEGER	:: ND05,	L
INTEGER	:: ND06,	L
INTEGER	:: ND07,	L
INTEGER	:: NDO8,	L
INTEGER	:: ND09,	L
INTEGER	:: ND10,	I
INTEGER	:: ND10,	_ L
INTEGER	:: ND12,	I
INTEGER	:: ND13,	I
INTEGER	:: ND14,	- I
INTEGER	:: ND15,	I
INTEGER	:: ND16,	_ L
INTEGER	:: ND17,	_ L
INTEGER	:: ND18,	_ L
INTEGER	:: ND19,	_ L
INTEGER	:: ND20,	I
INTEGER	:: ND21,	I
INTEGER	:: ND22,	I
INTEGER	:: ND23,	I
INTEGER	:: ND24,	L
INTEGER	:: ND25,	I
INTEGER	:: ND26,	L
INTEGER	:: ND27,	L
INTEGER	:: ND28,	L
INTEGER	:: ND29.	I
INTEGER	:: ND30,	I
INTEGER	:: ND31,	I
INTEGER	:: ND32,	I
INTEGER	:: ND33,	I
INTEGER	:: ND34,	I
INTEGER	:: ND35,	I
INTEGER	:: ND36,	I
INTEGER	:: ND37,	I
INTEGER	:: ND38,	L
INTEGER	:: ND39,	L
INTEGER	:: ND40,	L
INTEGER	:: ND41,	L
INTEGER	:: ND42,	L
INTEGER	:: ND43,	I
INTEGER	:: ND44,	L
INTEGER	:: ND45,	L

INTEGER	:	:	ND46,	LD46
INTEGER	:	:	ND47,	LD47
INTEGER	:	:	ND48,	LD48
INTEGER	:	:	ND49,	LD49
INTEGER	:	:	ND50,	LD50
INTEGER	:	:	ND51,	LD51
INTEGER	:	:	ND52,	LD52
INTEGER	:	:	ND53,	LD53
INTEGER	:	:	ND54,	LD54
INTEGER			ND55,	LD55
INTEGER			ND56,	LD56
INTEGER			ND57,	LD57
INTEGER			ND58,	LD58
INTEGER			ND59,	LD59
INTEGER			ND60,	LD60
INTEGER			ND61,	LD61
INTEGER			ND62,	LD62
INTEGER			ND63,	LD63
INTEGER			ND64,	LD64
INTEGER			ND66,	LD66
INTEGER			ND67,	LD67
INTEGER			ND68,	LD68
INTEGER			ND69,	LD69
INTEGER			ND70,	LD70
INTEGER			ND71,	LD71
INTEGER			ND71,	LD72
INTEGEIL	•	•	ND/Z,	ED12
INTEGER	:	:	TS_DIAG	
LOGICAL			LPRT	
INTEGER,			TINDEX(:,:)	
INTEGER,	POINTER:			
INTEGER,	POINTER:		, ,	
LOGICAL			DO_DIAG_WRITE	
	·		20_21114	
! Collection ids				
INTEGER	:	:	DIAG_COLLECTION	
INTEGER	:	:	GC_RST_COLLECTION	! Used only for NetCDF
				•
<pre>#if defined(NC_DIAG)</pre>				
! New diagnostic gr				
CHARACTER(LEN=15)			TRANSPORT_OUTPUT_	
CHARACTER(LEN=15)			WETSCAV_OUTPUT_TY	
CHARACTER (LEN=15)	:	:	DRYDEP_OUTPUT_TYPI	E
CHARACTER(LEN=15)	:	:	SPECIES_CONC_OUTPO	UT_TYPE
CHARACTER(LEN=15)	:	:	SPECIES_EMIS_OUTPO	UT_TYPE
CHARACTER(LEN=15)	:	:	MET_OUTPUT_TYPE	

[!] Placeholders pending grouping of diagnostics

```
CHARACTER(LEN=15)
                         :: NDO1_OUTPUT_TYPE
   CHARACTER (LEN=15)
                         :: NDO2_OUTPUT_TYPE
   CHARACTER (LEN=15)
                        :: ND12_OUTPUT_TYPE
                        :: ND14_OUTPUT_TYPE
   CHARACTER (LEN=15)
   CHARACTER (LEN=15)
                        :: ND15_OUTPUT_TYPE
                        :: ND16_OUTPUT_TYPE
   CHARACTER (LEN=15)
                        :: ND17_OUTPUT_TYPE
   CHARACTER (LEN=15)
                        :: ND18_OUTPUT_TYPE
   CHARACTER (LEN=15)
                        :: ND19_OUTPUT_TYPE
   CHARACTER (LEN=15)
   CHARACTER (LEN=15)
                         :: ND30_OUTPUT_TYPE
#endif
    !-----
    ! PLANEFLIGHT MENU fields
   1-----
   LOGICAL
                        :: DO_PF
                       :: PF_IFILE
   CHARACTER (LEN=255)
   CHARACTER(LEN=255) :: PF_OFILE
   ļ-----
   ! ND48 MENU fields
   ļ-----
   LOGICAL
                        :: DO_ND48
   CHARACTER (LEN=255)
                        :: ND48_FILE
   INTEGER
                         :: ND48_FREQ
   INTEGER
                         :: ND48_N_STA
             POINTER :: ND48_IARR(:)
   INTEGER,
                  POINTER :: ND48_JARR(:)
   INTEGER,
                   POINTER :: ND48_LARR(:)
   INTEGER,
   INTEGER,
                  POINTER :: ND48_NARR(:)
   ļ-----
   ! ND49 MENU fields
   ļ-----
   LOGICAL
                        :: DO_ND49
   CHARACTER(LEN=255) :: ND49_FILE
   INTEGER, POINTER :: ND49_TRACERS(:)
   INTEGER
                         :: ND49_FREQ
   INTEGER
                         :: ND49_IMIN
   INTEGER
                         :: ND49_IMAX
   INTEGER
                         :: ND49_JMIN
   INTEGER
                         :: ND49_JMAX
   INTEGER
                         :: ND49_LMIN
   INTEGER
                         :: ND49_LMAX
    !-----
   ! ND50 MENU fields
```

```
LOGICAL
                        :: DO_ND50
CHARACTER (LEN=255)
                        :: ND50_FILE
                        :: LND50_HDF
LOGICAL
                 POINTER :: ND50_TRACERS(:)
INTEGER,
INTEGER
                       :: ND50_IMIN
                        :: ND50_IMAX
INTEGER
INTEGER
                        :: ND50_JMIN
INTEGER
                        :: ND50_JMAX
INTEGER
                        :: ND50_LMIN
INTEGER
                        :: ND50_LMAX
I -----
! ND51 MENU fields
1-----
LOGICAL
                        :: DO_ND51
                        :: ND51_FILE
CHARACTER (LEN=255)
LOGICAL
                        :: LND51_HDF
                 POINTER :: ND51_TRACERS(:)
INTEGER,
REAL(fp)
                        :: ND51_HR_WRITE
REAL(fp)
                        :: ND51_HR1
REAL(fp)
                        :: ND51_HR2
INTEGER
                        :: ND51_IMIN
INTEGER
                        :: ND51_IMAX
INTEGER
                        :: ND51_JMIN
INTEGER
                        :: ND51_JMAX
INTEGER
                        :: ND51_LMIN
INTEGER
                        :: ND51_LMAX
1-----
! ND51b MENU fields
!-----
                        :: DO_ND51b
LOGICAL
                        :: ND51b_FILE
CHARACTER (LEN=255)
LOGICAL
                       :: LND51b_HDF
INTEGER,
                 POINTER :: ND51b_TRACERS(:)
REAL(fp)
                        :: ND51b_HR_WRITE
REAL(fp)
                        :: ND51b_HR1
REAL(fp)
                        :: ND51b_HR2
INTEGER
                        :: ND51b_IMIN
INTEGER
                        :: ND51b_IMAX
INTEGER
                        :: ND51b_JMIN
                        :: ND51b_JMAX
INTEGER
INTEGER
                        :: ND51b_LMIN
INTEGER
                        :: ND51b_LMAX
!-----
! ND63 MENU fields
```

```
LOGICAL
                        :: DO_ND63
CHARACTER (LEN=255)
                       :: ND63_FILE
         POINTER :: ND63_TRACERS(:)
INTEGER,
INTEGER
                       :: ND63_FREQ
INTEGER
                       :: ND63_IMIN
                        :: ND63_IMAX
INTEGER
INTEGER
                        :: ND63_JMIN
INTEGER
                        :: ND63_JMAX
! PROD LOSS MENU fields
!-----
LOGICAL
                       :: DO_SAVE_PL
LOGICAL
                       :: LFAMILY
INTEGER
                       :: ND65, LD65
LOGICAL
                      :: DO_SAVE_03
INTEGER
                       :: NFAM
          POINTER :: FAM_COEF(:,:)
REAL(fp),
CHARACTER(LEN=255), POINTER :: FAM_MEMB(:,:)
CHARACTER(LEN=255), POINTER :: FAM_NAME(: )
INTEGER,
                POINTER :: FAM_NMEM(: )
CHARACTER(LEN=255), POINTER :: FAM_TYPE(: )
! UNIX CMDS fields
!-----
                   :: BACKGROUND
CHARACTER (LEN=255)
CHARACTER (LEN=255)
                      :: REDIRECT
                      :: REMOVE_CMD
CHARACTER (LEN=255)
CHARACTER (LEN=255)
                      :: SEPARATOR
                      :: WILD_CARD
CHARACTER (LEN=255)
                      :: UNZIP_CMD
CHARACTER (LEN=255)
                      :: ZIP_SUFFIX
CHARACTER (LEN=255)
CHARACTER (LEN=1)
                      :: SPACE
1-----
! NESTED GRID MENU fields
!-----
                       :: ITS_A_NESTED_GRID
LOGICAL
                       :: LWINDO
LOGICAL
LOGICAL
                      :: LWIND02x25
LOGICAL
                      :: LWINDO_NA
CHARACTER (LEN=255)
                     :: TPBC_DIR_NA
LOGICAL
                      :: LWINDO_EU
CHARACTER (LEN=255)
                     :: TPBC_DIR_EU
LOGICAL
                       :: LWINDO_CH
                    :: TPBC_DIR_CH
CHARACTER (LEN=255)
LOGICAL
                       :: LWINDO_AS
```

CHARACTER(LEN=255)	:: TPBC_DIR_AS
LOGICAL	:: LWINDO_CU
CHARACTER(LEN=255)	:: TPBC_DIR
INTEGER	:: NESTED_TS
INTEGER	:: NESTED_I1
INTEGER	:: NESTED_J1
INTEGER	:: NESTED_I2
INTEGER	:: NESTED_J2
INTEGER	:: NESTED_IOW
INTEGER	:: NESTED_JOW
INTEGER	:: NESTED_IOE
INTEGER	:: NESTED_JOE
!	
! BENCHMARK MENU fields	
!	
	:: LSTDRUN
	:: STDRUN_INIT_FILE
CHARACTER (LEN=255)	:: STDRUN_FINAL_FILE
!	
! MERCURY MENU fields	
!	
INTEGER	:: ANTHRO_Hg_YEAR
CHARACTER (LEN=255)	:: HG_SCENARIO
LOGICAL	:: USE_CHECKS
LOGICAL	:: LDYNOCEAN
LOGICAL	:: LPREINDHG
LOGICAL	:: LGTMM
CHARACTER (LEN=255)	:: GTMM_RST_FILE
LOGICAL	:: LARCTICRIV
LOGICAL	:: LKRedUV
1	
! CH4 MENU fields	
! CH4 MENO lields	
LOGICAL	:: LCH4BUD
LOGICAL	:: LGAO
LOGICAL	:: LCOL
LOGICAL	:: LLIV
LOGICAL	:: LWAST
LOGICAL	:: LBFCH4
LOGICAL	:: LRICE
LOGICAL	:: LOTANT
LOGICAL	:: LBMCH4
LOGICAL	:: LWETL
LOGICAL	:: LSOABS
LOGICAL	:: LOTNAT
FOGTONE	LUINAI

```
!-----
! POPS MENU fields
ļ-----
CHARACTER(LEN=3)
                    :: POP_TYPE
LOGICAL
                    :: CHEM_PROCESS
REAL(fp)
                    :: POP_XMW
REAL(fp)
                     :: POP_KOA
REAL(fp)
                     :: POP_KBC
REAL(fp)
                     :: POP_K_POPG_OH
REAL(fp)
                     :: POP_K_POPP_O3A
REAL(fp)
                     :: POP_K_POPP_03B
REAL(fp)
                     :: POP_HSTAR
REAL(fp)
                     :: POP_DEL_H
REAL(fp)
                     :: POP_DEL_Hw
ļ-----
! Fields for drydep and dust. These get
! set in the init stage based on info
! from file "input.geos". (mlong, 1/5/13)
ļ-----
INTEGER
                     :: N_DUST_BINS
            POINTER :: NTRAIND(:)
INTEGER,
INTEGER,
              POINTER :: IDDEP(:)
           POINTER :: DUSTREFF(:)
POINTER :: DUSTDEN(:)

DEDNAMF(:)
INTEGER,
              POINTER :: IDEP(:)
REAL(fp),
REAL(fp),
CHARACTER(LEN=14), POINTER :: DEPNAME(:)
l -----
! Fields for interface to GEOS-5 GCM
ļ-----
LOGICAL
                     :: haveImpRst
! Fields for LINOZ strat chem
1-----
INTEGER
                     :: LINOZ_NLEVELS
INTEGER
                     :: LINOZ_NLAT
                     :: LINOZ_NMONTHS
INTEGER
INTEGER
                     :: LINOZ_NFIELDS
              POINTER :: LINOZ_TPARM(:,:,:,:)
REAL(fp),
!-----
! Fields for overhead 03
! This gets set in main.F based on met
! field and year (mpayer, 12/13/13)
ļ-----
```

LOGICAL :: USE_03_FROM_MET

END TYPE OptInput

REMARKS:

This will eventually replace the switches in logical_mod.F.

REVISION HISTORY:

```
01 Nov 2012 - R. Yantosca - Initial version, based on logical_mod.F
                           newer Olson 2001 land map & drydep inputs
07 Nov 2012 - R. Yantosca - Added Input_Opt%ITS_A_*_SIM fields
08 Nov 2012 - R. Yantosca - Added APM MENU fields
09 Nov 2012 - R. Yantosca - Added LD* variables for diagnostic levels
28 Nov 2012 - R. Yantosca - Add USE_OLSON_2001 logical flag
22 May 2013 - M. Payer - Add GAMMA_HO2 variable for chemistry menu
26 Feb 2013 - M. Long
                        - Add extra fields from input.geos
26 Feb 2013 - M. Long - Bug fix: timesteps are now INTEGER, not LOGICAL
28 Feb 2013 - R. Yantosca - Add haveImpRst field for GEOS-5 GCM interface
08 Mar 2013 - R. Yantosca - Add myCpu field to pass CPU \# to GEOS-Chem
15 Mar 2013 - R. Yantosca - Add fields for LINOZ strat chemistry
27 Mar 2013 - R. Yantosca - Add extra fields for tagged CO2
27 Mar 2013 - R. Yantosca - Add extra fields for tagged EDGAR
29 Mar 2013 - R. Yantosca - Add DO_DIAG_WRITE field (to shut diags in MPI)
22 Jul 2013 - M. Sulprizio- Add extra fields for RCP emissions
31 Jul 2013 - M. Sulprizio- Add extra field for AEIC aircraft emissions and
                            remove LAIRNOX field
13 Aug 2013 - M. Sulprizio- Add extra fields for semivolatile POA (H. Pye)
22 Aug 2013 - R. Yantosca - Add fields for soil NOx & species restart files
17 Sep 2013 - M. Sulprizio- Add LDSTUP flag for acid uptake on dust aerosols
26 Sep 2013 - R. Yantosca - Renamed GEOS_57_DIR to GEOS_FP_DIR
03 Oct 2013 - M. Sulprizio- Removed obsolete LMFCT for flux correction
03 Oct 2013 - M. Sulprizio- Removed obsolete LAVHRRLAI and LMODISLAI
13 Dec 2013 - M. Sulprizio- Add USE_03_FROM_MET logical flag
16 Apr 2014 - M. Sulprizio- Add field for PSC restart file
23 Jun 2014 - R. Yantosca - Add POP_EMISDIR field for POPs simlulation
25 Jun 2014 - R. Yantosca - Now add Input_Opt%SIM_TYPE field
29 Sep 2014 - R. Yantosca - Now add Input_Opt%N_DUST_BINS field
03 Dec 2014 - M. Yannetti - Added PRECISION_MOD
03 Dec 2014 - M. Sulprizio- Add fields for Radiation Menu
16 Dec 2014 - R. Yantosca - Removed JLOP, JLOP_PREV; these are in State_Chm
01 Apr 2015 - R. Yantosca - Add extra nested-grid fields
09 Apr 2015 - M. Sulprizio- Removed fields for NAPEMISS, POAEMISSSCALE,
                            and PST_RST_FILE. These options are now handled
                            by HEMCO.
11 Aug 2015 - R. Yantosca - Add MERRA2_DIR field to OptInput
26 Jan 2016 - E. Lundgren - Add fields for netcdf diagnostics
```

04 Feb 2016 - C. Keller - Add LINITSPEC. Used in ESMF to initialize species

```
concentrations from globchem.dat.
04 Feb 2016 - M. Sulprizio- Add Hg_CAT and Hg_CAT_FULL arrays for tagged Hg
                            simulations
27 Apr 2016 - R. Yantosca - Remove Hg_Cat, Hg_Cat_Full fields
17 May 2016 - R. Yantosca - Remove TRACER_N_CONST, TRACER_CONST, ID_EMITTED,
                            TRACER_COEFF
31 May 2016 - E. Lundgren - Remove TRACER_MW_KG, TRACER_MW_G, and XNUMOL
23 Jun 2016 - R. Yantosca - Remove references to APM code; it is no longer
                            compatible with the FlexChem implementation
13 Jul 2016 - R. Yantosca - Remove some unused drydep fields
16 Aug 2016 - M. Sulprizio- Rename from gigc_input_opt_mod.F90 to
                            input_opt_mod.F90. The "gigc" nomenclature is
                            no longer used.
29 Aug 2016 - M. Sulprizio- Rename N_TRACERS to N_ADVECT and TRACER_NAME to
                            AdvectSpc_Name to reflect that we now refer to
                            tracers as advected species
20 Sep 2016 - R. Yantosca - LND51_HDF and LND51b_HDF are now declared
```

03 Oct 2016 - R. Yantosca - LWINDO_CU has to be LOGICAL, not INTEGER

as LOGICAL, not INTEGER. This chokes Gfortran.

1.6.1 Set_Input_Opt

Subroutine SET_INPUT_OPT intializes all GEOS-Chem options carried in Input Options derived type object.

INTERFACE:

SUBROUTINE Set_Input_Opt(am_I_Root, Input_Opt, RC)

USES:

USE ErrCode_Mod

USE CMN_SIZE_Mod, ONLY : NDSTBIN, NVEGTYPE

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input Options object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

Set the following fields of Input_Opt outside of this routine:

(1) Input_Opt%MAX_DIAG : Max # of diagnostics

(2) Input_Opt%MAX_TRCS : Max # of tracers

```
(3 ) Input_Opt%MAX_MEMB : Max # of members per family tracer
(4 ) Input_Opt%MAX_FAMS : Max # of P/L diagnostic families
(5 ) Input_Opt%MAX_DEP : Max # of dry depositing species
(6 ) Input_Opt%LINOZ_NLEVELS : Number of levels in LINOZ climatology
(7 ) Input_Opt%LINOZ_NLAT : Number of latitudes in LINOZ climatology
(8 ) Input_Opt%LINOZ_NMONTHS : Number of months in LINOZ climatology
(9 ) Input_Opt%LINOZ_NFIELDS : Number of species in LINOZ climatology
```

We also need to implement better error checking.

```
01 Nov 2012 - R. Yantosca - Initial version
07 Nov 2012 - R. Yantosca - Now add size parameter fields to Input_Opt
                            that can be set prior to calling this routine
09 Nov 2012 - R. Yantosca - Now zero LD* fields for diagnostic levels
28 Nov 2012 - R. Yantosca - Now set USE_OLSON_2001 logical flag
29 Nov 2012 - M. Payer
                         - Add Input_Opt%ITS_A_POPS_SIM
26 Feb 2013 - M. Long
                        - Add extra fields from input.geos
28 Feb 2013 - R. Yantosca - Add haveImpRst field for GEOS-5 GCM interface
08 Mar 2013 - R. Yantosca - Now initialize the myCpu field
15 Mar 2013 - R. Yantosca - Now initialize the LINOZ_TPARM field
27 Mar 2013 - R. Yantosca - Add extra fields for tagged CO2
27 Mar 2013 - R. Yantosca - Add extra fields for EDGAR
29 Mar 2013 - R. Yantosca - Add DO_DIAG_WRITE field (to shut diags in MPI)
22 Apr 2013 - R. Yantosca - Now dimension ND48_*ARR to 1000 so that we are
                            consistent with the settings in diag48_mod.F
22 Jul 2013 - M. Sulprizio- Add extra fields for RCP emissions
07 Aug 2013 - M. Sulprizio- Add extra fields for SOA + SVPOA simulation
22 Aug 2013 - R. Yantosca - Add fields for soil NOx & species restart files
12 Sep 2013 - M. Sulprizio- Double size of IDDEP to account for dust
                            alkalinity (tdf 04/10/08)
17 Sep 2013 - M. Sulprizio- Add LDSTUP flag for acid uptake on dust aerosols
26 Sep 2013 - R. Yantosca - Renamed GEOS_57_DIR to GEOS_FP_DIR
25 Jun 2014 - R. Yantosca - Now initialize Input_Opt%SIM_TYPE field
03 Dec 2014 - M. Yannetti - Added PRECISION_MOD
05 Mar 2015 - R. Yantosca - Added RES_DIR, CHEM_INPUTS_DIR fields
06 Mar 2015 - R. Yantosca - Now initialize directory names with './'
01 Apr 2015 - R. Yantosca - Now initialize extra nested-grid fields
04 Mar 2016 - C. Keller - Added WETD_CONV_SCAL, LSYNOZ, LCAPTROP, and
                            OZONOPAUSE. These are only used within ESMF.
17 May 2016 - R. Yantosca - Remove TRACER_N_CONST, TRACER_CONST, ID_EMITTED,
                            TRACER_COEFF
31 May 2016 - E. Lundgren - Remove TRACER_MW_G, TRACER_MW_KG, and XNUMOL
13 Jul 2016 - R. Yantosca - Remove some obsolete drydep fields
13 Jul 2016 - R. Yantosca - Remove ID_TRACER, NUMDEP
```

1.6.2 Cleanup_Input_Opt

Subroutine CLEANUP_INPUT_OPT deallocates all allocatable fields of the Input Options object.

INTERFACE:

```
SUBROUTINE Cleanup_Input_Opt( am_I_Root, Input_Opt, RC )
```

USES:

USE ErrCode_Mod

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(OptInput), INTENT(INOUT) :: Input_Opt    ! Input Options object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure
```

REVISION HISTORY:

1.7 Fortran: Module Interface passive_tracer_mod.F90

Module passive_tracer_mod.F90 contains variables and routines for using passive tracers in GEOS-Chem. Passive tracers are tracers that are passively transported by GEOS-Chem, with a simple first order loss rate being applied to each tracer. The number of passive tracers, corresponding tracer properties as well as loss rates and default initial concentrations can be specified by the user via the GEOS-Chem input file (input.geos).

The passive tracer module is designed to work in combination with any existing GEOS-Chem simulation type, even though it has only been tested with the Radon simulation at this point. **REMARKS**:

```
Passive tracers are defined in input.geos in the PASSIVE TRACERS menu. For instance, to use the Radon simulation with two passive tracers ('Rn_ps' and 'Dummy') with atmospheric lifetimes of 3.8 days and 1 hour, respectively, add the following entries to input.geos:

%%% PASSIVE TRACERS %%%:
```

```
Number of pass. tracers : 2
   Passive tracer #1
                      : Rn_ps 328320.0 1.0e-20
                          : Dummy 3600.0
   Passive tracer #2
                                            1.0e-20
   The 3rd column of the tracer definition denotes the default initial
   concentration (in v/v) of the species of interest (1.0e-20 v/v in this
   case). This value will be used if the GEOS-Chem tracer restart file has
   no concentration field for the given tracer.
   There must be a matching entry in the tracers menu for every passive tracer
   defined in the passive tracers menu:
   %%% TRACER MENU %%%
   Type of simulation
                          : 1
                          : 4
   Number of Tracers
   Tracer Entries ----> : TR#
                                   Name g/mole
                                                 Tracer Members; () = emitted
   Tracer #1
                                   Rn
                                         222.0
                              1
   Tracer #2
                               2
                                   Pb
                                          210.0
   Tracer #3
                                            7.0
                          : 3
                                   Be7
   Tracer #4
                          : 4
                                   Rn_ps 222.0
                          : 5
   Tracer #5
                                   Dummy 100.0
   In this example, tracers 1-3 are the default tracers for this simulation type
   while tracers 4-5 are the user-specific passive tracers.
   As for regular GEOS-Chem tracers, emissions can be assigned to passive
   tracers via the HEMCO configuration file. For example, to assign a uniform
   flux of 0.1 kg/m2/s to passive tracer 'Dummy', add the following line to
   section base emissions of your HEMCO_Config.rc:
   0 DUMMY_EMIS 0.1 - - - xy kg/m2/s Dummy - 1 1
  //
 //
INTERFACE:
MODULE PASSIVE_TRACER_MOD
USES:
  USE PRECISION_MOD
  IMPLICIT NONE
  PRIVATE
```

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: INIT_PASSIVE_TRACER

PUBLIC :: ADD_PASSIVE_TRACER

PUBLIC :: PASSIVE_TRACER_GETRATE

PUBLIC :: PASSIVE_TRACER_INQUIRE

PUBLIC :: CLEANUP_PASSIVE_TRACER

PRIVATE MEMBER FUNCTIONS:

REVISION HISTORY:

```
04 Sep 2015 - C. Keller - Initial version.
```

1.7.1 Init_Passive_Tracer

Subroutine INIT_PASSIVE_TRACER initializes the passive tracers arrays.

INTERFACE:

```
SUBROUTINE INIT_PASSIVE_TRACER ( am_I_Root, NPT, RC )
```

USES:

USE ErrCode_Mod

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root ! root CPU?
```

INTEGER, INTENT(IN) :: NPT ! # of passive tracers

INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC ! Failure or success
```

REMARKS:

REVISION HISTORY:

```
04 Sep 2015 - C. Keller - Initial version
```

1.7.2 Add_Passive_Tracer

Subroutine ADD_PASSIVE_TRACER registers a passive tracer based on the passed input arguments.

INTERFACE:

```
SUBROUTINE ADD_PASSIVE_TRACER ( am_I_Root, TrcName, TrcTau, & TrcInitConc, TrcMW, RC )
```

USES:

USE ErrCode_Mod

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root ! root CPU?

CHARACTER(LEN=*), INTENT(IN ) :: TrcName ! Tracer name

REAL(fp), INTENT(IN ) :: TrcTau ! Tracer lifetime (s)

REAL(fp), INTENT(IN ) :: TrcInitConc ! Tracer default init conc (v/v)

REAL(fp), INTENT(IN ) :: TrcMW ! Tracer molec. weight (g/mol)
```

INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC ! Failure or success

REMARKS:

REVISION HISTORY:

```
04 Sep 2015 - C. Keller - Initial version
```

1.7.3 Passive_Tracer_Getrate

Subroutine PASSIVE_TRACER_GETRATE returns the unitless decay rate for the given tracer and chemistry time step. on all passive tracers.

INTERFACE:

```
SUBROUTINE PASSIVE_TRACER_GETRATE ( am_I_Root, TrcName, DT, Rate, RC )

USES:
```

USE ErrCode_Mod

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root ! root CPU?

CHARACTER(LEN=*), INTENT(IN ) :: TrcName ! Passive tracer name

REAL(fp), INTENT(IN ) :: DT ! Time step in s
```

OUTPUT PARAMETERS:

```
REAL(fp), INTENT( OUT) :: Rate ! Decay rate (unitless
```

INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC ! Failure or success
```

REMARKS:

```
04 Sep 2015 - C. Keller - Initial version
```

1.7.4 Passive_Tracer_Inquire

Function PASSIVE_TRACER_INQUIRE is a wrapper routine to inquire information about a passive tracer.

INTERFACE:

```
SUBROUTINE PASSIVE_TRACER_INQUIRE ( TrcName, IsPassive, MW, InitConc )
```

USES:

USE ErrCode_Mod

INPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(IN ) :: TrcName ! GC tracer name
```

OUTPUT PARAMETERS:

```
LOGICAL, OPTIONAL, INTENT( OUT) :: IsPassive ! Is TrcID a passive tracer?

REAL(fp), OPTIONAL, INTENT( OUT) :: MW ! Molecular weight (g/mol)

REAL(fp), OPTIONAL, INTENT( OUT) :: InitConc ! Initial concentration (v/v)
```

REMARKS:

REVISION HISTORY:

```
04 Sep 2015 - C. Keller - Initial version
```

1.7.5 Cleanup_Passive_Tracer

Subroutine CLEANUP_PASSIVE_TRACER finalizes the passive tracers arrays.

INTERFACE:

```
SUBROUTINE CLEANUP_PASSIVE_TRACER ( am_I_Root, RC )
```

USES:

USE ErrCode_Mod

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root ! root CPU?
```

INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC ! Failure or success
```

REMARKS:

```
04 Sep 2015 - C. Keller - Initial version
```

1.8 Fortran: Module Interface physiconstants.F

PhysConstants contains GEOS-Chem specific PHYSICAL CONSTANTS and DERIVED QUANTITIES.

INTERFACE:

MODULE PHYSCONSTANTS

USES:

```
USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

IMPLICIT NONE

PUBLIC
```

DEFINED PARAMETERS:

```
! AIRMW : Average molecular weight of dry air [g/mol]
REAL(fp), PARAMETER :: AIRMW = 28.97e+0_fp
! H2OMW : Molecular weight of water [g/mol]
REAL(fp), PARAMETER :: H20MW = 18.016e+0_fp
      : Avogadro's number [particles/mol]
! Now use more precise value 6.022140857e+23 instead of 6.022e+23?
! Source: NIST, 2014 (ewl, 1/7/16) (NEED TO CHANGE HEMCO)
REAL(fp), PARAMETER :: AVO
                               = 6.022140857e+23_fp
        : Acceleration due to gravity at earth's surface [m/s^2]
! Now use more precise value of 9.80665 instead of 9.8 (ewl, 1/7/16)
! Source: NIST, 2014 (NEED TO CHANGE HEMCO)
REAL(fp), PARAMETER :: g0
                                    9.80665e+0_fp
! g0_100 : 100 / g0
REAL(fp), PARAMETER :: g0_100 = 100.e+0_fp / g0
       : Double-Precision value of PI
! PI
REAL(fp), PARAMETER :: PI
                               = 3.14159265358979323e+0_fp
! PI_180 : Number of radians per degree
REAL(fp), PARAMETER :: PI_180 = PI / 180e+0_fp
! Re
       : Radius of Earth [m]
REAL(fp), PARAMETER :: Re
                               = 6.375e+6_{fp}
       : Gas Constant in Dry Air [J/K/kg]
REAL(fp), PARAMETER :: Rd
                                = 287.0e+0_fp
! Rv : Gas Constant for water vapor [J/K/kg]
```

REAL(fp), $PARAMETER :: Rv = 461.0e+0_fp$

```
! Rdg0 = Rd
                       / g0
      REAL(fp), PARAMETER :: Rdg0
                                    = Rd / g0
       ! SCALE_HEIGHT : Scale height of atmosphere [m]
      REAL(fp), PARAMETER :: SCALE_HEIGHT = 7600.e+0_fp
       ! VON_KARMAN : Von Karman's constant [.]
      REAL(fp), PARAMETER :: VON_KARMAN = 0.4e+0_fp
       ! RSTARG : Molar gas constant [J/K/mol]
       ! Now use more precise value 8.3144598 instead of 8.31450? (ewl, 1/7/16)
       ! Source: NIST, 2014 (NEED TO CHANGE HEMCO)
      REAL(fp), PARAMETER :: RSTARG
                                      = 8.3144598e+0_fp
       ! XNUMOLAIR : Molecules dry air per kg dry air
      REAL(fp), PARAMETER :: XNUMOLAIR = AVO / ( AIRMW * 1.e-3_fp)
       ! BOLTZ : Boltzmann's constant [J/K] (Source: NIST, 2014)
      REAL(fp), PARAMETER :: BOLTZ = 1.38064852e-23_{fp}
       ! ATM : Standard atmosphere [Pa] (Source: NIST, 2014)
      REAL(fp), PARAMETER :: ATM
                                  = 1.01325e+5_fp
       ! Condensation vapor pressure
       ! ** NEED SOURCE **
       ! We think 6.1078 hPa is the saturation vapor pressure at 273.16 K, the
         triple point of water, but this needs to be confirmed (mps, 4/21/16)
       ! Use BOLTZ [J/K] rather than BOLTG [ergs/K] from comode_loop_mod
          (ewl, 1/4/16)
      REAL(fp), PARAMETER :: CONSVAP = 6.1078e+03_fp /
                                        (BOLTZ * 1e+7_fp)
   !REFERENCES:
   (1) NIST, 2014. Website: http://physics.nist.gov/cuu/Constants/index.html
REVISION HISTORY:
    25 Jun 2002 - R. Yantosca - Initial version
    23 Aug 2011 - M. Long - Converted to Module from Header file
    23 Jul 2014 - R. Yantosca - Add Von Karman's constant here
   23 Jul 2014 - R. Yantosca - Add Avogadro's number here
   23 Jul 2014 - R. Yantosca - List constants in alphabetical order
   02 Dec 2014 - M. Yannetti - Added PRECISION_MOD
   06 Jan 2014 - E. Lundgren - Added constants and clarified comments
   24 Mar 2015 - E. Lundgren - Add xnumolair, previously in tracer_mod
   08 Jan 2016 - E. Lundgren - Update values to NIST 2014 and use AIRMW in
                               definition of XNUMOLAIR. Add BOLTZ.
   08 Jan 2016 - E. Lundgren - Rename this file to physconstants.F. Previously
```

```
it was called CMN_GCTM_mod.F
21 Apr 2016 - M. Sulprizio- Move CONSVAP here from comode_loop_mod.F
```

1.9 Fortran: Module Interface precision_mod.F

Module PRECISION_MOD is used to change the precision of many variables throughout GEOS-Chem at compile-time.

INTERFACE:

MODULE PRECISION_MOD

USES:

IMPLICIT NONE PRIVATE

DEFINED PARAMETERS:

```
! ------
    ! Set parameters for floating precision
    ! FP will be set to either 4-byte or 8-byte precision at compile
    ! time. Most variables can now declared with REAL(fp).
    #if defined( USE_REAL8 )
    ! Use 8-byte floating point precision when asked.
    INTEGER, PARAMETER, PUBLIC :: fp = KIND( REAL( 0.0, 8 ) )
#else
    ! Use 4-byte floating point by default.
    INTEGER, PARAMETER, PUBLIC :: fp = KIND( REAL( 0.0, 4 ) )
#endif
    |-----
    ! Set parameters for fixed precision
    ! Not all variables can be converted into the flexible precision.
    ! Some may have to be still declared as either 4-byte or 8-byte
    ! floating point. Use these parameters for such variables.
    ! KIND parameter for 4-byte precision
    INTEGER, PARAMETER, PUBLIC :: f4 = KIND( REAL( 0.0, 4 ) )
    ! KIND parameter for 8-byte precision
    INTEGER, PARAMETER, PUBLIC :: f8 = KIND( REAL( 0.0, 8 ) )
```

REMARKS:

This module is designed to help avoid hard-coding precision.

REVISION HISTORY:

1.10 Fortran: Module Interface species_database_mod.F90

Module SPECIES_DATABASE_MOD contains routines to set up a database object containing physical properties for each GEOS-Chem species. This allows us to consolidate all species properties into a single data structure, for convenience.

INTERFACE:

```
MODULE Species_Database_Mod
```

USES:

```
USE Precision_Mod
```

IMPLICIT NONE PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: Init_Species_Database
PUBLIC :: Cleanup_Species_Database

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: TranUc

%%% Uncomment this if you want to use the new henry's law constants

%%% compiled by Katie Travis and posted on this wiki page:

#define NEW_HENRY_CONSTANTS 1

REMARKS:

```
28 Aug 2015 - R. Yantosca - Initial version
02 Aug 2016 - M. Sulprizio- Add KppSpcId to store all KPP species incices.
```

1.10.1 Init_Species_Database

Initializes the GEOS-Chem species database object. You can add information about new species to this routine.

INTERFACE:

```
SUBROUTINE Init_Species_Database( am_I_Root, Input_Opt, SpcData, RC )
```

USES:

```
USE ErrCode_Mod
USE Input_Opt_Mod, ONLY : OptInput
USE Passive_Tracer_Mod, ONLY : PASSIVE_TRACER_INQUIRE
USE Species_Mod
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(SpcPtr), POINTER :: SpcData(:) ! Vector with species info
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REMARKS:

For detailed information about the species database (and the physical properties that are specified there), please see the following GEOS-Chem wiki pages:

- (1) wiki.geos-chem.org/GEOS_Chem_species_database
- (2) wiki.geos-chem.org/Physical_properties_of_GEOS-Chem_species References for the new Henry's law constants:
- (1) Sander et al [2015]: http://henrys-law.org The Hcp (aka KO) parameter listed on the wiki page:

http://wiki.geos-chem.org/Physical_properties_of_GEOS-Chem_species have units of [mol m-3 Pa-1]. But the GEOS-Chem species object expects this parameter to have units of [M atm-1]. Therefore, when we pass the Hcp parameter to routine Spc_Create via the HENRY_KO argument, we will multiply by the proper conversion factor (9.86923e-3) to convert [mol m-3 Pa-1] to [M atm-1].

```
22 Jul 2015 - R. Yantosca - Initial version
01 Sep 2015 - R. Yantosca - Add Henry KO, CR constants for DMS, ACET
02 Sep 2015 - R. Yantosca - Corrected typos for some SOA species
24 Sep 2015 - R. Yantosca - WD_RainoutEff is now a 3-element vector
24 Sep 2015 - R. Yantosca - Add WD_KcScaleFAc, a 3-element vector
```

```
30 Sep 2015 - R. Yantosca - DD_A_Density is renamed to Density
30 Sep 2015 - R. Yantosca - DD_A_Radius is renamed to Radius
01 Oct 2015 - R. Yantosca - Added DD_DvzMinVal field to put a minimum
                            deposition velocity for sulfate aerosols
14 Oct 2015 - E. Lundgren - Treat H2SO4 as an aerosol for TOMAS
18 Nov 2015 - M. Sulprizio- Add passive tracers PASV to RnPbBe simulation
16 Dec 2015 - R. Yantosca - Use MW_g = 31.4 g/mol for SO4s and NITs
15 Mar 2016 - R. Yantosca - Added tagged CO tracer names
22 Apr 2016 - R. Yantosca - Now define Is_HgO, Is_Hg2, Is_HgP fields
19 May 2016 - R. Yantosca - Remove DryDepId_PAN and DryDepId_HN03; we shall
                            now explicitly compute a drydep velocity for
                            all GEOS-Chem species.
21 Jun 2016 - M. Sulprizio- Set Is_Photolysis to T for all species included
                            in FAST-JX photolysis. Also added new species
                            that are in FAST-JX photolysis but not already
                            defined here.
18 Jul 2016 - M. Sulprizio- Remove family tracers ISOPN, MMN, CFCX, HCFCX
                            and replace with their constituents.
02 Aug 2016 - M. Sulprizio- Add KppSpcId as argument passed to Spc_Create
11 Aug 2016 - E. Lundgren - Define special background conc for some species
22 Nov 2016 - M. Sulprizio- Move aerosol densities for BC, OC, and SO4 here
                            from aerosol_mod.F
```

1.10.2 Cleanup_Species_Database

Finalizes the vector with species information.

INTERFACE:

```
SUBROUTINE Cleanup_Species_Database( am_I_Root, SpcData, RC )
USES:
```

USE ErrCode_Mod USE Species_Mod

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(SpcPtr), POINTER :: SpcData(:) ! Species database object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

REVISION HISTORY:

22 Jul 2015 - R. Yantosca - Initial version

1.10.3 TranUc

Tranlate a character variable to all upper case letters. Non-alphabetic characters are not affected. The original "text" is destroyed.

INTERFACE:

```
SUBROUTINE TranUc( text )
```

INPUT/OUTPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(INOUT) :: text
```

AUTHOR:

```
Robert D. Stewart, May 19, 1992 (part of CHARPAK)
```

REMARKS:

Keep a private shadow copy of this routine here so as not to incur a dependency with GeosUtil/charpak_mod.F. This lets us keep species_datbase_mod.F90 in the Headers/ folder together with state_chm_mod.F90 and species_mod.F90.

REVISION HISTORY:

```
06 Jan 2015 - R. Yantosca - Initial version
```

1.10.4 Unique_Species_Names

Stores the list of unique species names (i.e. removing duplicates from the list of advected species and the list of KPP species) for later use. Also computes the corresponding indices for the KPP variable and fixed species arrays (VAR and FIX, respectively).

INTERFACE:

```
SUBROUTINE Unique_Species_Names( am_I_Root, Input_Opt, nSpecies, RC )
```

USES:

```
USE ErrCode_Mod
```

USE Input_Opt_Mod, ONLY : OptInput

USE GcKpp_Monitor, ONLY : Spc_Names

USE GcKpp_Parameters, ONLY: NFIX, NSPEC, NVAR

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: nSpecies ! Number of unique species
```

INTEGER, INTENT(OUT) :: RC ! Success or failure

REMARKS:

This may not be the fastest search algorithm (because it relies on string comparisons). But it is only executed at startup so we can live with it. We could make it faster by hashing but that seems like overkill.

REVISION HISTORY:

```
09 May 2016 - R. Yantosca - Initial version
02 Aug 2016 - M. Sulprizio- Add KppSpcId; Also only set KppVarId if loop indexis <= NVAR.
```

1.10.5 Cleanup_Work_Arrays

Stores the list of unique species names (i.e. removing duplicates from the list of advected species and the list of KPP species) for later use. Also computes the indices for KPP variable and fixed indices.

INTERFACE:

```
SUBROUTINE Cleanup_Work_Arrays()
```

REMARKS:

This may not be the fastest search algorithm, but it is only executed once, at startup.

REVISION HISTORY:

```
06 May 2016 - R. Yantosca - Initial version
```

1.11 Fortran: Module Interface species_mod.F90

Module SPECIES_MOD contains types and routines to define the GEOS-Chem species object.

INTERFACE:

```
MODULE Species_Mod
USES:
USE Precision_Mod
IMPLICIT NONE
PRIVATE
```

PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: Str2Hash

PUBLIC :: SpcData_Init

PUBLIC :: SpcData_Cleanup

PUBLIC :: Spc_Create

PUBLIC :: Spc_GetIndx

PUBLIC :: Spc_GetNumSpecies
```

PUBLIC TYPES:

PUBLIC :: Spc_Print

```
! Counters for the species indices
INTEGER, PRIVATE :: AdvectCount = 0
                               ! Counter of advected species
INTEGER, PRIVATE :: DryDepCount = 0
                              ! Counter of dry-deposited species
INTEGER, PRIVATE :: KppSpcCount = 0
                               ! Counter of species in KPP matrix
INTEGER, PRIVATE :: WetDepCount = 0
                              ! Counter of wet-deposited species
                           ! Counter of active chem species
! Counter of fixed chem species
! Counter of photolysis species
INTEGER, PRIVATE :: ActiveCount = 0
                               ! Counter of active chem species
INTEGER, PRIVATE :: FixedCount = 0
INTEGER, PRIVATE :: PhotolCount = 0
                       = 0
= 0
INTEGER, PRIVATE :: HgOCount = 0
                              ! Number of HgO tracers
INTEGER, PRIVATE :: Hg2Count
                               ! Number of Hg2 tracers
INTEGER, PRIVATE :: HgPCount
                               ! Number of HgP tracers
!-----
! Type for the Species Database object (vector of type Species)
TYPE, PUBLIC :: SpcPtr
  END TYPE SpcPtr
! Type for individual species information
! (i.e. this is a single entry in the Species Database)
TYPE, PUBLIC :: Species
  ! Indices
  INTEGER
                :: ModelID
                              ! Model species ID
  INTEGER
                :: AdvectID
                              ! Advection index
  INTEGER
                :: DryDepID
                               ! Dry deposition index
  INTEGER
                :: WetDepID
                              ! Wet deposition index
                            ! KPP species
! KPP variable species index
! KPP fixed species index
! Photolysis index
                :: KppSpcID
  INTEGER
                :: KppVarId
                               ! KPP variable species index
  INTEGER
               :: KppFixId
  INTEGER
  INTEGER
               :: PhotolID
  ! Names
  CHARACTER(LEN=31) :: Name
                              ! Short name
```

```
CHARACTER(LEN=80) :: FullName
                                   ! Long name
INTEGER
                 :: NameHash
                                   ! Integer hash for short name
! Logical switches
LOGICAL
         :: Is_Gas
                                   ! Is it a gas? If not, aerosol.
LOGICAL
                :: Is_Advected
                                  ! Is it advected?
                :: Is_DryDep
                                  ! Is it dry-deposited?
LOGICAL
                 :: Is_WetDep
                                  ! Is it wet-deposited?
LOGICAL
                :: Is_Kpp
                                  ! Is it in the KPP mechanism?
LOGICAL
LOGICAL
                :: Is_ActiveChem ! Is it an active chemical species?
                :: Is_FixedChem ! Is it a fixed chemical species?
LOGICAL
LOGICAL
                :: Is_Photolysis
                                  ! Is it an photolysis species?
                :: Is_InRestart
                                  ! Is it in the restart file?
LOGICAL
! Molecular weights
REAL(fp)
                                   ! Species molecular weight [g/mol]
                :: MW_g
                                   ! Emitted molecular weight [g/mol]
REAL(fp)
                :: EmMW_g
REAL(fp)
                :: MolecRatio
                                   ! Mol carbon / mol species [1
! Default background concentration
REAL(fp)
                :: BackgroundVV
                                   ! Background conc [v/v]
! Density and radius
REAL(fp)
                                   ! Density [kg/m3]
                :: Density
REAL(fp)
                :: Radius
                                   ! Radius
                                            [m]
! Henry's law parameters
REAL(f8)
                :: Henry_KO
                                  ! Liq./gas Henry const [M/atm]
                :: Henry_CR
                                  ! d(ln KO) / d(1/T)
REAL(f8)
                                                       [K
                :: Henry_PKA
                                  ! pKa for Henry const. correction
REAL(f8)
! Drydep parameters
LOGICAL
                :: DD_AeroDryDep
                                  ! Use AERO_SFCRSII for drydep?
LOGICAL
                :: DD_DustDryDep
                                  ! Use DUST_SFCRSII for drydep?
                :: DD_DvzAerSnow ! Vd for aerosols on snow [cm/s]
REAL(fp)
                :: DD_DvzMinVal(2) ! Min Vd for aerosols [cm/s]
REAL(fp)
REAL(fp)
                :: DD_F0
                                   ! FO (reactivity) factor [1]
REAL(fp)
                 :: DD_KOA
                                   ! KOA factor for POPG
!%%% NOTE: We will eventually replace this with the common Henry's law
! ///// parameters. But in order to replicate the prior behavior,
! % we will need to supply the dry deposition code with the same
!%%% HSTAR values that are currently set in INIT_DRYDEP. Therefore,
!%%% add this field as a temporary placeholder for the Hstar quantity
!%%% from drydep_mod.F. We will remove this later on. (bmy, 8/24/15)
! %%%
REAL(fp)
                 :: DD_Hstar_Old
                                   ! HSTAR value in drydep_mod [M/atm]
```

```
! Wetdep parameters, gas-phase species
                 :: WD_LiqAndGas ! Consider liquid and gas phases?
  LOGTCAL.
                 :: WD_ConvFacI2G ! Conv. factor for ice/gas ratio
  REAL(fp)
  REAL(fp)
                 :: WD_RetFactor
                                  ! Retention factor [1]
  ! Wetdep parameters, aerosol-phase species
  LOGICAL
                 :: WD_Is_H2SO4
                                 ! Flag to denote H2SO4 wetdep
  LOGICAL
                 :: WD_Is_HNO3
                                 ! Flag to denote HNO3 wetdep
  LOGICAL
                :: WD_Is_SO2
                                 ! Flag to denote SO2 wetdep
                 :: WD_CoarseAer
  LOGICAL
                                 ! T=coarse aerosol; F=fine aerosol
                 :: WD_AerScavEff
                                  ! Aerosol scavenging efficiency
  REAL(fp)
  REAL(fp)
                 :: WD_KcScaleFac(3) ! Temperature-dependent scale
                                  ! factors to multiply Kc rate
                                  ! (conv of condensate -> precip)
                                  ! in F_AEROSOL (wetscav_mod.F)
  REAL(fp)
                :: WD_RainoutEff(3) ! Temperature-dependent scale
                                  ! factors for rainout efficiency
  ! Microphysics parameters
  LOGICAL
                 :: MP_SizeResAer
                                  ! T=size-resolved aerosol (TOMAS)
  LOGICAL
                 :: MP_SizeResNum
                                  ! T=size-resolved aerosol number
  ! Tagged mercury parameters
                               ! T=total or tagged HgO species
! T=total or tagged HgO species
  LOGICAL
              :: Is_HgO
  LOGICAL
                 :: Is_Hg2
  LOGICAL
                 :: Is_HgP
                                 ! T=total or tagged HgP species
  INTEGER
                 :: Hg_Cat
                                  ! Tagged Hg category number
END TYPE Species
!DEFINED PARAMETERS
! Missing value parameters
INTEGER, PARAMETER :: MISSING_INT = -999 ! Integer
REAL(fp), PARAMETER :: MISSING = -999e+0_fp ! Flexible precision
REAL(f8), PARAMETER :: MISSING_R8 = -999e+0_f8 ! 8-byte precision
REAL(fp), PARAMETER :: ZERO = 0.0e+0_fp ! Flexible precision
REAL(f8), PARAMETER :: ZERO_R8 = 0.0e+0_f8 ! 8-byte precision
REAL(fp), PARAMETER :: MISSING_MW = -1.0_fp ! Missing MW values
!-----
! Missing species concentration value if not in restart file and special
! background value not defined
REAL(fp), PARAMETER, PUBLIC :: MISSING_VV = 1.0e-20_fp ! Missing spc conc
```

REMARKS:

- (1) The emission molecular weight is the molecular weight of the emitted compound. This value is only different to MW_g if the emitted compound does not correspond to the transported species, e.g. if emissions are in kg C4H10 but the corresponding species is transported as mass Carbon.
- (2) MolecRatio is the ratio between # of species molecules per emitted molecule, e.g. 4 if emissions are kg C4H10 but model species are kg C.

REVISION HISTORY:

```
28 Feb 2014 - C. Keller - Initial version
22 Jul 2015 - R. Yantosca - Updated and cleaned up a bit
18 Aug 2015 - R. Yantosca - Added indices for drydep, wetdep, transport
18 Aug 2015 - R. Yantosca - Added missing value parameters
31 Aug 2015 - R. Yantosca - Add AdvectId
24 Sep 2015 - R. Yantosca - Make WD_RainoutEff a 3-element vector:
                            (1) T < 237K; (2) 237K < T < 258 K (3) T > 258K
24 Sep 2015 - R. Yantosca - Rename WD_ConvFactor to WD_ConvFacI2G
25 Sep 2015 - R. Yantosca - Rename WD_SizeResAer to MP_SizeResAer
25 Sep 2015 - R. Yantosca - Add MP_SizeResBin for microphysics size bins
30 Sep 2015 - R. Yantosca - Renamed DD_A_Density to Density
30 Sep 2015 - R. Yantosca - Renamed DD_A_Radius to Radius
30 Sep 2015 - R. Yantosca - Added WD_Is_HNO3 and WD_Is_SO2 fields to flag
                            special cases of HNO3 and SO2 wet deposition
01 Oct 2015 - R. Yantosca - Add field DD_DvzMinVal
16 Oct 2015 - E. Lundgren - Add WD_Is_H2SO4 field to flag special case of
                            H2SO4 wet deposition for microphysics
22 Apr 2016 - R. Yantosca - Added Is_HgO, Is_Hg2, Is_HgP species
04 May 2016 - R. Yantosca - Added fast name lookup via hashing
09 May 2016 - R. Yantosca - Add Is_Kpp, KppVarId, KppFixId to type Species
21 Jun 2016 - M. Sulprizio- Add Is_Photolysis, Is_ActiveChem, and
                            Is_FixedChem to type Species
25 Jul 2016 - E. Lundgren - Add Is_InRestart to track which species are
                            read in versus set to default background values
02 Aug 2016 - M. Sulprizio- Remove function Get_KPPIndx, it is not used.
                            KppSpcId is set in species_database_mod.F90 where
                            KppVarId and KppFixId are set.
04 Aug 2016 - R. Yantosca - Add parameter MISSING_MW = -1.0
10 Aug 2016 - E. Lundgren - Add BackgroundVV field for default background
                            and missing background concentration param [v/v]
```

1.11.1 Str2Hash

Returns a unique integer hash for a given character string. This allows us to implement a fast name lookup algorithm.

INTERFACE:

```
FUNCTION Str2Hash( Str ) RESULT( Hash )
```

INPUT PARAMETERS:

```
CHARACTER(LEN=14), INTENT(IN) :: Str    ! String (14 chars long)
```

RETURN VALUE:

```
INTEGER :: Hash ! Hash value from string
```

REMARKS:

- (1) Algorithm taken from this web page: https://fortrandev.wordpress.com/2013/07/06/fortran-hashing-algorithm/
- (2) For now, we only use the first 14 characters of the character string to compute the hash value. Most GEOS-Chem species names only use at most 14 unique characters. We can change this later if need be.

REVISION HISTORY:

```
04 May 2016 - R. Yantosca - Initial version
05 May 2016 - R. Yantosca - Now make the input string 14 chars long
```

1.11.2 SpcData_Init

Routine SpcData_Init initializes species database object. This is an array where each element is of type Species. This object holds the metadata for each species (name, molecular weight, Henry's law constants, drydep info, wetdep info, etc.

INTERFACE:

```
SUBROUTINE SpcData_Init( am_I_Root, nSpecies, SpecDB, RC )
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! root CPU?
INTEGER, INTENT(IN) :: nSpecies ! # of species
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(SpcPtr), POINTER :: SpecDB(:) ! Species database INTEGER, INTENT(INOUT) :: RC ! Return code
```

```
20 Aug 2013 - C. Keller - Adapted from gigc_state_chm_mod.F90 22 Jul 2015 - R. Yantosca - Cosmetic changes
```

1.11.3 Spc_GetIndx

Function Spc_GetIndx returns the index of a given species in the species data base object. You can search by the short name or the full name of the species.

INTERFACE:

```
FUNCTION Spc_GetIndx( Name, SpecDB ) RESULT( Indx )
```

USES:

USE CHARPAK_MOD, ONLY : TRANUC

INPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(IN) :: Name ! Species name
```

TYPE(SpcPtr), POINTER :: SpecDB(:) ! Species Database object

RETURN VALUE:

INTEGER :: Indx ! Index of this species

REMARKS:

The input name field has will get copied to an internal string that is 14 characters long, for input into the Str2Hash function. 14 characters is about the longest species name for GEOS-Chem. We can modify this if need be.

REVISION HISTORY:

```
09 Oct 2012 - M. Long - Initial version, based on gc_esmf_utils_mod.F90
```

22 Jul 2015 - R. Yantosca - Cosmetic changes

04 May 2016 - R. Yantosca - Now use hash comparison, it's faster

04 May 2016 - R. Yantosca - Renamed to Spc_GetIndx

05 May 2016 - R. Yantosca - The NAME argument is now of variable length

15 Jun 2016 - M. Sulprizio- Make species name uppercase before computing hash

1.11.4 SpcData_Cleanup

Routine SpcData_Cleanup cleans up the passed species collection object

INTERFACE:

```
SUBROUTINE SpcData_Cleanup( SpecDB )
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(SpcPtr), POINTER :: SpecDB(:) ! Species database object
```

REVISION HISTORY:

```
20 Aug 2013 - C. Keller - Adapted from gigc_state_chm_mod.F90
```

22 Jul 2015 - R. Yantosca - Cosmetic changes

08 Oct 2015 - R. Yantosca - Bug fix, make sure the size of SpecDb is zero before deallocating each element

1.11.5 Spc_Create

Routine Spc_Create creates a new object that holds information about a given species, and assigns values to it.

INTERFACE:

```
SUBROUTINE Spc_Create( am_I_Root,
                                       ThisSpc,
                                                       ModelID,
                                                                       &
                        DryDepID,
                                       Name,
                                                       FullName,
                                                                        &
                        MW_g,
                                       EmMW_g,
                                                       MolecRatio,
                                                                        &
                        BackgroundVV,
                                       Henry_KO,
                                                       Henry_CR,
                                                                       &
                        Henry_PKA,
                                       Density,
                                                       Radius,
                                                                       &
                        DD_AeroDryDep, DD_DustDryDep, DD_DvzAerSnow,
                                                                       &
                        DD_DvzMinVal,
                                       DD_FO,
                                                       DD_KOA,
                                                                       &
                        DD_HStar_Old,
                                       MP_SizeResAer, MP_SizeResNum,
                                                                       &
                        WD_RetFactor,
                                       WD_LiqAndGas,
                                                       WD_ConvFacI2G,
                        WD_AerScavEff, WD_KcScaleFac, WD_RainoutEff,
                        WD_CoarseAer,
                                       Is_Advected,
                                                       Is_Gas,
                                                                       &
                        Is_Drydep,
                                       Is_Wetdep,
                                                       Is_Photolysis,
                                                                       &
                        Is_InRestart,
                                       Is_Hg0,
                                                       Is_Hg2,
                                                                       &
                        Is_HgP,
                                       KppSpcId,
                                                       KppVarId,
                                                                       &
                        KppFixId,
                                       RC
                                                       )
```

USES:

```
USE CHARPAK_MOD, ONLY: TRANUC! String manipulation
USE PhysConstants, ONLY: AIRMW, AVO! Physical constants
```

INPUT PARAMETERS:

```
:: am_I_Root
                                                    ! Are we on the root CPU?
LOGICAL,
                  INTENT(IN)
                                                    ! Model ID number
INTEGER,
                  OPTIONAL
                               :: ModelID
INTEGER,
                  OPTIONAL
                               :: DryDepID
                                                    ! Drydep ID number
CHARACTER(LEN=*), OPTIONAL
                               :: Name
                                                    ! Short name of species
                                                    ! Long name of species
CHARACTER(LEN=*), OPTIONAL
                               :: FullName
REAL(fp),
                                                    ! Molecular weight [g]
                  OPTIONAL
                               :: MW_g
REAL(fp),
                               :: EmMW_g
                                                    ! Emissions mol. wt [g]
                  OPTIONAL
                               :: MolecRatio
REAL(fp),
                                                    ! Molec ratio
                  OPTIONAL
REAL(fp),
                  OPTIONAL
                               :: BackgroundVV
                                                    ! Background conc [v/v]
                                                    ! Henry's law KO [M/atm]
                               :: Henry_KO
REAL(f8),
                  OPTIONAL
                               :: Henry_CR
                                                    ! Henry's law CR [K]
REAL(f8),
                  OPTIONAL
                               :: Henry_PKA
                                                    ! Henry's law pKa [1]
REAL(f8),
                  OPTIONAL
REAL(fp),
                               :: Density
                                                    ! Density [kg/m3]
                  OPTIONAL
REAL(fp),
                               :: Radius
                                                    ! Radius [m]
                  OPTIONAL
                               :: DD_AeroDryDep
                                                    ! Use AERO_SFCRSII?
LOGICAL,
                  OPTIONAL
LOGICAL,
                               :: DD_DustDryDep
                                                    ! Use DUST_SFCRSII?
                  OPTIONAL
                                                    ! Vd for aerosols
REAL(fp),
                  OPTIONAL
                               :: DD_DvzAerSnow
                                                    ! on snow/ice [cm/s]
REAL(fp),
                  OPTIONAL
                               :: DD_DvzMinVal(2)
                                                    ! Min Vd for aerosols
                                                    ! (cf GOCART) [cm/s]
```

```
REAL(fp),
                OPTIONAL
                           :: DD_F0
                                             ! Drydep reactivity [1]
REAL(fp),
                OPTIONAL
                           :: DD_KOA
                                             ! Drydep KOA parameter
!%%% NOTE: We will eventually replace this with the common Henry's law
!%%% parameters. But in order to replicate the prior behavior,
1\%\% we will need to supply the dry deposition code with the same
!%%% HSTAR values that are currently set in INIT_DRYDEP. Therefore,
!%%% add this field as a temporary placeholder for the Hstar quantity
!%%% from drydep_mod.F. We will remove this later on. (bmy, 8/24/15)
! %%%
                           :: DD_Hstar_Old
                                             ! HSTAR, drydep [M/atm]
REAL(fp),
                OPTIONAL
:: MP_SizeResAer
                                             ! Size resolved aerosol?
LOGICAL,
                OPTIONAL
                OPTIONAL
                          :: MP_SizeResNum
                                             ! Size resolved aer #?
LOGICAL,
REAL(fp),
                OPTIONAL
                           :: WD_RetFactor
                                             ! Wetdep retention factor
                          :: WD_LiqAndGas
                                             ! Liquid and gas phases?
LOGICAL,
                OPTIONAL
REAL(fp),
                OPTIONAL
                          :: WD_ConvFacI2G
                                             ! Factor for ice/gas ratio
                OPTIONAL :: WD_AerScavEff
REAL(fp),
                                             ! Aerosol scavenging eff.
REAL(fp),
                OPTIONAL :: WD_KcScaleFac(3) ! Factor to multiply Kc
                                             ! rate in F_AEROSOL
                OPTIONAL
                          :: WD_RainoutEff(3) ! Rainout efficiency
REAL(fp),
                          :: WD_CoarseAer
                                             ! Coarse aerosol?
LOGICAL,
                OPTIONAL
                                             ! Is it advected?
LOGICAL,
                OPTIONAL
                          :: Is_Advected
                          :: Is_Gas
                                             ! Gas (T) or aerosol (F)?
LOGICAL,
                OPTIONAL
                OPTIONAL :: Is_Drydep
                                             ! Is it dry deposited?
LOGICAL,
                         :: Is_Wetdep
                                             ! Is it wet deposited?
LOGICAL,
                OPTIONAL
LOGICAL,
                          :: Is_Photolysis
                                             ! Is it photolysis spc?
                OPTIONAL
LOGICAL,
                OPTIONAL
                          :: Is_InRestart
                                             ! Is it in restart file?
                         :: Is_Hg0
                                             ! Denotes HgO species
LOGICAL,
                OPTIONAL
LOGICAL,
                OPTIONAL
                          :: Is_Hg2
                                             ! Denotes Hg2 species
LOGICAL,
                OPTIONAL
                          :: Is_HgP
                                             ! Denotes HgP species
                          :: KppSpcId
                                             ! KPP species ID
INTEGER,
                OPTIONAL
                         :: KppVarId
                                             ! KPP variable species ID
INTEGER,
                OPTIONAL
INTEGER,
                OPTIONAL
                          :: KppFixId
                                             ! KPP fixed species ID
```

INPUT/OUTPUT PARAMETERS:

TYPE(Species), POINTER :: ThisSpc ! Object w/ species info

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Return code

REMARKS:

- (1) If Fullname is not specified, it will use the value assigned to Name.
- (2) If EmMw_g is not specified, it will use the value assigned to MW_g.
- (3) If MolecRatio is not specified, it will be set to 1.
- (4) WD_Is_HNO3 is automatically set according to Name.

- (5) WD_Is_SO2 is automatically set according to Name.
- (6) All other fields, if not specified, will be set to MISSING
- (7) If Is_Gas = T, aerosol-specific fields will be set to MISSING. (except for HNO3 and SO2, which wet scavenge as aerosols).
- (8) If Is_Gas = F, gas-phase specific-fields will be set to MISSING.
- (9) If Is_Advected = T, this will automatically update AdvectId.
- (10) If Is_Drydep = T, this will automatically update DryDepId.
- (11) If Is_Wetdep = T, this will automatically update WetDepId.

20 Aug 2013 - C. Keller - Adapted from gigc_state_chm_mod.F90

REVISION HISTORY:

21 Jun 2016 - M. Sulprizio- Add optional argument Is_Photolysis. Also set
Is_ActiveChem and Is_Fixed Chem according to
KppVarId and KPPFixId.

06 Jul 2016 - R. Yantosca - Add more error checks to avoid uninit'd fields
18 Jul 2016 - M. Sulprizio- Remove special handling of ISOPN and MMN for
DryDepCount. Family tracers have been eliminated.

25 Jul 2016 - E. Lundgren - Add optional argument Is_InRestart

02 Aug 2016 - M. Sulprizio- Add optional argument KppSpcId

04 Aug 2016 - R. Yantosca - Now set missing molecular weights to -1, which seems to avoid numerical roundoff

10 Aug 2016 - E. Lundgren - Add default background concentration argument

1.11.6 Spc_Print

Routine Spc_Create prints the fields of the species object.

INTERFACE:

SUBROUTINE Spc_Print(am_I_Root, ThisSpc, RC)

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(Species), POINTER :: ThisSpc ! Object w/ species info

INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC ! Return code

REMARKS:

Optional fields are not printed out if they are not defined (i.e. if they have a "missing data value" of -999).

REVISION HISTORY:

```
27 Jul 2015 - R. Yantosca - Initial version
```

1.11.7 Spc_GetNumSpecies

Routine Spc_GetNumSpecies returns the number of advected, dry-deposited, and wet-deposited species to an external routine.

INTERFACE:

```
SUBROUTINE Spc_GetNumSpecies( nAdvect, nDryDep, nKppSpc, nWetDep, & nHgOCats, nHg2Cats, nHgPCats )
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: nAdvect   ! # of advected species
INTEGER, INTENT(OUT) :: nDryDep   ! # of dry-deposited species
INTEGER, INTENT(OUT) :: nKppSpc   ! # of species in the KPP mechanism
INTEGER, INTENT(OUT) :: nWetDep   ! # of wet-deposited species
INTEGER, INTENT(OUT) :: nHgOCats   ! # of HgO categories
INTEGER, INTENT(OUT) :: nHgPCats   ! # of HgO categories
INTEGER, INTENT(OUT) :: nHgPCats   ! # of HgO categories
```

REVISION HISTORY:

```
02 Sep 2015 - R. Yantosca - Initial version
25 Apr 2016 - R. Yantosca - Also return the # of HgO, Hg2, HgP categories
18 May 2016 - R. Yantosca - Also return the # of KPP chemical species
```

1.12 Fortran: Module Interface state_chm_mod.F90

Module STATE_CHM_MOD contains the derived type used to define the Chemistry State object for GEOS-Chem.

This module also contains the routines that allocate and deallocate memory to the Chemistry State object. The chemistry state object is not defined in this module. It must be be declared as variable in the top-level driver routine, and then passed to lower-level routines as an argument.

INTERFACE:

```
MODULE State_Chm_Mod
  USES:
  USE PhysConstants ! Physical constants
  USE Precision_Mod    ! GEOS-Chem precision types
  USE Species_Mod    ! For species database object
  IMPLICIT NONE
  PRIVATE
PUBLIC MEMBER FUNCTIONS:
  PUBLIC :: Ind_
  PUBLIC :: Init_State_Chm
  PUBLIC :: Cleanup_State_Chm
   !PRIVATE DATA MEMBERS:
  TYPE(SpcPtr), PRIVATE, POINTER :: SpcDataLocal(:) ! Local version of StateChm for
PUBLIC DATA MEMBERS:
   ! Derived type for Chemistry State
   !-----
  TYPE, PUBLIC :: ChmState
      ! Count of each type of species
                                                     ! # of species
     INTEGER
                                :: nSpecies
                                                    ! # of advected species
! # of drydep species
                                :: nAdvect
     INTEGER
     INTEGER
                                :: nDryDep
                                :: nKppSpc
                                                       ! # of KPP chem species
     INTEGER
                                                       ! # of wetdep species
     INTEGER
                                :: nWetDep
      ! Mapping vectors to subset types of species
                POINTER :: Map_Advect (: ) ! Advected species ID's
POINTER :: Map_DryDep (: ) ! Drydep species ID's
POINTER :: Map_KppSpc (: ) ! KPP chem species ID's
POINTER :: Map_WetDep (: ) ! Wetdep species IDs'
     INTEGER,
     INTEGER,
     INTEGER,
                        POINTER :: Map_WetDep (:
                                                      ) ! Wetdep species IDs'
     INTEGER,
      ! Physical properties & indices for each species
     TYPE(SpcPtr),
                        POINTER :: SpcData (:
                                                      ) ! GC Species database
     ! Chemical species
     INTEGER, POINTER :: Spec_Id (: ) ! Species ID # CHARACTER(LEN=14), POINTER :: Spec_Name (: ) ! Species names
     REAL(fp), POINTER :: Species (:,:,:,:) ! Species [molec/cm3]
     CHARACTER (LEN=20)
                                :: Spc_Units
                                                       ! Species units
      ! Aerosol quantities
     INTEGER
                                :: nAero
                                                        ! # of Aerosol Types
     REAL(fp), POINTER :: AeroArea (:,:,:)! Aerosol Area [cm2/cm3]
```

```
(:,:,:) ! Aerosol Radius [cm]
    REAL(fp),
                     POINTER :: AeroRadi
    REAL(fp),
                   POINTER :: WetAeroArea(:,:,:,:) ! Aerosol Area [cm2/cm3]
    REAL(fp),
                    POINTER :: WetAeroRadi(:,:,:,:) ! Aerosol Radius [cm]
#if defined( ESMF_ )
    ! Chemical rates & rate parameters
              POINTER :: JLOP
                                        (:,:,: ) ! 1-D SMVGEAR index
                     POINTER :: JLOP_PREV (:,:,: ) ! JLOP, prev timestep
    INTEGER,
#endif
    ! Fields for UCX mechanism
    REAL(f4),
                     POINTER :: STATE_PSC (:,:,: ) ! PSC type (see Kirner
                                                 ! et al. 2011, GMD)
                    POINTER :: KHETI_SLA (:,:,:) ! Strat. liquid aerosol
    REAL(fp),
                                                 ! reaction cofactors
    ! For the tagged Hg simulation
    INTEGER
                            :: N_HG_CATS
                                                 ! # of Hg categories
                     POINTER :: HgO_Id_List(: ) ! HgO cat <-> tracer #
    INTEGER.
    INTEGER,
                    POINTER :: Hg2_Id_List(:
                                               ) ! Hg2 cat <-> tracer #
    ) ! HgP cat <-> tracer #
```

END TYPE ChmState

REMARKS:

```
19 Oct 2012 - R. Yantosca - Initial version, based on "gc_type2_mod.F90"
26 Oct 2012 - R. Yantosca - Add fields for stratospheric chemistry
26 Feb 2013 - M. Long - Add DEPSAV to derived type ChmState
07 Mar 2013 - R. Yantosca - Add Register_Tracer subroutine
07 Mar 2013 - R. Yantosca - Now make POSITION a locally SAVEd variable
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
19 May 2014 - C. Keller - Removed Trac_Btend. DepSav array covers now
                            all species.
03 Dec 2014 - M. Yannetti - Added PRECISION_MOD
11 Dec 2014 - R. Yantosca - Keep JLOP and JLOP_PREV for ESMF runs only
17 Feb 2015 - E. Lundgren - New tracer units kg/kg dry air (previously kg)
13 Aug 2015 - E. Lundgren - Add tracer units string to ChmState derived type
28 Aug 2015 - R. Yantosca - Remove strat chemistry fields, these are now
                           handled by the HEMCO component
05 Jan 2016 - E. Lundgren - Use global physical constants
28 Jan 2016 - M. Sulprizio- Add STATE_PSC, KHETI_SLA. These were previously
                            local arrays in ucx_mod.F, but now need to be
                            accessed in gckpp_HetRates.F90.
12 May 2016 - M. Sulprizio- Add WetAeroArea, WetAeroRadi to replace 1D arrays
```

```
WTARE, WERADIUS previously in comode_mod.F

18 May 2016 - R. Yantosca - Add mapping vectors for subsetting species

07 Jun 2016 - M. Sulprizio- Remove routines Get_Indx, Register_Species, and Register_Tracer made obsolete by the species database.

22 Jun 2016 - R. Yantosca - Rename Id_HgO to HgO_Id_List, Id_Hg2 to Hg2_Id_List, and Id_HgP to HgP_Id_List

16 Aug 2016 - M. Sulprizio- Rename from gigc_state_chm_mod.F90 to state_chm_mod.F90. The "gigc" nomenclature is no longer used.

23 Aug 2016 - M. Sulprizio- Remove tracer fields from State_Chm. These are now entirely replaced with the species fields.
```

1.12.1 Ind_

Function IND₋ returns the index of an advected species or chemical species contained in the chemistry state object by name.

INTERFACE:

```
FUNCTION Ind_( name, flag ) RESULT( Indx )
```

USES:

```
USE CHARPAK_MOD, ONLY : TRANUC
```

INPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(IN) :: name ! Species name CHARACTER(LEN=*), OPTIONAL, INTENT(IN) :: flag ! Species type
```

RETURN VALUE:

```
INTEGER :: Indx ! Index of this species !REMARKS
```

REVISION HISTORY:

```
07 Oct 2016 - M. Long - Initial version
15 Jun 2016 - M. Sulprizio- Make species name uppercase before computing hash
17 Aug 2016 - M. Sulprizio- Tracer flag 'T' is now advected species flag 'A'
```

1.12.2 Init_State_Chm

Routine INIT_STATE_CHM allocates and initializes the pointer fields of the chemistry state object.

INTERFACE:

```
SUBROUTINE Init_State_Chm( am_I_Root, IM, JM, & LM, Input_Opt, State_Chm, & nAerosol, RC )
```

USES:

```
USE ErrCode_Mod
```

USE GCKPP_Parameters, ONLY : NSPEC
USE Input_Opt_Mod, ONLY : OptInput
USE Species_Mod, ONLY : Species

USE Species_Mod, ONLY : Spc_GetNumSpecies
USE Species_Database_Mod, ONLY : Init_Species_Database

INPUT PARAMETERS:

```
LOGICAL,
             INTENT(IN)
                         :: am_I_Root
                                         ! Is this the root CPU?
INTEGER,
                                         ! # longitudes on this PET
             INTENT(IN)
                          :: IM
INTEGER,
              INTENT(IN) :: JM
                                         ! # longitudes on this PET
INTEGER,
                                         ! # longitudes on this PET
             INTENT(IN)
                          :: LM
              INTENT(IN) :: nAerosol ! # aerosol species
INTEGER,
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(OptInput), INTENT(INOUT) :: Input_Opt   ! Input Options object
TYPE(ChmState), INTENT(INOUT) :: State_Chm   ! Chemistry State object
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Return code

REMARKS:

In the near future we will put some error trapping on the allocations so that we can stop the simulation if the allocations cannot be made.

```
19 Oct 2012 - R. Yantosca - Renamed from gc_type2_mod.F90

19 Oct 2012 - R. Yantosca - Now pass all dimensions as arguments

26 Oct 2012 - R. Yantosca - Now allocate Strat_P, Strat_k fields

26 Oct 2012 - R. Yantosca - Add nSchem, nSchemBry as arguments

01 Nov 2012 - R. Yantosca - Don't allocate strat chem fields if nSchm=0

and nSchmBry=0 (i.e. strat chem is turned off)

26 Feb 2013 - M. Long - Now pass Input_Opt via the argument list

26 Feb 2013 - M. Long - Now allocate the State_Chm%DEPSAV field

11 Dec 2014 - R. Yantosca - Remove TRAC_TEND and DEPSAV fields

13 Aug 2015 - E. Lundgren - Initialize trac_units to ''

28 Aug 2015 - R. Yantosca - Remove stratospheric chemistry fields;

these are all now read in via HEMCO

28 Aug 2015 - R. Yantosca - Also initialize the species database object

09 Oct 2015 - R. Yantosca - Bug fix: set State_Chm%SpcData to NULL
```

```
16 Dec 2015 - R. Yantosca - Now overwrite the Input_Opt%TRACER_MW_G and related fields w/ info from species database

29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts

02 May 2016 - R. Yantosca - Nullify Hg index fields for safety's sake

18 May 2016 - R. Yantosca - Now determine the # of each species first, then allocate fields of State_Chm

18 May 2016 - R. Yantosca - Now populate the species mapping vectors

30 Jun 2016 - M. Sulprizio- Remove nSpecies as an input argument. This is now initialized as the size of SpcData.

22 Jul 2016 - E. Lundgren - Initialize spc_units to ''

28 Nov 2016 - R. Yantosca - Only allocate STATE_PSC and KHETI_SLA for UCX simulations; set to NULL otherwise

28 Nov 2016 - R. Yantosca - Only allocate State_Chm%*Aero* fields for fullchem and/or aerosol-only simulations
```

1.12.3 Cleanup_State_Chm

Routine CLEANUP_STATE_CHM deallocates all fields of the chemistry state object.

INTERFACE:

```
SUBROUTINE Cleanup_State_Chm( am_I_Root, State_Chm, RC ) USES:
```

USE ErrCode_Mod

USE Species_Database_Mod, ONLY : Cleanup_Species_Database

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Return code

REMARKS:

For now the am_I_Root and RC arguments are not used. We include these for consistency and also to facilitate future expansion. (bmy, 10/16/12)

```
15 Oct 2012 - R. Yantosca - Initial version
26 Oct 2012 - R. Yantosca - Now deallocate Strat_P, Strat_k fields
26 Feb 2013 - M. Long - Now deallocate State_Chm%DEPSAV
11 Dec 2014 - R. Yantosca - Remove TRAC_TEND and DEPSAV fields
28 Aug 2015 - R. Yantosca - Remove stratospheric chemistry fields;
these are all now read in via HEMCO
28 Aug 2015 - R. Yantosca - Also initialize the species database object
```

1.13 Fortran: Module Interface state_met_mod.F90

Module STATE_MET_MOD contains the derived type used to define the Meteorology State object for GEOS-Chem.

This module also contains the routines that allocate and deallocate memory to the Meteorology State object. The Meteorology State object is not defined in this module. It must be be declared as variable in the top-level driver routine, and then passed to lower-level routines as an argument.

INTERFACE:

```
MODULE State_Met_Mod
USES:
USE PRECISION_MOD
IMPLICIT NONE
PRIVATE
```

PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: Init_State_Met
PUBLIC :: Cleanup_State_Met
```

PUBLIC DATA MEMBERS:

```
! Derived type for Meteorology State
TYPE, PUBLIC :: MetState
  !-----
  ! Surface fields
  I-----
  REAL(fp), POINTER :: ALBD
                            (:,: ) ! Visible surface albedo [1]
  REAL(fp), POINTER :: CLDFRC
                             (:,: ) ! Column cloud fraction [1]
                             (:,: ) ! Max cloud top height [levels]
  INTEGER, POINTER :: CLDTOPS
  REAL(fp), POINTER :: EFLUX
                             (:,: ) ! Latent heat flux [W/m2]
  REAL(fp), POINTER :: EVAP
                             (:,: ) ! Surface evap [kg/m2/s]
  REAL(fp), POINTER :: FRCLND
                             (:,: ) ! Olson land fraction [1]
  REAL(fp), POINTER :: FRLAKE
                             (:,: ) ! Fraction of lake [1]
  REAL(fp), POINTER :: FRLAND
                             (:,: )! Fraction of land [1]
  REAL(fp), POINTER :: FRLANDIC
                             (:,: ) ! Fraction of land ice [1]
  REAL(fp), POINTER :: FROCEAN
                             (:,: ) ! Fraction of ocean [1]
  REAL(fp), POINTER :: FRSEAICE
                            (:,: )! Sfc sea ice fraction
  REAL(fp), POINTER :: FRSNO
                             (:,: ) ! Sfc snow fraction
  REAL(fp), POINTER :: GRN
                             (:,: ) ! Greenness fraction
  REAL(fp), POINTER :: GWETROOT
                            (:,: ) ! Root soil wetness [1]
  REAL(fp), POINTER :: GWETTOP
                             (:,: ) ! Top soil moisture [1]
  REAL(fp), POINTER :: HFLUX
                             (:,: ) ! Sensible heat flux [W/m2]
```

(:,:)! Leaf area index [m2/m2]

```
REAL(fp), POINTER :: LAI
REAL(fp), POINTER :: ITY
                               (:,: ) ! Land surface type index
REAL(fp), POINTER :: LWI
                               (:,: ) ! Land/water indices [1]
REAL(fp), POINTER :: LWI_GISS
                               (:,: ) ! Land fraction [1]
REAL(fp), POINTER :: MOLENGTH
                              (:,: ) ! Monin-Obhukov length [m]
REAL(fp), POINTER :: OICE
                               (:,: ) ! Fraction of ocean ice [1]
REAL(fp), POINTER :: PARDR
                               (:,: ) ! Direct photsyn active rad [W/m2]
REAL(fp), POINTER :: PARDF
                               (:,: ) ! Diffuse photsyn active rad [W/m2]
REAL(fp), POINTER :: PBLH
                               (:,: ) ! PBL height [m]
INTEGER, POINTER :: PBL_TOP_L (:,: ) ! PBL top layer [1]
                               (:,: ) ! Sfc geopotential height [m2/s2]
REAL(fp), POINTER :: PHIS
REAL(fp), POINTER :: PRECANV
                               (:,: ) ! Anvil previp @ ground [kg/m2/s]
REAL(fp), POINTER :: PRECCON
                               (:,: ) ! Conv precip @ ground [kg/m2/s]
                               (:,: ) ! Total precip @ ground [kg/m2/s]
REAL(fp), POINTER :: PRECTOT
REAL(fp), POINTER :: PRECLSC
                               (:,: ) ! LS precip @ ground [kg/m2/s]
REAL(fp), POINTER :: PRECSNO
                               (:,: ) ! Snow precip [kg/m2/s]
REAL(fp), POINTER :: PS1_WET
                               (:,: ) ! Wet sfc press at dt start[hPa]
REAL(fp), POINTER :: PS2_WET
                               (:,: ) ! Wet sfc press at dt end [hPa]
REAL(fp), POINTER :: PSC2_WET
                               (:,: ) ! Wet interpolated sfc press [hPa]
REAL(fp), POINTER :: PS1_DRY
                               (:,: ) ! Dry sfc press at dt start[hPa]
REAL(fp), POINTER :: PS2_DRY
                               (:,: ) ! Dry sfc press at dt end [hPa]
REAL(fp), POINTER :: PSC2_DRY
                               (:,: ) ! Dry interpolated sfc press [hPa]
REAL(fp), POINTER :: RADLWG
                               (:,: ) ! Net LW radiation @ ground [W/m2]
REAL(fp), POINTER :: RADSWG
                               (:,: ) ! Solar radiation @ ground [W/m2]
REAL(fp), POINTER :: SEAICE00
                               (:,: ) ! Sea ice coverage 00-10%
REAL(fp), POINTER :: SEAICE10
                               (:,: ) ! Sea ice coverage 10-20%
REAL(fp), POINTER :: SEAICE20
                               (:,: ) ! Sea ice coverage 20-30%
REAL(fp), POINTER :: SEAICE30
                              (:,: ) ! Sea ice coverage 30-40%
REAL(fp), POINTER :: SEAICE40
                               (:,: ) ! Sea ice coverage 40-50%
REAL(fp), POINTER :: SEAICE50
                              (:,: ) ! Sea ice coverage 50-60%
REAL(fp), POINTER :: SEAICE60
                               (:,: ) ! Sea ice coverage 60-70%
REAL(fp), POINTER :: SEAICE70
                               (:,: ) ! Sea ice coverage 70-80%
REAL(fp), POINTER :: SEAICE80
                               (:,: ) ! Sea ice coverage 80-90%
REAL(fp), POINTER :: SEAICE90
                              (:,: ) ! Sea ice coverage 90-100%
REAL(fp), POINTER :: SLP
                               (:,: ) ! Sea level pressure [hPa]
REAL(fp), POINTER :: SNICE
                               (:,: ) ! Fraction of snow/ice [1]
REAL(fp), POINTER :: SNODP
                               (:,: ) ! Snow depth [m]
REAL(fp), POINTER :: SNOMAS
                               (:,:)! Snow mass [kg/m2]
                               (:,: ) ! Snow depth (H2O equiv) [mm H2O]
REAL(fp), POINTER :: SNOW
REAL(fp), POINTER :: SST
                               (:,: ) ! Sea surface temperature [K]
REAL(fp), POINTER :: SUNCOS
                               (:,: ) ! COS(SZA), current time
REAL(fp), POINTER :: SUNCOSmid (:,: ) ! COS(SZA), midpt of chem timestep
REAL(fp), POINTER :: SUNCOSmid5(:,: ) ! COS(SZA), midpt of chem timestep
                                        ! 5 hrs ago (for PARANOX)
REAL(fp), POINTER :: SWGDN
                               (:,: ) ! Incident radiation @ grnd [W/m2]
REAL(fp), POINTER :: TO3
                               (:,: ) ! Total overhead O3 column [DU]
REAL(fp), POINTER :: TO31
                               (:,: ) ! Total O3 at timestep start [DU]
REAL(fp), POINTER :: TO32
                               (:,: ) ! Total O3 at timestep end [DU]
```

```
REAL(fp), POINTER :: TROPP
                               (:,: ) ! Tropopause pressure [hPa]
REAL(fp), POINTER :: TROPP1
                               (:,: ) ! Trop P at timestep start [hPa]
REAL(fp), POINTER :: TROPP2
                               (:,: ) ! Trop P at timestep end [hPa]
REAL(fp), POINTER :: TS
                               (:,: ) ! Surface temperature [K]
REAL(fp), POINTER :: TSKIN
                               (:,: ) ! Surface skin temperature [K]
REAL(fp), POINTER :: TTO3
                               (:,: ) ! Tropospheric ozone column [DU]
REAL(fp), POINTER :: U10M
                               (:,: ) ! E/W wind speed @ 10m height [m/s]
REAL(fp), POINTER :: USTAR
                               (:,: ) ! Friction velocity [m/s]
REAL(fp), POINTER :: UVALBEDO (:,: ) ! UV surface albedo [1]
REAL(fp), POINTER :: V10M
                               (:,: ) ! N/S wind speed @ 10m height [m/s]
REAL(fp), POINTER :: ZO
                               (:,: ) ! Surface roughness height [m]
REAL(fp), POINTER :: CNV_FRC
                              (:,: ) ! Convective fraction [1]
                    -----
! 3-D Fields
REAL(fp), POINTER :: AREA_M2
                               (:,:,:) ! Grid box surface area [cm2]
REAL(fp), POINTER :: CLDF
                               (:,:,:) ! 3-D cloud fraction [1]
REAL(fp), POINTER :: CMFMC
                               (:,:,:)! Cloud mass flux [kg/m2/s]
REAL(fp), POINTER :: DETRAINE
                              (:,:,:) ! Detrainment (entrain plume) [Pa/s]
REAL(fp), POINTER :: DETRAINN
                               (:,:,:) ! Detrainment (non-entr plume)[Pa/s]
REAL(fp), POINTER :: DNDE
                               (:,:,:) ! Downdraft (entr plume) [Pa/s]
REAL(fp), POINTER :: DNDN
                               (:,:,:) ! Downdraft (non-entr plume) [Pa/s]
REAL(fp), POINTER :: DQRCU
                               (:,:,:) ! Conv precip prod rate [kg/kg/s]
                                      ! (assume per dry air)
                               (:,:,:) ! LS precip prod rate [kg/kg/s]
REAL(fp), POINTER :: DQRLSAN
                                      ! (assume per dry air)
REAL(fp), POINTER :: DQIDTMST
                               (:,:,:) ! Ice tendency, mst proc [kg/kg/s]
REAL(fp), POINTER :: DQLDTMST
                               (:,:,:) ! H2O tendency, mst proc [kg/kg/s]
REAL(fp), POINTER :: DQVDTMST
                               (:,:,:) ! Vapor tendency, mst proc [kg/kg/s]
REAL(fp), POINTER :: DTRAIN
                               (:,:,:) ! Detrainment flux [kg/m2/s]
REAL(fp), POINTER :: ENTRAIN
                               (:,:,:) ! GCAP entrainment [Pa/s]
REAL(fp), POINTER :: HKBETA
                               (:,:,:) ! Hack overshoot parameter [1]
REAL(fp), POINTER :: HKETA
                               (:,:,:)! Hack conv mass flux [kg/m2/s]
REAL(fp), POINTER :: MOISTQ
                               (:,:,:) ! Tendency in sp. humidity
                                       ! [kg/kg tot air/s]
REAL(fp), POINTER :: OPTD
                               (:,:,:) ! Visible optical depth [1]
REAL(fp), POINTER :: PEDGE
                               (:,:,:) ! Wet air press @ level edges [hPa]
REAL(fp), POINTER :: PFICU
                               (:,:,:) ! Dwn flux ice prec:conv [kg/m2/s]
REAL(fp), POINTER :: PFILSAN
                               (:,:,:)! Dwn flux ice prec:LS+anv [kg/m2/s]
REAL(fp), POINTER :: PFLCU
                               (:,:,:) ! Dwn flux liq prec:conv [kg/m2/s]
                               (:,:,:) ! Dwn flux ice prec:LS+anv [kg/m2/s]
REAL(fp), POINTER :: PFLLSAN
REAL(fp), POINTER :: PV
                               (:,:,:) ! Potential vort [kg*m2/kg/s]
                               (:,:,:) ! Ice mixing ratio [kg/kg dry air]
REAL(fp), POINTER :: QI
REAL(fp), POINTER :: QL
                               (:,:,:) ! Water mixing ratio [kg/kg dry air]
REAL(fp), POINTER :: REEVAPCN
                              (:,:,:) ! Evap of precip conv [kg/kg/s]
                                       ! (assume per dry air)
REAL(fp), POINTER :: REEVAPLS (:,:,:) ! Evap of precip LS+anvil [kg/kg/s]
```

```
! (assume per dry air)
REAL(fp), POINTER :: RH
                               (:,:,:) ! Relative humidity [%]
REAL(fp), POINTER :: RH1
                               (:,:,:) ! RH at timestep start [%]
REAL(fp), POINTER :: RH2
                               (:,:,:) ! RH at timestep end [%]
REAL(fp), POINTER :: SPHU
                               (:,:,:) ! Spcfc humidity [g H2O/kg tot air]
REAL(fp), POINTER :: SPHU1
                               (:,:,:) ! Spec hum at timestep start [g/kg]
REAL(fp), POINTER :: SPHU2
                               (:,:,:) ! Spec hum at timestep end [g/kg]
REAL(fp), POINTER :: T
                               (:,:,:) ! Temperature [K]
                               (:,:,:) ! Opt depth of ice clouds [1]
REAL(fp), POINTER :: TAUCLI
REAL(fp), POINTER :: TAUCLW
                               (:,:,:) ! Opt depth of H2O clouds [1]
REAL(fp), POINTER :: TMPU1
                               (:,:,:) ! Temperature at timestep start [K]
REAL(fp), POINTER :: TMPU2
                               (:,:,:) ! Temperature at timestep end [K]
REAL(fp), POINTER :: U
                               (:,:,:) ! E/W component of wind [m s-1]
REAL(fp), POINTER :: UPDE
                               (:,:,:) ! Updraft (entraining plume) [Pa/s]
REAL(fp), POINTER :: UPDN
                               (:,:,:) ! Updraft (non-entr'n plume) [Pa/s]
REAL(fp), POINTER :: UPDVVEL
                               (:,:,:) ! Updraft vertical velocity [hPa/s]
REAL(fp), POINTER :: V
                               (:,:,:) ! N/S component of wind [m s-1]
REAL(fp), POINTER :: ZMEU
                               (:,:,:) ! Z/M updraft entrainment [Pa/s]
REAL(fp), POINTER :: ZMMD
                               (:,:,:) ! Z/M downdraft mass flux [Pa/s]
REAL(fp), POINTER :: ZMMU
                               (:,:,:) ! Z/M updraft
                                                       mass flux [Pa/s]
! Air quantities assigned in AIRQNT
! Note on pressures: PMID is calculated from PEDGE,
! and dry air pressures assume constant RH and T across grid box
REAL(fp), POINTER :: PEDGE_DRY (:,:,:) ! Dry air partial pressure [hPa]
                                       ! @ level edges [hPa]
REAL(fp), POINTER :: PMID
                               (:,:,:) ! Average wet air pressure [hPa]
                                       ! defined as arithmetic
                                       ! average of edge pressures
REAL(fp), POINTER :: PMID_DRY
                               (:,:,:) ! Dry air partial pressure [hPa]
                                       ! defined as arithmetic average
                                       ! of edge pressures
REAL(fp), POINTER :: TV
                               (:,:,:) ! Virtual temperature [K]
REAL(fp), POINTER :: MAIRDEN
                               (:,:,:) ! Moist air density [kg/m3]
REAL(fp), POINTER :: AIRDEN
                               (:,:,:)! Dry air density [kg/m3]
REAL(fp), POINTER :: AIRNUMDEN (:,:,:) ! Dry air density [molec/m3]
REAL(fp), POINTER :: AVGW
                               (:,:,:) ! Water vapor volume mixing ratio
                                       ! [vol H2O / vol dry air]
REAL(fp), POINTER :: BXHEIGHT
                               (:,:,:) ! Grid box height [m] (dry air)
REAL(fp), POINTER :: DELP
                               (:,:,:) ! Delta-P (wet) across box [hPa]
REAL(fp), POINTER :: DELP_DRY
                               (:,:,:) ! Delta-P (dry) across box [hPa]
                               (:,:,:) ! Dry air mass [kg] in grid box
REAL(fp), POINTER :: AD
REAL(fp), POINTER :: AIRVOL
                               (:,:,:) ! Grid box volume [m3] (dry air)
REAL(fp), POINTER :: DELP_PREV (:,:,:) ! Previous State_Met%DELP
REAL(fp), POINTER :: DP_DRY_PREV (:,:,:) ! Previous State_Met%DELP_DRY
REAL(fp), POINTER :: SPHU_PREV (:,:,:) ! Previous State_Met%SPHU
```

```
-----
! Land type and leaf area index (LAI) fields for dry deposition
INTEGER, POINTER :: IREG
                             (:,: ) ! # of landtypes in grid box (I,J)
INTEGER, POINTER :: ILAND
                             (:,:,:) ! Land type at (I,J); 1.. IREG(I,J)
                             (:,:,:) ! Fraction (per mil) of grid box
INTEGER, POINTER :: IUSE
                                     ! (I,J) occupied by each land type
REAL(fp), POINTER :: XLAI
                             (:,:,:) ! LAI per land type, this month
REAL(fp), POINTER :: XLAI2
                             (:,:,:) ! LAI per land type, next month
REAL(fp), POINTER :: XCHLR
                             (:,:,:) ! CHLR per land type, this month
REAL(fp), POINTER :: XCHLR2
                             (:,:,:) ! CHLR per land type, next month
```

END TYPE MetState

REMARKS:

In MERRA2, PS and SLP are kept in Pa (not converted to hPa).

```
19 Oct 2012 - R. Yantosca - Initial version, split off from gc_type_mod.F90
23 Oct 2012 - R. Yantosca - Added QI, QL met fields to the derived type
15 Nov 2012 - M. Payer
                       - Added all remaining met fields
12 Dec 2012 - R. Yantosca - Add IREG, ILAND, IUSE fields for dry deposition
13 Dec 2012 - R. Yantosca - Add XLAI, XLAI2 fields for dry deposition
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
15 Nov 2013 - R. Yantosca - Now denote that RH fields have units of [%]
10 Oct 2014 - C. Keller - Added ITY (needed for GIGC). For now, this value
                            is just initialized to 1.0 and not modified any
                            more.
05 Nov 2014 - M. Yannetti - Changed REAL*8 to REAL(fp)
12 Feb 2015 - C. Keller
                        - Added UPDVVEL (for use in wet scavenging).
24 Feb 2015 - E. Lundgren - Add PEDGE_DRY, PMID_DRY, and MAIRDEN
03 Mar 2015 - E. Lundgren - Add TV (virtual temperature)
16 Apr 2015 - E. Lundgren - Add mean pressures PMEAN and PMEAN_DRY. Clarify
                            definition of PMID as arithmetic average P.
                            Add MOISTMW to use TCVV with moist mixing ratio.
25 May 2015 - C. Keller - Removed SUNCOSmid5 (now calculated by HEMCO).
08 Jul 2015 - E. Lundgren - Add XCHLR and XCHLR2 for organic marine aerosols
11 Aug 2015 - R. Yantosca - Extend #ifdefs for MERRA2 met fields
22 Sep 2015 - E. Lundgren - Add SWGDN for incident radiation at ground
28 Oct 2015 - E. Lundgren - Add previous delta-P and specific humidity for
                            tracer mass conservation in mixing ratio update
04 Mar 2016 - C. Keller
                          - Add CNV_FRC for convective fraction. Currently
                            not a standard GEOS-FP output, only used in
                            online model (ESMF).
```

```
21 Dec 2015 - M. Sulprizio- Add AIRNUMDEN, which is the same as AIRDEN but has units molec/cm3 for the chemistry routines.

17 Mar 2016 - M. Sulprizio- Remove OPTDEP. Instead, we now solely use OPTD.

03 May 2016 - E. Lundgren - Add PSC2_DRY, PS1_DRY, and PS2_DRY

06 Jul 2016 - E. Lundgren - Rename PS1, PS2, and PSC1: add '_WET' suffix

06 Jul 2016 - E. Lundgren - Add DELP_DRY and DP_DRY_PREV

19 Jul 2016 - E. Lundgren - Remove PMEAN, PMEAN_DRY, MOISTMW, and ADMOIST

16 Aug 2016 - M. Sulprizio- Rename from gigc_state_chm_mod.F90 to state_chm_mod.F90. The "gigc" nomenclature is no longer used.
```

1.13.1 Init_State_Met

Subroutine INIT_STATE_MET allocates all fields of the meteorology state object.

INTERFACE:

```
SUBROUTINE Init_State_Met( am_I_Root, IM, JM, LM, State_Met, RC )
```

USES:

```
USE ErrCode_Mod ! Error codes
USE CMN_SIZE_MOD, ONLY : NTYPE ! # of land types
```

INPUT PARAMETERS:

```
LOGICAL,
               INTENT(IN)
                          :: am_I_Root
                                            ! Is this the root CPU?
INTEGER,
               INTENT(IN)
                             :: IM
                                            ! # longitudes on this PET
                                            ! # longitudes on this PET
INTEGER,
               INTENT(IN)
                            :: JM
                                            ! # longitudes on this PET
INTEGER,
               INTENT(IN)
                             :: LM
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met  ! Obj for meteorology state
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Return code
```

REMARKS:

For consistency, maybe this should be moved to a different module.

```
19 Oct 2012 - R. Yantosca - Initial version, based on gc_environment_mod.F90
19 Oct 2012 - R. Yantosca - Now pass all dimensions as arguments
23 Oct 2012 - R. Yantosca - Now allocate QI, QL fields
15 Nov 2012 - M. Payer - Added all remaining met fields
16 Nov 2012 - R. Yantosca - Now zero all fields after allocating
27 Nov 2012 - R. Yantosca - Now allocate SUNCOS fields (IM,JM)
```

```
12 Dec 2012 - R. Yantosca - Now allocate the IREG, ILAND, IUSE fields
13 Dec 2012 - R. Yantosca - Now allocate the XLAI, XLAI2 fields
07 Mar 2013 - R. Yantosca - Now allocate PF*LSAN, PF*CU fields properly
for GEOS-5.7.x met (they are edged)
26 Sep 2013 - R. Yantosca - Renamed GEOS_57 Cpp switch to GEOS_FP
22 Aug 2014 - R. Yantosca - Allocate PBL_TOP_L field
05 Nov 2014 - R. Yantosca - Now use 0.0_fp instead of 0d0
06 Nov 2014 - R. Yantosca - Now make all fields (IM,JM,LM) instead of
(LM,JM,IM), to facilitate use w/in GEOS-5 GCM
05 Oct 2016 - R. Yantosca - Swapped order of HKETA and HKBETA allocation
28 Nov 2016 - R. Yantosca - Nullify fields that may or may not be allocated
```

1.13.2 Cleanup_State_Met

Subroutine CLEANUP_STATE_MET deallocates all fields of the meteorology state object.

INTERFACE:

```
SUBROUTINE Cleanup_State_Met( am_I_Root, State_Met, RC )  {\bf USES:}
```

USE ErrCode_Mod ! Error codes

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(MetState), INTENT(INOUT) :: State_Met ! Obj for meteorology state

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Return code

REVISION HISTORY:

```
19 Oct 2012 - R. Yantosca - Initial version, based on gc_environment_mod.F90
23 Oct 2012 - R. Yantosca - Now deallocate QI, QL fields
15 Nov 2012 - M. Payer - Added all remaining met fields
19 Nov 2012 - R. Yantosca - Segregate DEALLOCATE statements w/ #ifdefs
for each met field data product type
27 Nov 2012 - R. Yantosca - Now deallocate the SUNCOS fields
12 Dec 2012 - R. Yantosca - Now deallocate the IREG, ILAND, IUSE fields
26 Sep 2013 - R. Yantosca - Renamed GEOS_57 Cpp switch to GEOS_FP
22 Aug 2014 - R. Yantosca - Deallocate PBL_TOP_L field
```

2 GEOS-Chem driver and other operations

These modules contain routines to perform core operations such as initializing a GEOS-Chem simulation, timestepping, reading data from restart files, and cleanup.

2.1 Fortran: Module Interface main.F

Program GEOS_CHEM is the main level driver program for the GEOS-Chem model of atmospheric chemistry and composition.

INTERFACE:

PROGRAM GEOS_CHEM

USES:

```
1-----
! Parameters to define floating-point variables
!-----
USE PRECISION_MOD, ONLY : fpp => fp  ! Flexible precision
USE PRECISION_MOD, ONLY: f4 ! 4-byte floating point
USE PRECISION_MOD, ONLY: f8 ! 8-byte floating point
!-----
! Basic GEOS-Chem modules
!-----
                  ! Size parameters
! Error codes for success or failure
! For error checking
USE CMN_SIZE_MOD
USE ErrCode_Mod
USE ERROR_MOD
USE FILE_MOD
                     ! For file I/O
USE GC_Environment_Mod ! For allocating derived type objects
                       ! For defining the lons/lats/areas of the grid
USE GC_GRID_MOD
                    ! Derived type for Input Options
USE Input_Opt_Mod
                       ! For reading settings from "input.geos"
USE INPUT_MOD
                       ! For regridding MODIS LAI
USE MAPPING_MOD
                     ! Computes IREG, ILAND, IUSE from Olson map
USE OLSON_LANDMAP_MOD
USE PhysConstants
                       ! Physical constants
USE PRESSURE_MOD
                       ! For computing pressure at grid boxes
                       ! For horizontal regridding
USE REGRID_A2A_MOD
USE RESTART_MOD
                       ! For restart file I/O
                       ! Derived type for Chemistry State object
USE State_Chm_Mod
USE State_Met_Mod
                       ! Derived type for Meteorology State object
                       ! For computing date & time
USE TIME_MOD
USE UnitConv_Mod
                       ! For gas concentration unit conversion
I-----
! GEOS-Chem chemistry modules
I-----
USE CARBON_MOD
                       ! For SOA simulation
                    ! For SUA simulation
! Driver routines for chemistry
USE CHEMISTRY_MOD
USE GLOBAL_CH4_MOD ! For offline CH4 simulation
USE MERCURY_MOD ! For offline Hg simulation (driver)
USE OCEAN_MERCURY_MOD ! For offline Hg simulation (ocean model)
USE STRAT_CHEM_MOD ! For linearized stratospheric chemistry
```

```
USE TOMS_MOD
                      ! For overhead O3 columns (for FAST-J)
USE UCX_MOD
                    ! For unified trop-strat chemistry (SDE)
USE UVALBEDO_MOD ! For reading UV albedoes (for FAST-J)
!-----
! GEOS-Chem deposition modules
!-----
USE DEPO_MERCURY_MOD ! Deposition for offline Hg simulation
USE DRYDEP_MOD
                    ! For dry deposition
USE WETSCAV_MOD
                ! For wet deposition (rainout & washout)
I-----
! GEOS-Chem diagnostics modules
!-----
USE BENCHMARK_MOD
                      ! For the 1-month benchmark simulations
                  ! Logical switches for G-C diagnostics
! G-C diagnostic arrays & counters
! For ND41 (afternoon PBL ) diag
USE CMN_DIAG_MOD
USE DIAG_MOD
USE DIAG41_MOD
                    ! For ND42 (SOA products ) diag
USE DIAG42_MOD
USE DIAG48_MOD
                    ! For ND48 (station timeseries ) diag
USE DIAG49_MOD
                    ! For ND49 (inst. timeseries ) diag
                   ! For ND50 (24h avg timeseries ) diag
USE DIAG50_MOD
USE DIAG51_MOD
                    ! For ND51 (satellite timeseries) diag
                    ! For ND51b (satellite timeseries) diag
USE DIAG51b_MOD
                    ! For ND63 (PARANOX timeseries ) diag
USE DIAG63_MOD ! For ND63 (PARANOX timeseries ) diag
USE DIAG_OH_MOD ! For ND43 (OH,HO2,etc. prod ) diag
USE DIAGNOSTICS_MOD ! NetCDF diagnostics module (C. Keller)
USE PLANEFLIGHT_MOD ! For ND40 (plane flight track ) diag
USE DIAG63_MOD
!-----
! GEOS-Chem dynamics modules
!-----
USE CHEMGRID_MOD ! For the dynamic tropopause
                   ! For deep cloud convection
! For LINOX linear strat chemistry
USE CONVECTION_MOD
USE LINOZ_MOD
USE PBL_MIX_MOD
USE PBL_MIX_MOD ! To compute PBL height
USE TPCORE_BC_MOD ! For nested-grid boundary conditions
USE TRANSPORT_MOD
USE VDIFF_MOD
                  ! Driver routines for advection
                     ! For non-local PBL mixing (J. Lin)
!-----
! GEOS-Chem emissions modules
1-----
USE EMISSIONS_MOD ! For interfacing with HEMCO emissions USE MIXING_MOD ! performs tracer mixing
USE MODIS_LAI_MOD ! For MODIS leaf area indices (replacement)
!-----
```

```
! GEOS-Chem met field I/O modules
     USE DAO_MOD
                                ! Met field definitions
     USE GCAP_READ_MOD
                                ! For reading GCAP met data
     USE GEOSFP_READ_MOD
                                ! For reading GEOS-FP data
     USE MERRA2_READ_MOD
                                ! For reading MERRA2 data
                                ! For reading MERRA A1 data
     USE MERRA_A1_MOD
     USE MERRA_A3_MOD
                                ! For reading MERRA A3 data
     USE MERRA_CN_MOD
                                ! For reading MERRA CN data
     USE MERRA_I6_MOD
                                ! For reading MERRA I6 data
     USE A3_READ_MOD
                                ! For reading A3 data (all other met)
                                ! For reading A6 data (all other met)
     USE A6_READ_MOD
                                ! For reading I6 data (all other met)
     USE I6_READ_MOD
#if defined( EXCHANGE )
      USE EXCHANGE_MOD
                                ! For two-way coupled simulations
#endif
#if defined( RRTMG )
      ! Radiation modules
     USE RRTMG_RAD_TRANSFER_MOD, ONLY: DO_RRTMG_RAD_TRANSFER,
                                        LW_UFLUX, LW_DFLUX,
     &
                                        SW_UFLUX, SW_DFLUX,
                                        LW_UFLUXC, LW_DFLUXC,
     &
     &
                                        SW_UFLUXC, SW_DFLUXC,
     &
                                        INIT_SURFACE_RAD,
                                        READ_SURFACE_RAD,
                                        INIT_STRAT_CLIM,
     &
     &
                                        READ_STRAT_CLIM,
                                        INIT_MCICA_CLOUDS,
                                        SET_SPECMASK
     USE CMN_FJX_MOD,
                                  ONLY: NSPECRADMENU,
                                        LSPECRADMENU
     USE rrtmg_lw_init, ONLY : rrtmg_lw_ini
     USE rrtmg_sw_init,
                          ONLY : rrtmg_sw_ini
#endif
```

IMPLICIT NONE

REMARKS:

GG(GGGG	EEEEEEE	00000	SSSSSS	CCCCCC	Н Н	EEEEEEE	М		М
G		E	0 0	S	C	H H	E	М	M M	М
G	GGG	EEEEEE	0 0	SSSSSSS	C	нннннн	EEEEEE	М	М	М
G	G	E	0 0	S	C	H H	E	М		M
GGO	GGGG	EEEEEEE	00000	SSSSSS	CCCCCC	н н	EEEEEEE	М		Μ

```
(formerly known as the Harvard-GEOS model) for 4 x 5, 2 x 2.5 global grids and hi-res nested grids
```

Contact: GEOS-Chem Support Team (geos-chem-support@as.harvard.edu)

See the GEOS-Chem Web Site:

http://acmg.seas.harvard.edu/geos/

and the GEOS-Chem User's Guide:

http://acmg.seas.harvard.edu/geos/doc/man/

and the GEOS-Chem wiki:

http://wiki.seas.harvard.edu/geos-chem/

for the most up-to-date GEOS-Chem documentation on the following topics:

- installation, compilation, and execution
- coding practice and style
- input files and met field data files
- horizontal and vertical resolution
- modification history

- 13 Aug 2010 R. Yantosca Added ProTeX headers
- 13 Aug 2010 R. Yantosca Add modifications for MERRA (treat like GEOS-5)
- 19 Aug 2010 R. Yantosca Now call MERRA met field reader routines
- 02 Feb 2011 S. Kim Call Compute_OD after wet deposition
- 05 Oct 2011 R. Yantosca Now get SUNCOS30 array from routine COSSZA
- 07 Oct 2011 R. Yantosca Rename SUNCOS30 to SUNCOS_MID, which is the cos(SZA) at the midpt of the chemistry timestep
- 02 Feb 2012 R. Yantosca Added modifications for GEOS-5.7.x met fields
- 06 Feb 2012 R. Yantosca Reorganize USE statements for clarity
- 06 Feb 2012 R. Yantosca Renamed NN to NNN to avoid name confusion
- 07 Feb 2012 R. Yantosca Split off met field I/O into internal routines READ_INITIAL_MET_FIELDS and READ_MET_FIELDS
- 07 Feb 2012 M. Payer Replace call to COSSZA with GET_COSINE_SZA
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 06 Mar 2012 R. Yantosca Now call READ_TOMS every month (this was formerly done within routine "fast_j.F")
- 06 Mar 2012 R. Yantosca Add subroutine GET_OVERHEAD_03_FOR_FASTJ which calls COMPUTE_OVERHEAD_03 (in toms_mod.F) to pre-compute the overhead 03 columns for

```
FAST-J photolysis. This removes code from
                            "set_prof.F" to facilitate the GI model.
19 Mar 2012 - R. Yantosca - Now call routines from olson_landmap_mod.F90
                            to read the Olson land map data
04 Apr 2012 - R. Yantosca - Now call updated LAI routines from new module
                            modis_lai_mod.F90. Retire routine RDLAI.
05 Apr 2012 - R. Yantosca - Removed reference to LXTRA, it's obsolete
11 Apr 2012 - R. Yantosca - Replace lai_mod.F with modis_lai_mod.F90
11 Apr 2012 - R. Yantosca - Now call INIT_MODIS_LAI (in modis_lai_mod.F90)
                           here so that we don't have to call it from
                            megan_mod.F and mercury_mod.F separately.
17 Apr 2012 - R. Yantosca - Need to set the mapping variable to NULL()
10 Jun 2012 - L. Murray - Remove references to UPBDFLX_MOD.F
31 Jul 2012 - R. Yantosca - Now pass am_I_Root variable to lower-level
                            routines in order to allow PRINT and WRITE
                            statements to execute on the root CPU. This
                            is needed for compatibility w/ the GEOS-5 GCM.
13 Aug 2012 - R. Yantosca - Now call FILL_CHEM_STATE_IDs to populate
                            the CHEM_STATE object ID and name fields
18 Oct 2012 - R. Yantosca - Rename LOCAL_MET object to State_Met
18 Oct 2012 - R. Yantosca - Rename CHEM_STATE object to State_Chm
18 Oct 2012 - R. Yantosca - Now pass am_I_Root, RC arguments to routines
                            ALLOCATE_ALL, INIT_ALL when using -DDEVEL
19 Oct 2012 - R. Yantosca - Now reference gigc_state_chm_mod.F90
19 Oct 2012 - R. Yantosca - Now reference gigc_state_met_mod.F90
25 Oct 2012 - R. Yantosca - Define logical doDebugPrt for ND70 output
25 Oct 2012 - R. Yantosca - Add descriptive comments for DEVEL #ifdefs
25 Oct 2012 - R. Yantosca - Now reference gigc_errcode_mod.F90
01 Nov 2012 - R. Yantosca - Now read soil NOx restart file
01 Nov 2012 - R. Yantosca - Now reference gigc_input_opt_mod.F90
08 Nov 2012 - R. Yantosca - Now pass Input_Opt as an arg to DO_CHEMISTRY
01 Nov 2012 - R. Yantosca - Now read soil NOx restart file
14 Nov 2012 - R. Yantosca - Add am_I_Root, Input_Opt, RC as arguments
                            to various subroutines
                          - Replaced all met field arrays with State_Met
15 Nov 2012 - M. Payer
                            derived type object
15 Nov 2012 - R. Yantosca - Bring Input_Opt out of the DEVEL tags
26 Feb 2013 - R. Yantosca - Add placeholder tag for Input_Opt%MAX_DEP
05 Mar 2013 - R. Yantosca - Now pass am_I_Root, Input_Opt, RC to routine
                            DO_PBL_MIX_2 (for non-local PBL mixing)
15 Mar 2013 - R. Yantosca - Now set Input_Opt%LINOZ_N* fields here
26 Mar 2013 - S.D. Eastham- Added initialization of rare tracers
29 Mar 2013 - R. Yantosca - Bring code out of DEVEL blocks
30 May 2013 - R. Yantosca - Now pass Input_Opt object to STDRUN routine
03 Jun 2013 - R. Yanosca - Use routines from updated mercury_mod.F
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
23 Oct 2013 - R. Yantosca - Now pass am_I_root, Input_Opt, RC to INIT_DAO
13 Dec 2013 - M. Sulprizio- Now set USE_03_FROM_MET logical flag during
```

```
initialization stage
11 Apr 2014 - R. Yantosca - Now remove call to INIT_GLOBAL_CH4; this is
                           now done from routine GIGC_Init_Extra
19 May 2014 - C. Keller - Added INIT_CHEMISTRY
19 May 2014 - C. Keller - Added HEMCO
23 Jun 2014 - R. Yantosca - Removed references to unix_cmds_mod.F
23 Jun 2014 - R. Yantosca - Removed references to directory_mod.F
23 Jun 2014 - R. Yantosca - Removed references to logical_mod.F
15 Jul 2014 - R. Yantosca - Now reference grid_mod.F90, regrid_a2a_mod.F90
15 Jul 2014 - R. Yantosca - Now call Init_Map_A2A to store shadow variables
                            within regrid_a2a_mod.F90. This helps to
                            break dependencies for the HEMCO implementation.
25 Jul 2014 - R. Yantosca - Remove reference to commsoil_mod.F90
22 Aug 2014 - R. Yantosca - Now save areas [m2] in State_Met%AREA_M2
15 Dec 2014 - M. Yannetti - Added PRECISION_MOD
06 Jan 2015 - R. Yantosca - Added two-way coupled simulation options
17 Feb 2015 - E. Lundgren - Remove STT and TCVV pointers
25 Feb 2015 - E. Lundgren - Remove MAKE-RH call since now in AIRQNT
16 Mar 2015 - E. Lundgren - Change tracer main units from kg to kg/kg
24 Mar 2015 - E. Lundgren - Now pass Input_Opt to Check_STT
31 Mar 2015 - E. Lundgren - Move post-transport AIRQNT call to transport_mod
16 Apr 2015 - R. Yantosca - Remove call to INIT_DAO; it's obsolete
12 Aug 2015 - R. Yantosca - Add support for MERRA2 meteorology
03 Sep 2015 - R. Yantosca - Now call SETUP_WETSCAV instead of INIT_WETSCAV
25 Jan 2016 - R. Yantosca - Call LINE_BUFFER to force PGI compiler to flush
                             STDOUT (unit=6) output to disk during a run
03 Feb 2016 - E. Lundgren - Use routine MAKE_RESTART_FILES for all GC rsts
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
02 May 2016 - R. Yantosca - Now pass Input_Opt to cleanup_gigc_state_chm
18 May 2016 - M. Sulprizio- Remove call to INIT_COMODE; it's obsolete
06 Jun 2016 - M. Sulprizio- Remove call to FILL_CHEM_STATE_IDs; this routine
                            was made obsolete by the species database
22 Jun 2016 - R. Yantosca - Add error checks to prevent calling UCX routines
                            when we are running specialty simulations
12 Jul 2016 - E. Lundgren - Remove binary punch restart file option
29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90
```

2.1.1 display_grid_and_model

Internal Subroutine DISPLAY_GRID_AND_MODEL displays the appropriate messages for the given model grid and machine type. It also prints the starting time and date (local time) of the GEOS-Chem simulation.

INTERFACE:

SUBROUTINE DISPLAY_GRID_AND_MODEL

REVISION HISTORY:

```
02 Dec 2003 - R. Yantosca - Initial version
13 Aug 2010 - R. Yantosca - Added ProTeX headers
13 Aug 2010 - R. Yantosca - Added extra output
02 Feb 2012 - R. Yantosca - Added output for GEOS-5.7.x met fields
28 Feb 2012 - R. Yantosca - Removed support for GEOS-3
19 Mar 2012 - R. Yantosca - Now echo info for 0.25 x 0.3125 runs
19 Mar 2012 - R. Yantosca - Now echo info if ISORROPIA is turned off
22 Oct 2012 - R. Yantosca - Now echo info if -DDEVEL is used
```

2.1.2 ctm_flush

Internal subroutine CTM_FLUSH flushes certain diagnostic file buffers to disk.

CTM_FLUSH should normally be called after each diagnostic output, so that in case the run dies, the output files from the last diagnostic timestep will not be lost.

FLUSH is an intrinsic FORTRAN subroutine and takes as input the unit number of the file to be flushed to disk.

INTERFACE:

SUBROUTINE CTM_FLUSH

REVISION HISTORY:

```
31 Aug 2000 - R. Yantosca - Initial version
13 Aug 2010 - R. Yantosca - Added ProTeX headers
06 Aug 2012 - R. Yantosca - IU_BPCH is only global file LUN still needed
```

2.1.3 display_end_time

Internal subroutine DISPLAY_END_TIME prints the ending time of the GEOS-Chem simulation.

INTERFACE:

SUBROUTINE DISPLAY_END_TIME

```
03 May 2005 - R. Yantosca - Initial version
13 Aug 2010 - R. Yantosca - Added ProTeX headers
```

2.1.4 read_initial_met_fields

Internal subroutine READ_INITIAL_MET_FIELDS calls the various routines to read met fields at the beginning of a GEOS-Chem simulation. This code was moved out of the main routine for clarity, due to the many #if defined() blocks that are required.

INTERFACE:

SUBROUTINE READ_INITIAL_MET_FIELDS()

REMARKS:

All variables used in this routine are declared above in the main program, and as such, are visible here.

Also calls the following routines:

- (1) AVGPOLE (average pressure @ poles) when I3 or I6 fields are read
- (2) LIGHTNING (lightning NOx emissions) when A3 or A6 fields are read

REVISION HISTORY:

```
07 Feb 2012 - R. Yantosca - Initial version
28 Feb 2012 - R. Yantosca - Removed support for GEOS-3
23 Oct 2013 - R. Yantosca - Now pass Input_Opt to GET_A6_FIELDS
23 Oct 2013 - R. Yantosca - Now pass Input_Opt to GET_MERRA_A3_FIELDS
24 Jun 2014 - R. Yantosca - Now pass Input_Opt to other routines
24 Jun 2014 - R. Yantosca - Cosmetic changes, line up arguments
12 Aug 2015 - R. Yantosca - Call routines for reading MERRA2 fields
```

2.1.5 read_met_fields

Internal subroutine READ_MET_FIELDS calls the various routines to read met fields in the main GEOS-Chem timestepping loop. This code was moved out of the main routine for clarity, due to the many #if defined() blocks that are required.

INTERFACE:

SUBROUTINE READ_MET_FIELDS()

REMARKS:

All variables used in this routine are declared above in the main program, and as such, are visible here.

Also calls the following routines:

- (1) AVGPOLE (average pressure @ poles) when I3 or I6 fields are read
- (2) LIGHTNING (lightning NOx emissions) when A3 or A6 fields are read

```
07 Feb 2012 - R. Yantosca - Initial version
28 Feb 2012 - R. Yantosca - Removed support for GEOS-3
04 Jan 2013 - M. Payer - Call UPDATE_T_DAY for MERRA and GEOS-5.7.2 (tmf)
23 Oct 2013 - R. Yantosca - Now pass Input_Opt to GET_A6_FIELDS
24 Jun 2014 - R. Yantosca - Now pass Input_Opt to other routines
24 Jun 2014 - R. Yantosca - Cosmetic changes, line up arguments
12 Aug 2015 - R. Yantosca - Now call routines to read MERRA2 met data
```

2.1.6 get_overhead_o3_for_fastj

Internal subroutine GET_OVERHEAD_O3_FOR_FASTJ

INTERFACE:

```
SUBROUTINE GET_OVERHEAD_O3_FOR_FASTJ( am_I_Root )
INPUT ARGUMENTS:

LOGICAL, INTENT(IN ) :: am_I_Root ! Root CPU?
```

REMARKS:

This routine makes use of variables declared in above in the main program (which are visible in all sub-programs below the CONTAINS statement).

The original code was done in FAST-J routine "set_prof.F", but has been split off to facilitate development of the grid-independent model.

REVISION HISTORY:

```
07 Mar 2012 - R. Yantosca - Initial version
14 Nov 2013 - R. Yantosca - For GEOS-FP, read 03 from met field files
13 Dec 2013 - M. Sulprizio- Moved USE_03_FROM_MET to the Input_Opt object and
set in initialization stage of GEOS_CHEM
22 Oct 2014 - C. Keller - Added am_I_Root
```

2.1.7 initialize_regridding

Internal subroutine Initialize_Regridding passes several variables to regrid_a2a_mod.F90, where they are locally shadowed.

INTERFACE:

```
SUBROUTINE Initialize_Regridding( am_I_Root, Input_Opt, RC )
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

OUTPUT PARAMETERS:

REMARKS:

This routine is a wrapper for Init_Map_A2A in regrid_a2a_mod.F90. Passing variables via Init_Map_A2A helps us to remove dependencies on other GEOS-Chem routines from regrid_a2a_mod.F90. This in turn facilitates the implementation of the HEMCO emissions package.

REVISION HISTORY:

```
15 Jul 2014 - R. Yantosca - Initial version
05 Mar 2015 - R. Yantosca - Now read data w/r/t ExtData/HEMCO
```

2.2 Fortran: Module Interface input_mod.F

Module INPUT_MOD contains routines that read the GEOS-Chem input file at the start of the run and pass the information to several other GEOS-Chem F90 modules.

INTERFACE:

```
MODULE INPUT_MOD
```

USES:

```
USE inquireMod, ONLY : findFreeLUN
USE PRECISION_MOD ! For GEOS-Chem Precision (fp)
```

IMPLICIT NONE PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: INITIALIZE_GEOS_GRID
PUBLIC :: READ_INPUT_FILE
PUBLIC :: GC_Init_Extra

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: READ_ONE_LINE
PRIVATE :: SPLIT_ONE_LINE

PRIVATE :: READ_SIMULATION_MENU

PRIVATE :: READ_ADVECTED_SPECIES_MENU

PRIVATE :: READ_AEROSOL_MENU
PRIVATE :: READ_EMISSIONS_MENU
PRIVATE :: READ_FUTURE_MENU
PRIVATE :: READ_CHEMISTRY_MENU
PRIVATE :: READ_RADIATION_MENU

PRIVATE :: READ_TRANSPORT_MENU
PRIVATE :: READ_CONVECTION_MENU
PRIVATE :: READ_DEPOSITION_MENU
PRIVATE :: READ_OUTPUT_MENU
PRIVATE :: READ_DIAGNOSTIC_MENU

PRIVATE :: SET_TINDEX

PRIVATE :: READ_ND49_MENU

PRIVATE :: READ_ND50_MENU

PRIVATE :: READ_ND51_MENU

PRIVATE :: READ_ND51b_MENU

PRIVATE :: READ_ND63_MENU

PRIVATE :: READ_PROD_LOSS_MENU
PRIVATE :: READ_UNIX_CMDS_MENU
PRIVATE :: READ_NESTED_GRID_MENU
PRIVATE :: READ_BENCHMARK_MENU

PRIVATE :: READ_CH4_MENU

PRIVATE :: READ_PASSIVE_TRACER_MENU
PRIVATE :: VALIDATE_DIRECTORIES

PRIVATE :: CHECK_DIRECTORY
PRIVATE :: CHECK_TIME_STEPS
PRIVATE :: IS_LAST_DAY_GOOD

#if defined(TOMAS)

PRIVATE :: INIT_TOMAS_MICROPHYSICS

#endif

- 20 Jul 2004 R. Yantosca Initial version
- (1) Now references LSOA in READ_AEROSOL_MENU (bmy, 9/28/04)
- (2) Fixed error checks and assign LSPLIT for tagged Hg. Also now refernces LAVHRRLAI from "logical_mod.f" (eck, bmy, 12/20/04)
- (3) Updated for crystalline/aqueous aerosol tracers. Also moved routine IS_LAST_DAY_GOOD here from "main.f". Also now references "ocean_mercury_mod.f". Also now open the bpch file for output in READ_DIAGNOSTIC_MENU instead of in "main.f". (cas, sas, bmy, 2/3/05)
- (4) Now references "diag03_mod.f" and "diag41_mod.f". Fixed minor bugs. Now references FILE_EXISTS from "file_mod.f". Updated comments. (bmy, 3/28/05)
- (5) Now modified for GEOS-5 and GCAP met fields. Also now set LSPLIT correctly for HCN/CH3CN simulation. (swu, xyp, bmy, 6/30/05)
- (6) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (7) Now read LMEGAN switch for MEGAN biogenics. Now read variable
 DATA_DIR_1x1 for 1x1 emissions files, etc. Now reference XNUMOL and
 XNUMOLAIR from "tracer_mod.f" (tmf, bmy, 10/25/05)
- (8) Now read LEMEP switch for EMEP emissions (bdf, bmy, 11/1/05)
- (9) Now added MERCURY MENU section. Also fixed bug in READ_ND48_MENU. (eck, cdh, bmy, 3/6/06)
- (10) Now read LGFED2BB switch for GFED2 biomass emissions (bmy, 4/5/06)

- (11) Bug fix for GCAP in IS_LAST_DAY_GOOD. Also now read LCTH, LMFLUX, LPRECON in READ_EMISSIONS_MENU. (bmy, 5/10/06)
- (12) Updated for ND42 SOA concentration diagnostic (dkh, bmy, 5/22/06)
- (13) Modified for future emissions (swu, bmy, 6/1/06)
- (14) Modified for BRAVO emissions (rjp, kfb, bmy, 6/26/06)
- (15) Remove support for GEOS-1 and GEOS-STRAT met fields. Also modified for David Streets' emissions. (bmy, 8/17/06)
- (16) Modified for variable tropopause. Also set dimension of ND28 diag for GFED2 or default biomass burning. Now read if Time Spent in Troposphere is wanted (phs, bmy, 10/17/06)
- (17) Now modified for OTD-LIS local redistribution. Remove references to GEOS-1 and GEOS-STRAT run dirs. (bmy, 11/5/07)
- (18) New error traps for OTD-LIS scaling, dependent on met field type.

 Bug fix, create string variables for ERROR_STOP. Bug fix: use ND52
 in call to SET_TINDEX in READ_DIAGNOSTIC_MENU. (ltm, bmy, 2/11/08)
- (19) Bug fix: use (0,0) in call to INIT_TRANSFER (phs, 6/17/08)
- (20) Minor fix in READ_TRANSPORT_MENU (cdh, bmy, 7/7/08)
- (21) Fixed typo READ_EMISSIONS_MENU for GEOS-3 (bmy, 10/30/08)
- (22) Set upper limit on dynamic timestep for 0.5 x 0.666 nested grids (yxw, bmy, dan, 11/6/08)
- (23) Now read LCAC switch for CAC emissions (amv, 1/09/2008)
- (24) Move the call to NDXX_SETUP (phs, 11/18/08)
- (25) Minor bug fix in READ_DIAGNOSTIC_MENU (tmf, 2/10/09)
- (26) Add LMEGANMONO switch in emission menu (ccc, 3/2/09)
- (27) Add LDICARB switch in aerosol menu (ccc, tmf, 3/10/09)
- (28) Now read LCOOKE in aerosol menu (phs, 5/18/09)
- (29) Add CH4_MENU in input.geos (kjw, 8/18/09)
- (30) Corrected typos in CHECK_TIME_STEPS (bmy, 8/21/09)
- (31) Now read LLINOZ in READ_SIMULATION_MENU (dbm, bmy, 10/16/09)
- (32) Remove reference to obsolete embedded chemistry stuff (bmy, 2/25/10)
- (33) Remove depreciated lightning options (ltm, bmy, 1/24/11)
- 25 Aug 2010 R. Yantosca Added modifications for MERRA
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 16 Feb 2011 R. Yantosca Add modifications for APM from G. Luo
- 29 Jul 2011 R. Yantosca Bug fix in READ_EMISSIONS_MENU for nested NA
- 07 Sep 2011 P. Kasibhatla Modified to include monthly GFED3
- 17 Jan 2012 P. Kasibhatla Modified to include daily and 3-hourly GFED3
- 08 Feb 2012 R. Yantosca Add modifications for GEOS-5.7.x met data
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 01 Mar 2012 R. Yantosca Now reference new grid_mod.F90
- 30 Jul 2012 R. Yantosca READ_INPUT_FILE now accepts am_I_Root from both the ESMF interface and main.F
- 03 Aug 2012 R. Yantosca Move calls to findFreeLUN out of DEVEL block
- 03 Aug 2012 R. Yantosca Now make IU_GEOS a global module variable so that we can define it with findFreeLun
- 02 Nov 2012 R. Yantosca Now pass the Input Options object to routines; this will eventually replace logical_mod, etc.
- 26 Feb 2013 M. Long Now make INITIALIZE_GEOS_GRID a public routine

```
04 Mar 2013 - R. Yantosca - Add routine GIGC_Init_Extra to move some init
                            calls out of the run stage when using ESMF
23 Apr 2013 - R. Yantosca - For TOMAS, rename READ_MICROPHYSICS_MENU to
                            INIT_TOMAS_MICROPHYSICS
13 Aug 2013 - M. Sulprizio- Add modifications for updated SOA and SOA +
                            semivolatile POA simulations (H. Pye)
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
17 Sep 2013 - R. Yantosca - Increase MAXDIM from 255 to 500 for more tracers
26 Sep 2013 - R. Yantosca - Renamed GEOS_57 Cpp switch to GEOS_FP everywhere
26 Sep 2013 - R. Yantosca - Now read GEOS_FP_DIR from Input_Opt everywhere
23 Jun 2014 - R. Yantosca - Remove references to logical_mod.F
23 Jun 2014 - R. Yantosca - Removed INIT_INPUT routine
14 Nov 2014 - M. Yannetti - Added PRECISION_MOD
24 Nov 2014 - C. Keller - Updates on timestep handling in ESMF environment
23 Jun 2016 - R. Yantosca - Remove references to APM code; it is no longer
                            compatible with the FlexChem implementation
28 Jul 2016 - M. Sulprizio- Rename subroutine READ_TRACER_MENU to
                            READ_ADVECTED_SPECIES_MENU
29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90
```

2.2.1 read_input_file

Subroutine READ_INPUT_FILE is the driver program for reading the GEOS-Chem input file "input.geos" from disk.

In an ESMF environment, all time steps (chemistry, convection, emissions, dynamics) must be specified externally before calling this routine. This is done in routine GIGC_Init_Simulation (gigc_initialization_mod.F90). The time steps specified in input.geos are ignored.

INTERFACE:

```
SUBROUTINE READ_INPUT_FILE( am_I_Root, Input_Opt, RC )
```

USES:

```
USE CHARPAK_MOD, ONLY : STRREPL

USE ErrCode_Mod

USE FILE_MOD, ONLY : IOERROR

USE GAMAP_MOD, ONLY : DO_GAMAP

USE Input_Opt_Mod, ONLY : OptInput

USE SEASALT_MOD, ONLY : INIT_SEASALT
```

INPUT PARAMETERS:

USE CMN_SIZE_MOD

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(OptInput), INTENT(INOUT) :: Input_Opt   ! Input options
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REVISION HISTORY:

```
20 Jul 2004 - R. Yantosca - Initial version
(1 ) Now call DO_GAMAP from "gamap_mod.f" to create "diaginfo.dat" and
      "tracerinfo.dat" files after all diagnostic menus have been read in
(2) Now call NDXX_setup from this routine (phs, 11/18/08)
(3 ) Now call READ_ND51b_MENU (amv, bmy, 12/18/09)
27 Aug 2010 - R. Yantosca - Added ProTeX headers
30 Jul 2012 - R. Yantosca - Now accept am_I_Root from main.F, so that we
                            can get rid of duplicate code in DEVEL blocks
03 Aug 2012 - R. Yantosca - Move calls to findFreeLUN out of DEVEL block
03 Aug 2012 - R. Yantosca - Now make IU_GEOS a global module variable
                            so that we can define it with findFreeLun
15 Oct 2012 - R. Yantosca - Add EXTERNAL_GRID, XTERNAL_FORCING to #ifdef
16 Oct 2012 - R. Yantosca - Don't call CHECK_TIME_STEPS if we are calling
                            READ_INPUT_FILE from the ESMF interface
09 Nov 2012 - R. Yantosca - Now pass Input_Opt to lower-level routines
06 Dec 2012 - R. Yantosca - Now call CHECK_TIME_STEPS when we are connecting
                            to the GEOS-5 GCM via the ESMF environment,
19 Mar 2013 - R. Yantosca - When using ESMF interface to GEOS-5, append
                            ".rc" to input.geos (instead of ___.rc)
04 Apr 2013 - R. Yantosca - Now pass objects to DO_GAMAP routine
23 Jun 2014 - R. Yantosca - Now do not call INIT_INPUT, this is replaced
                            by the INIT_GIGC_INPUT_OPT routine
15 Apr 2015 - R. Yantosca - Also define Input_Opt%ITS_A_NESTED_GRID here
                            so that we can pass it to INITIALIZE_GEOS_GRID
04 Aug 2015 - M. Long
                        - Removed ".rc" file specifier. Not necessary.
16 Dec 2015 - R. Yantosca - Now pass State_Chm to READ_TRACER_MENU
04 Sep 2015 - C. Keller - Added passive tracer menu
16 Jun 2016 - E. Lundgren - Move TOMAS init to GIGC_INIT_EXTRA
```

2.2.2 read_one_line

Subroutine READ_ONE_LINE reads a line from the input file. If the global variable VERBOSE is set, the line will be printed to stdout. READ_ONE_LINE can trap an unexpected EOF if LOCATION is passed. Otherwise, it will pass a logical flag back to the calling routine, where the error trapping will be done.

INTERFACE:

FUNCTION READ_ONE_LINE(EOF, LOCATION) RESULT(LINE)

USES:

USE FILE_MOD, ONLY : IOERROR

INPUT PARAMETERS:

CHARACTER(LEN=*), INTENT(IN), OPTIONAL :: LOCATION ! Msg to display

OUTPUT PARAMETERS:

LOGICAL, INTENT(OUT) :: EOF ! Denotes EOF

REVISION HISTORY:

```
20 Jul 2004 - R. Yantosca - Initial version
```

27 Aug 2010 - R. Yantosca - Added ProTeX headers

03 Aug 2012 - R. Yantosca - Now make IU_GEOS a global module variable so that we can define it with findFreeLun

17 Sep 2013 - R. Yantosca - Extend line length to read in more tracers

2.2.3 split_one_line

Subroutine SPLIT_ONE_LINE reads a line from the input file (via routine READ_ONE_LINE), and separates it into substrings.

SPLIT_ONE_LINE also checks to see if the number of substrings found is equal to the number of substrings that we expected to find. However, if you don't know a-priori how many substrings to expect a-priori, you can skip the error check.

INTERFACE:

SUBROUTINE SPLIT_ONE_LINE(SUBSTRS, N_SUBSTRS, N_EXP, LOCATION)

USES:

USE CHARPAK_MOD, ONLY: STRSPLIT

INPUT PARAMETERS:

```
! Number of substrings we expect to find INTEGER, INTENT(IN) :: N_EXP
```

! Name of routine that called SPLIT_ONE_LINE CHARACTER(LEN=*), INTENT(IN) :: LOCATION

OUTPUT PARAMETERS:

```
! Array of substrings (separated by " ")
CHARACTER(LEN=255), INTENT(OUT) :: SUBSTRS(MAXDIM)
```

```
! Number of substrings actually found INTEGER, INTENT(OUT) :: N_SUBSTRS
```

REVISION HISTORY:

```
20 Jul 2004 - R. Yantosca - Initial version
27 Aug 2010 - R. Yantosca - Added ProTeX headers
17 Sep 2013 - R. Yantosca - Extend LINE to 500 chars to allow more tracers
```

2.2.4 read_simulation_menu

Subroutine READ_SIMULATION_MENU reads the SIMULATION MENU section of the GEOS-Chem input file.

INTERFACE:

```
SUBROUTINE READ_SIMULATION_MENU( am_I_Root, Input_Opt, RC )
```

USES:

```
USE CMN_SIZE_MOD
     USE ErrCode_Mod
                          ONLY : SET_XOFFSET, SET_YOFFSET
     USE GC_GRID_MOD,
     USE Input_Opt_Mod,
                          ONLY : OptInput
     USE TIME_MOD,
                            ONLY : SET_BEGIN_TIME,
                                                    SET_END_TIME
                          ONLY : SET_CURRENT_TIME, SET_DIAGb
     USE TIME_MOD,
     USE TIME_MOD,
                           ONLY : SET_NDIAGTIME,
                                                    GET_TAU
     USE TRANSFER_MOD,
                            ONLY : INIT_TRANSFER
#if defined( EXTERNAL_GRID ) || defined( EXTERNAL_FORCING )
                            ONLY : Accept_External_Date_Time
     USE TIME_MOD,
#endif
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(OptInput), INTENT(INOUT) :: Input_Opt  ! Input options
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

```
20 Jul 2004 - R. Yantosca - Initial version
```

- (1) Bug fix: Read LSVGLB w/ the * format and not w/ '(a). (bmy, 2/23/05)
- (2) Now read GEOS_5_DIR and GCAP_DIR from input.geos (swu, bmy, 5/25/05)
- (3) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (4) Now references DATA_DIR_1x1 for 1x1 emissions files (bmy, 10/24/05)
- (5) Now read switch for using variable tropopause or not (phs, 9/14/06)
- (6) Remove references to GEOS-1 and GEOS-STRAT run dirs. Now calls

```
INIT_TRANSFER (bmy, 11/5/07)
(7) Fix typo in "print to screen" section (phs, 6/1/08)
(8) Call INIT_TRANSFER w/ (0,0) instead of (I0,J0) (phs, 6/17/08)
(10) Now read LLINOZ switch from input.geos file (dbm, bmy, 10/16/09)
13 Aug 2010 - R. Yantosca - Now read MERRA_DIR
19 Aug 2010 - R. Yantosca - Set LUNZIP=F for MERRA met fields.
27 Aug 2010 - R. Yantosca - Added ProTeX headers
01 Feb 2012 - R. Yantosca - Now read GEOS_57_DIR for GEOS-5.7.x met
08 Feb 2012 - R. Yantosca - Set LUNZIP=F for GEOS-5.7.x met fields
28 Feb 2012 - R. Yantosca - Removed support for GEOS-3
01 Mar 2012 - R. Yantosca - Now call routine INITIALIZE_GEOS_GRID to
                            initialize horizontal grid parameters
10 Jun 2012 - L. Murray - Move Linoz to chemistry menu
30 Jul 2012 - R. Yantosca - Now accept am_I_Root as an argument when
                            running with the traditional driver main.F
01 Nov 2012 - R. Yantosca - Now pass Input_Opt, RC as arguments
06 Dec 2012 - R. Yantosca - Now get NYMDb, NHMSb, NYMDe, NHMSe from the ESMF
                            environment when connecting to the GEOS-5 GCM
11 Dec 2012 - R. Yantosca - ACCEPT_DATE_TIME_FROM_ESMF has now been renamed
                            to ACCEPT_EXTERNAL_DATE_TIME
19 May 2014 - C. Keller - Now read HEMCO configuration file.
23 Jun 2014 - R. Yantosca - Remove references to logical_mod.F
12 Aug 2015 - R. Yantosca - Add support for MERRA2
12 Aug 2015 - R. Yantosca - Add support for 05x0625 grids
13 Aug 2015 - R. Yantosca - Bug fix: prefix RES_DIR in front of MERRA2_DIR
27 Jul 2016 - M. Sulprizio- Remove LSVGLB and OUT_RST_FILE options. Restart
                            files are now always saved out and the output
                            restart file name is hardcoded in restart_mod.F.
09 Aug 2016 - E. Lundgren - Remove call to routine set_restart; use input
                            rst filename directly in restart_mod.F.
```

2.2.5 initialize_geos_grid

Subroutine INITIALIZE_GEOS_GRID calls routines from grid_mod.F90 to initialize the horizontal grid parameters.

INTERFACE:

```
SUBROUTINE INITIALIZE_GEOS_GRID( am_I_Root, Input_Opt, RC )
```

USES:

```
USE CMN_SIZE_MOD

USE GC_GRID_MOD, ONLY : COMPUTE_GRID

USE GC_GRID_MOD, ONLY : INIT_GRID

USE Input_Opt_Mod, ONLY : OptInput
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

The module grid_mod.F90 has been modified to save grid parameters in 3D format, which will facilitate interfacing GEOS-Chem to a GCM.

The module global_grid_mod.F90 contains several of the global grid arrays (*_g) originally in grid_mod.F. These arrays are used in regridding GFED3 biomass emissions, which are available on a 0.5x0.5 global grid. The global arrays may need to be used in the future for regridding other emissions for nested grids.

REVISION HISTORY:

2.2.6 read_advected_species_menu

Subroutine READ_ADVECTED_SPECIES_MENU reads the ADVECTED SPECIES MENU section of the GEOS-Chem input file.

INTERFACE:

SUBROUTINE READ_ADVECTED_SPECIES_MENU(am_I_Root, Input_Opt, RC)

USES:

```
USE CHARPAK_MOD, ONLY : ISDIGIT

USE CMN_SIZE_MOD

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ALLOC_ERR

USE ERROR_MOD, ONLY : ERROR_STOP

USE Input_Opt_Mod, ONLY : OptInput
```

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REVISION HISTORY:

- 20 Jul 2004 R. Yantosca Initial version
- (1) Now set LSPLIT correctly for Tagged Hg simulation (eck, bmy, 12/13/04)
- (2) Now initialize ocean mercury module (sas, bmy, 1/20/05)
- (3) Now set LSPLIT correctly for Tagged HCN/CH3CN sim (xyp, bmy, 6/30/05)
- (4) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (5) Now reference XNUMOLAIR from "tracer_mod.f" (bmy, 10/25/05)
- (6) Now move call to INIT_OCEAN_MERCURY to READ_MERCURY_MENU (bmy, 2/24/06)
- (7) Now do not call SET_BIOTRCE anymore; it's obsolete (bmy, 4/5/06)
- (8) Add SET_BIOTRCE to initialize IDBxxxs. (fp, 2/26/10)
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 13 Aug 2012 R. Yantosca Now pass CHEM_STATE as an argument (DEVEL only)
- 01 Nov 2012 R. Yantosca Now pass Input_Opt, RC as arguments
- 07 Nov 2012 R. Yantosca Now define Input_Opt%ITS_A_*_SIM fields
- 28 Oct 2013 R. Yantosca Set Input_Opt%ITS_A_SPECIALTY_SIM = .FALSE.

 when running GEOS-Chem in an ESMF environment
- 25 Jun 2014 R. Yantosca Removed references to tracer_mod.F
- 21 Aug 2014 R. Yantosca Bug fix: add ITS_A_RnPbBe_SIM to the test that defines the ITS_A_SPECIALTY_SIM flag
- 24 Mar 2015 E. Lundgren Move init_tracer to within APM ifdef block
- 23 Jun 2016 R. Yantosca Remove call to TRACERID, it's obsolete
- 28 Jul 2016 M. Sulprizio- Rename TRACER MENU to ADVECTED SPECIES MENU; Remove ID, MW, and member columns from menu

2.2.7 read_aerosol_menu

Subroutine READ_AEROSOL_MENU reads the AEROSOL MENU section of the GEOS-Chem input file.

INTERFACE:

SUBROUTINE READ_AEROSOL_MENU(am_I_Root, Input_Opt, RC)

USES:

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP
USE Input_Opt_Mod, ONLY : OptInput
USE UCY MOD ONLY : T NAT SUPE

USE UCX_MOD, ONLY: T_NAT_SUPERCOOL, P_ICE_SUPERSAT

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REMARKS:

Move error checks that depend on species indices to the subroutine DO_ERROR_CHECKS. This is now called from GC_INIT_EXTRA, after the initialization of the species database.

- 20 Jul 2004 R. Yantosca Initial version
- (1) Now reference LSOA (bmy, 9/28/04)
- (2) Now stop run if LSOA=T and SOA tracers are undefined (bmy, 11/19/04)
- (3) Now reference LCRYST from "logical_mod.f". Also now check to make prevent aerosol tracers from being undefined if the corresponding logical switch is set. (cas, bmy, 1/14/05)
- (4) Now also require LSSALT=T when LSULF=T, since we now compute the production of SO4 and NIT w/in the seasalt aerosol (bec, bmy, 4/13/05)
- (5) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (6) Now update error check for SOG4, SOA4 (dkh, bmy, 6/1/06)
- (7) Add LDICARB switch to cancel SOG condensation onto OC aerosols. (ccc, tmf, 3/10/09)
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 01 Nov 2012 R. Yantosca Now pass Input_Opt, RC as arguments
- 11 Apr 2013 S.D. Eastham- Added gravitational settling flag
- 13 Aug 2013 M. Sulprizio- Add modifications for updated SOA and SOA + semivolatile POA simulations (H. Pye)
- 12 Sep 2013 M. Sulprizio- Add modifications for acid uptake on dust aerosols (T.D. Fairlie)
- 16 Apr 2014 M. Sulprizio- Now read path for PSC restart file
- 23 Jun 2014 R. Yantosca Removed references to logical_mod.F
- 25 Jun 2014 R. Yantosca Removed references to tracer_mod.F
- 09 Apr 2015 M. Sulprizio- Removed options for DEAD dust emissions, NAP emissions, POA emissions scale, and the PSC

restart file. These options are now handled by HEMCO.

```
08 Jul 2015 - E. Lundgren - Added LMPOA option for marine organic aerosols
16 Jun 2016 - K. Travis - Now define species ID's with the Ind_ function
22 Jun 2016 - R. Yantosca - Move error checks to DO_ERROR_CHECKS routine
```

BOC

LOCAL VARIABLES:

```
! Scalars
                                     LBRC, LSOA
              :: LSULF, LCARB,
:: LSVPOA, LDUST,
LOGICAL
                                      LDSTUP
LOGICAL
                           LCRYST,
LOGICAL
               :: LSSALT,
                                       LDICARB
               :: LGRAVSTRAT, LHOMNUCNAT, LSOLIDPSC
LOGICAL
LOGICAL
               :: LPSCCHEM, LSTRATOD, LMPOA
INTEGER
               :: N, T,
                                       Ι
CHARACTER(LEN=255) :: MSG, LOCATION
! Arrays
CHARACTER(LEN=255) :: SUBSTRS(MAXDIM)
!-----
! READ_AEROSOL_MENU begins here!
!-----
! Location string for ERROR_STOP
LOCATION = 'READ_AEROSOL_MENU ("input_mod.f")'
! Error check
IF ( CT1 /= 2 ) THEN
  MSG = 'SIMULATION MENU & ADVECTED SPECIES MENU ' //
       'must be read in first!'
  CALL ERROR_STOP( MSG, LOCATION )
ENDIF
! Use online sulfate aerosols?
CALL SPLIT_ONE_LINE( SUBSTRS, N, 1, 'read_aerosol_menu:1')
READ( SUBSTRS(1:N), * ) LSULF
! Use crystalline sulfate aerosols?
CALL SPLIT_ONE_LINE( SUBSTRS, N, 1, 'read_aerosol_menu:2')
READ( SUBSTRS(1:N), * ) LCRYST
! Use online carbon aerosols?
CALL SPLIT_ONE_LINE( SUBSTRS, N, 1, 'read_aerosol_menu:3')
READ( SUBSTRS(1:N), * ) LCARB
! Use brown carbon aerosols?
```

```
CALL SPLIT_ONE_LINE( SUBSTRS, N, 1, 'read_aerosol_menu:4')
READ( SUBSTRS(1:N), * ) LBRC
! Use secondary organic aerosols?
CALL SPLIT_ONE_LINE( SUBSTRS, N, 1, 'read_aerosol_menu:5')
READ( SUBSTRS(1:N), * ) LSOA
! SOAupdate: Add Semi-volatile POA switch (hotp 8/9/09)
CALL SPLIT_ONE_LINE( SUBSTRS, N, 1, 'read_aerosol_menu:6')
READ( SUBSTRS(1:N), * ) LSVPOA
! Use online dust aerosols ?
CALL SPLIT_ONE_LINE( SUBSTRS, N, 1, 'read_aerosol_menu:7')
READ( SUBSTRS(1:N), * ) LDUST
!tdf
! Use SO2 and HNO3 uptake on dust aerosols
CALL SPLIT_ONE_LINE( SUBSTRS, N, 1, 'read_aerosol_menu:9.5')
READ( SUBSTRS(1:N), * ) LDSTUP
! Use online sea-salt aerosols?
CALL SPLIT_ONE_LINE( SUBSTRS, N, 1, 'read_aerosol_menu:8')
READ( SUBSTRS(1:N), * ) LSSALT
! Accum mode seasalt radii bin edges [um]
CALL SPLIT_ONE_LINE( SUBSTRS, N, 2, 'read_aerosol_menu:9')
DO T = 1, N
   READ( SUBSTRS(T), * ) Input_Opt%SALA_REDGE_um(T)
ENDDO
! Coarse mode seasalt radii bin edges [um]
CALL SPLIT_ONE_LINE( SUBSTRS, N, 2, 'read_aerosol_menu:10')
DO T = 1, N
   READ( SUBSTRS(T), * ) Input_Opt%SALC_REDGE_um(T)
ENDDO
! Use marine organic aerosols?
CALL SPLIT_ONE_LINE( SUBSTRS, N, 1, 'read_aerosol_menu:11')
READ( SUBSTRS(1:N), * ) LMPOA
! Switch to comment the SOG condensation in carbon_mod.f (ccc, 3/10/09)
! Use online dicarbonyl chemistry
CALL SPLIT_ONE_LINE( SUBSTRS, N, 1, 'read_aerosol_menu:12')
READ( SUBSTRS(1:N), * ) LDICARB
! Apply gravitational settling in stratosphere?
CALL SPLIT_ONE_LINE( SUBSTRS, N, 1, 'read_aerosol_menu:13')
READ( SUBSTRS(1:N), * ) LGRAVSTRAT
```

```
! Use solid polar stratospheric clouds (PSCs)?
CALL SPLIT_ONE_LINE( SUBSTRS, N, 1, 'read_aerosol_menu:14')
READ( SUBSTRS(1:N), * ) LSOLIDPSC
! Allow homogeneous nucleation of NAT?
CALL SPLIT_ONE_LINE( SUBSTRS, N, 1, 'read_aerosol_menu:15')
READ( SUBSTRS(1:N), * ) LHOMNUCNAT
! NAT supercooling requirement (K)
CALL SPLIT_ONE_LINE( SUBSTRS, N, 1, 'read_aerosol_menu:16')
READ( SUBSTRS(1:N), * ) T_NAT_SUPERCOOL
! Ice supersaturation ratio requirement
CALL SPLIT_ONE_LINE( SUBSTRS, N, 1, 'read_aerosol_menu:17')
READ( SUBSTRS(1:N), * ) P_ICE_SUPERSAT
! Perform PSC-related heterogeneous chemistry?
CALL SPLIT_ONE_LINE( SUBSTRS, N, 1, 'read_aerosol_menu:18')
READ( SUBSTRS(1:N), * ) LPSCCHEM
! Include stratospheric aerosols optical depths?
CALL SPLIT_ONE_LINE( SUBSTRS, N, 1, 'read_aerosol_menu:19')
READ( SUBSTRS(1:N), * ) LSTRATOD
! Separator line
CALL SPLIT_ONE_LINE( SUBSTRS, N, 1, 'read_aerosol_menu:20')
! Error checks
! Make sure that SALA, SALC bins are contiguous
IF ( Input_Opt%SALA_REDGE_um(2) /=
    Input_Opt%SALC_REDGE_um(1)
                                ) THEN
  MSG = 'SALA and SALC bin edges are not contiguous!'
  CALL ERROR_STOP( MSG, LOCATION )
ENDIF
! Turn off switches for simulations that don't use aerosols
IF ( ( .not. Input_Opt%ITS_A_FULLCHEM_SIM ) .and.
    ( .not. Input_OPt%ITS_AN_AEROSOL_SIM ) ) THEN
  LSULF = .FALSE.
  LCRYST = .FALSE.
  LCARB = .FALSE.
  LBRC = .FALSE.
  LSOA = .FALSE.
  LDUST = .FALSE.
```

```
LSSALT = .FALSE.
  LMPOA = .FALSE.
  LSVPOA = .FALSE.
ENDIF
!%% The cryst/aq code is currently under development so make
!%%% sure that LCRYST = FALSE for now until further notice
!%%% (rjp, bmy, 3/15/05)
LCRYST = .FALSE.
!-----
! Set fields of Input Options object
!-----
Input_Opt%LSULF
                        = LSULF
Input_Opt%LCRYST
                        = LCRYST
Input_Opt%LCARB
                       = LCARB
Input_Opt%LBRC
                        = LBRC
Input_Opt%LSOA
                       = LSOA
Input_Opt%LSVPOA
                       = LSVPOA
Input_Opt%LDUST
                       = LDUST
Input_Opt%LDSTUP
                       = LDSTUP
Input_Opt%LSSALT
                       = LSSALT
Input_Opt%LMPOA
                       = LMPOA
Input_Opt%LDICARB
                        = LDICARB
Input_Opt%LGRAVSTRAT
                       = LGRAVSTRAT
Input_Opt%LSOLIDPSC
                       = LSOLIDPSC
Input_Opt%LHOMNUCNAT
                       = LHOMNUCNAT
Input_Opt%T_NAT_SUPERCOOL
                       = T_NAT_SUPERCOOL
Input_Opt%P_ICE_SUPERSAT
                       = P_ICE_SUPERSAT
Input_Opt%LPSCCHEM
                        = LPSCCHEM
Input_Opt%LSTRATOD
                        = LSTRATOD
! Return success
RC = GC\_SUCCESS
1-----
! Print to screen
IF ( am_I_Root ) THEN
  WRITE(6, '(/,a)') 'AEROSOL MENU'
  WRITE(6, '(a)') '----'
  WRITE( 6, 100
                 ) 'Online SULFATE AEROSOLS?
                                          : ', LSULF
  WRITE(6, 100 ) 'Brown Carbon Aerosol? : ', LBRC WRITE(6, 100 ) 'Online 2dy ORGANIC AEROSOLS?: ', LSOA WRITE(6, 100 ) 'Semivolatile POA? : ', LSVP
                                    : ', LSVPOA
  WRITE( 6, 100
                ) 'Online DUST AEROSOLS? : ', LDUST
```

```
WRITE( 6, 100
                         ) 'Acid uptake on dust?
                                                    : ', LDSTUP
         WRITE( 6, 100
                         ) 'Online SEA SALT AEROSOLS?
                                                    : ', LSSALT
         WRITE( 6, 110
                         ) 'Accum SEA SALT radii [um]
     &
                            Input_Opt%SALA_REDGE_um(1),
                            Input_Opt%SALA_REDGE_um(2)
     &
                         ) 'Coarse SEA SALT radii [um]
         WRITE( 6, 110
     &
                            Input_Opt%SALC_REDGE_um(1),
     &
                           Input_Opt%SALC_REDGE_um(2)
         WRITE( 6, 100
                         ) 'MARINE ORGANIC AEROSOLS?
                                                    : ', LMPOA
         WRITE( 6, 100
                         ) 'Settle strat. aerosols? : ',LGRAVSTRAT
         WRITE( 6, 100
                         ) 'Online SOLID PSC aerosols? : ',LSOLIDPSC
         WRITE( 6, 100
                         ) 'Allow hom. NAT nucleation? : ',LHOMNUCNAT
         WRITE( 6, 120
                         ) 'NAT supercooling requirement: ',
                                                  T_NAT_SUPERCOOL
         WRITE( 6, 120
                         ) 'Ice supersaturation req.
                                                    : ',
                                       ((P_ICE_SUPERSAT-1)*1.e+2_fp)
     &
        WRITE( 6, 100
                         ) 'Perform PSC het. chemistry? : ',LPSCCHEM
         WRITE( 6, 100
                         ) 'Use strat. aerosol OD? : ', LSTRATOD
      ENDIF
 100 FORMAT( A, L5 )
 110 FORMAT( A, f6.2, ' - ', f6.2)
 120 FORMAT( A, f6.2, 'K')
 105 FORMAT( A, f6.2)
 130 FORMAT(A, A)
      END SUBROUTINE READ_AEROSOL_MENU
 EOC
#if defined( TOMAS )
 ______
                  GEOS-Chem Global Chemical Transport Model
\mbox{}\hrulefill\
 \subsubsection [init\_tomas\_microphys] {init\_tomas\_microphys}
 Subroutine INIT\_TOMAS\_MICROPHYS will initialize the
   TOMAS microphysics package. This replaces the former subroutine
   READ\_MICROPHYSICS\_MENU.
 //
 \\{\bf INTERFACE:}
                    SUBROUTINE INIT_TOMAS_MICROPHYSICS( am_I_Root, Input_Opt,
\begin{verbatim}
                                      State_Chm, RC )
     &
```

USES:

USE ERROR_MOD, ONLY : ERROR_STOP
USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Chm_Mod, ONLY : Ind_

USE TOMAS_MOD, ONLY : INIT_TOMAS

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry state

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REMARKS:

We now invoke TOMAS by compiling GEOS-Chem and setting either the TOMAS=yes (30 bins, default) or TOMAS40=yes (40 bins, optional) switches. The old LTOMAS logical switch is now obsolete because all of the TOMAS code is segregated from the rest of GEOS-Chem with #ifdef blocks. Therefore, we no longer need to read the microphysics menu, but we still need to apply some error checks and then call INIT_TOMAS. (bmy, 4/23/13)

The Ind_() function now defines all species ID's. It returns -1 if a species cannot be found. The prior behavior was to return 0 if a species wasn't found. Therefore, in order to preserve the logic of the error checks, we must force any -1's returned by Ind_() to 0's in this subroutine.

- 20 Jul 2004 R. Yantosca Initial version
- (1) Now read LNEI99 -- switch for EPA/NEI99 emissions (bmy, 11/5/04)
- (2) Now read LAVHRRLAI-switch for using AVHRR-derived LAI (bmy, 12/20/04)
- (3) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (4) Now read LMEGAN -- switch for MEGAN biogenics (tmf, bmy, 10/20/05)
- (5) Now read LEMEP -- switch for EMEP emissions (bdf, bmy, 11/1/05)
- (6) Now read LGFED2BB -- switch for GFED2 biomass emissions (bmy, 4/5/06)
- (7) Now read LOTDLIS, LCTH, LMFLUX, LPRECON for lightning options (bmy, 5/10/06)
- (8) Now read LBRAVO for BRAVO Mexican emissions (rjp, kfb, bmy, 6/26/06)
- (9) Now read LEDGAR for EDGAR emissions (avd, bmy, 7/11/06)
- (10) Now read LSTREETS for David Streets' emissions (bmy, 8/17/06)
- (11) Kludge: Reset LMFLUX or LPRECON to LCTH, as the MFLUX and PRECON

lightning schemes have not yet been implemented. Rename LOTDLIS to LOTDREG. Also read LOTDLOC for the OTD-LIS local redistribution of lightning flashes (cf B. Sauvage). Make sure LOTDREG and LOTDLOC are not both turned on at the same time. (bmy, 1/31/07)

- (12) Add LOTDSCALE to the list of LNOx options (ltm, bmy, 9/24/07)
- (13) Add new error traps for OTD-LIS options, dependent on met field type (ltm, bmy, 11/29/07)
- (14) Bug fix, create string variables for ERROR_STOP (bmy, 1/24/08)
- (15) Now read LCAC for CAC emissions (amv, 1/09/2008)
- (16) Now read LEDGARSHIP, LARCSHIP and LEMEPSHIP (phs, 12/5/08)
- (17) Fixed typo in message for GEOS-3 (bmy, 10/30/08)
- (18) Now read LVISTAS (amv, 12/2/08)
- (19) Now read L8DAYBB, L3HRBB and LSYNOPBB for GFED2 8-days and 3hr emissions, and LICARTT for corrected EPA (phs, yc, 12/17/08)
- (20) Add a specific switch for MEGAN emissions for monoterpenes and MBO (ccc, 2/2/09)
- (21) Now read LICOADSSHIP (cklee, 6/30/09)
- (22) Bug fix: for now, if LEMEPSHIP is turned on but LEMEP is turned off, just turn off LEMEPSHIP and print a warning msg. (mak, bmy, 10/18/09)
- (23) Now accounts for NEI2005 (amv, phs, 10/9/09)
- (24) Included optional flag for using MODIS LAI data (mpb,2009).
- (25) Included optional flag for using PCEEA model (mpb, 2009)
- (26) Now force settings for EU, NA, CC nested grids (amv, bmy, 12/18/09)
- (27) Now force MEGAN to use MODIS LAI (ccarouge, bmy, 2/24/10)
- (28) Add separate switch for NOx fertilizer. (fp, 2/29/10)
- (29) Add scaling for isoprene and NOx emissions. (fp, 2/29/10)
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 23 Apr 2013 R. Yantosca Renamed to INIT_TOMAS_MICROPHYS
- 30 Jan 2014 R. Yantosca INIT_TOMAS accepts am_I_Root, Input_Opt, RC
- 16 Jun 2016 K. Travis Now define species ID's with the Ind_ function
- 16 Jun 2016 E. Lundgren INIT_TOMAS now accepts State_Chm
- 22 Jun 2016 R. Yantosca Force -1's returned by Ind_() to zeroes, in order to preserve the program logic

2.2.8 read_emissions_menu

Subroutine READ_EMISSIONS_MENU reads the EMISSIONS MENU section of the GEOS-Chem input file.

INTERFACE:

SUBROUTINE READ_EMISSIONS_MENU(am_I_Root, Input_Opt, RC)

USES:

USE CMN_03_MOD

USE CMN_SIZE_MOD USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP
USE Input_Opt_Mod, ONLY : OptInput
USE TIME_MOD, ONLY : SET_HISTYR
USE UCX_MOD, ONLY : CFCYEAR

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REMARKS:

The $Ind_{()}$ function now defines all species ID's. It returns -1 if a species cannot be found. Therefore now test for $Ind_{()} > 0$ for a valid species.

- 20 Jul 2004 R. Yantosca Initial version
- (1) Now read LNEI99 -- switch for EPA/NEI99 emissions (bmy, 11/5/04)
- (2) Now read LAVHRRLAI-switch for using AVHRR-derived LAI (bmy, 12/20/04)
- (3) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (4) Now read LMEGAN -- switch for MEGAN biogenics (tmf, bmy, 10/20/05)
- (5) Now read LEMEP -- switch for EMEP emissions (bdf, bmy, 11/1/05)
- (6) Now read LGFED2BB -- switch for GFED2 biomass emissions (bmy, 4/5/06)
- (7) Now read LOTDLIS, LCTH, LMFLUX, LPRECON for lightning options (bmy, 5/10/06)
- (8) Now read LBRAVO for BRAVO Mexican emissions (rjp, kfb, bmy, 6/26/06)
- (9) Now read LEDGAR for EDGAR emissions (avd, bmy, 7/11/06)
- (10) Now read LSTREETS for David Streets' emissions (bmy, 8/17/06)
- (11) Kludge: Reset LMFLUX or LPRECON to LCTH, as the MFLUX and PRECON lightning schemes have not yet been implemented. Rename LOTDLIS to LOTDREG. Also read LOTDLOC for the OTD-LIS local redistribution of lightning flashes (cf B. Sauvage). Make sure LOTDREG and LOTDLOC are not both turned on at the same time. (bmy, 1/31/07)
- (12) Add LOTDSCALE to the list of LNOx options (ltm, bmy, 9/24/07)
- (13) Add new error traps for OTD-LIS options, dependent on met field type (ltm, bmy, 11/29/07)
- (14) Bug fix, create string variables for ERROR_STOP (bmy, 1/24/08)
- (15) Now read LCAC for CAC emissions (amv, 1/09/2008)
- (16) Now read LEDGARSHIP, LARCSHIP and LEMEPSHIP (phs, 12/5/08)
- (17) Fixed typo in message for GEOS-3 (bmy, 10/30/08)

- (18) Now read LVISTAS (amv, 12/2/08)
- (19) Now read L8DAYBB, L3HRBB and LSYNOPBB for GFED2 8-days and 3hr emissions, and LICARTT for corrected EPA (phs, yc, 12/17/08)
- (20) Add a specific switch for MEGAN emissions for monoterpenes and MBO (ccc, 2/2/09)
- (21) Now read LICOADSSHIP (cklee, 6/30/09)
- (22) Bug fix: for now, if LEMEPSHIP is turned on but LEMEP is turned off, just turn off LEMEPSHIP and print a warning msg. (mak, bmy, 10/18/09)
- (23) Now accounts for NEI2005 (amv, phs, 10/9/09)
- (24) Included optional flag for using MODIS LAI data (mpb, 2009).
- (25) Included optional flag for using PCEEA model (mpb, 2009)
- (26) Now force settings for EU, NA, CC nested grids (amv, bmy, 12/18/09)
- (27) Now force MEGAN to use MODIS LAI (ccarouge, bmy, 2/24/10)
- (28) Add separate switch for NOx fertilizer. (fp, 2/29/10)
- (29) Add scaling for isoprene and NOx emissions. (fp, 2/29/10)
- (30) Remove depreciated lightning options. (ltm, 1/25,11)
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 27 Aug 2010 R. Yantosca Added warning msg for MERRA
- 29 Jul 2011 L. Zhang Fix bug that turns off CAC/BRAVO emissions inadvertently during nested NA simulations
- 11 Aug 2011 E. Leibensperger Added flag for historical emissions and base year
- 07 Sep 2011 P. Kasibhatla Add modifications for GFED3
- 14 Feb 2012 R. Yantosca Reorganize error checks for logical switches
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 05 Apr 2012 R. Yantosca Now call INIT_MODIS_LAI
- 05 Apr 2012 R. Yantosca Reorganized USE statements for clarity
- 10 Apr 2012 R. Yantosca Bug fix: do not turn off LAVHRRLAI or LMODISLAI when emissions are turned off. LAI is used in other areas of the code.
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 01 Nov 2012 R. Yantosca Now pass Input_Opt, RC as arguments
- 22 Jul 2013 M. Sulprizio- Now copy LRCP, LRCPSHIP, LRCPAIR to Input_Opt
- 31 Jul 2013 M. Sulprizio- Now copy LAEIC to Input_Opt; Add check to make sure LAEIC and LRCPAIR are not both on
- 22 Aug 2013 R. Yantosca Now read path for soil NOx restart file
- 26 Sep 2013 R. Yantosca Remove SEAC4RS C-preprocessor switch
- 03 Oct 2013 M. Sulprizio- Removed obsolete options for LAVHRRLAI and LMODISLAI. MODIS LAI data are now read from netCDF files.
- 03 Jun 2014 R. Yantosca Radically simplify this routine since most emissions options are now specified in HEMCO
- 23 Jun 2014 R. Yantosca Remove reference to logical_mod.F
- 25 Jun 2014 R. Yantosca Move call to INIT_MODIS_LAIT to GIGC_INIT_EXTRA
- 04 Sep 2014 R. Yantosca Bug fix: Now use Input_Opt%OTDLOC since we have now removed logical_mod.F
- 24 Jun 2015 R. Yantosca Now always turn off emissions for mass cons test

```
16 Jun 2016 - K. Travis
                         - Now define species ID's with the Ind_ function
```

- 22 Jun 2016 R. Yantosca Move some error checks to DO_ERROR_CHECKS
- 20 Sep 2016 R. Yantosca Use "I4" format to read in CFCYEAR

2.2.9 read_co2_sim_menu

Subroutine READ_CO2_SIM_MENU reads the CO2 SIM MENU section of the GEOS-Chem input file.

INTERFACE:

```
SUBROUTINE READ_CO2_SIM_MENU( am_I_Root, Input_Opt, RC )
```

USES:

```
USE CMN_03_MOD
```

USE CMN_SIZE_MOD

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP ONLY : OptInput

USE Input_Opt_Mod,

INPUT PARAMETERS:

INTENT(IN) :: am_I_Root ! Is this the root CPU? LOGICAL,

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REVISION HISTORY:

```
02 Mar 2009 - R. Nassar - Initial version
```

27 Aug 2010 - R. Yantosca - Added ProTeX headers

07 Sep 2011 - P. Kasibhatla - Modified for GFED3

30 Jul 2012 - R. Yantosca - Now accept am_I_Root as an argument when

running with the traditional driver main.F

01 Nov 2012 - R. Yantosca - Now pass Input_Opt, RC as arguments

03 Jun 2014 - R. Yantosca - Now specify biomass, biofuel options in HEMCO

23 Jun 2014 - R. Yantosca - Removed references to logical_mod.F

25 Jun 2014 - R. Yantosca - Removed references to tracer_mod.F

13 Apr 2015 - R. Nassar - Simplified CO2 menu since options are now in HEMCO

2.2.10 read_future_menu

Subroutine READ_FUTURE_MENU reads the FUTURE MENU section of the GEOS-Chem input file; this defines IPCC future emissions options.

INTERFACE:

```
SUBROUTINE READ_FUTURE_MENU( am_I_Root, Input_Opt, RC )
```

USES:

```
USE ErrCode_Mod
```

USE FUTURE_EMISSIONS_MOD, ONLY : DO_FUTURE_EMISSIONS

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(OptInput), INTENT(INOUT) :: Input_Opt  ! Input options
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure
```

REVISION HISTORY:

```
01 Jun 2006 - S. Wu - Initial version
```

27 Aug 2010 - R. Yantosca - Added ProTeX headers

30 Jul 2012 - R. Yantosca - Now accept am_I_Root as an argument when running with the traditional driver main.F

01 Nov 2012 - R. Yantosca - Now pass Input_Opt, RC as arguments

20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete

23 Jun 2014 - R. Yantosca - Removed reference to logical_mod.F

2.2.11 read_chemistry_menu

Subroutine READ_CHEMISTRY_MENU reads the CHEMISTRY MENU section of the GEOS-Chem input file.

INTERFACE:

```
SUBROUTINE READ_CHEMISTRY_MENU( am_I_Root, Input_Opt, RC )
```

USES:

```
USE CMN_SIZE_MOD
```

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP
USE Input_Opt_Mod, ONLY : OptInput
USE TIME_MOD, ONLY : SET_CT_CHEM

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REVISION HISTORY:

- 20 Jul 2004 R. Yantosca Initial version
- (1) added optional test on KPPTRACER (phs, 6/17/09)
- (2) Remove reference to obsolete embedded chemistry stuff in "CMN" (bmy, 2/25/10)
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 10 Jun 2012 L. Murray Move all strat chemistry switches here
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 01 Nov 2012 R. Yantosca Now pass Input_Opt, RC as arguments
- 06 Dec 2012 R. Yantosca Now get TS_CHEM from the ESMF environment when we are connecting to the GEOS-5 GCM
- 11 Dec 2012 R. Yantosca ACCEPT_DATE_TIME_FROM_ESMF has now been renamed to ACCEPT_EXTERNAL_DATE_TIME
- 22 May 2013 M. Payer Now read in GAMMA_HO2. Recommended value is 0.2 based on Jacon et al (2000) and Mao et al (2013).
- 22 Aug 2013 R. Yantosca Now read in path for species restart file
- 25 Jun 2014 R. Yantosca Removed references to tracer_mod.F
- 27 Jul 2016 M. Sulprizio- Remove LSVCSPEC and SPEC_RST_FILE. Restart files are now always saved out and the output restart file name is hardcoded in restart_mod.F.

2.2.12 read_radiation_menu

Subroutine READ_RADIATION_MENU reads the RADIATION MENU section of the GEOS-Chem input file.

INTERFACE:

SUBROUTINE READ_RADIATION_MENU(am_I_Root, Input_Opt, RC)

USES:

USE CMN_FJX_MOD ! Fast-JX flux diagnostics

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP
USE Input_Opt_Mod, ONLY : OptInput
USE TIME_MOD, ONLY : SET_CT_RAD

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REVISION HISTORY:

```
18 Jun 2013 - D. Ridley - Initial version
```

03 Dec 2014 - M. Sulprizio- Now save fields to the Input_Opt object

10 Dec 2014 - M. Sulprizio- Add error checks for RRTMG switches

2.2.13 read_transport_menu

Subroutine READ_TRANSPORT_MENU reads the TRANSPORT MENU section of the GEOS-Chem input file.

INTERFACE:

SUBROUTINE READ_TRANSPORT_MENU(am_I_Root, Input_Opt, RC)

USES:

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP USE Input_Opt_Mod, ONLY : OptInput

#if !defined(ESMF_)

USE TRANSPORT_MOD, ONLY : SET_TRANSPORT

#endif

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

- 20 Jul 2004 R. Yantosca Initial version

 (1) Now define MAX_DYN for 1 x 1.25 grid (bmy, 12/1/04)

 (2) Update text in error message (bmy, 2/23/05)

 (3) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)

 (4) Don't stop run if TS DYN > MAX_DYN but transport is turned of
- (4) Don't stop run if TS_DYN > MAX_DYN but transport is turned off (cdh, bmy, 7/7/08)
- (5) Set MAX_DYN for the 0.5 x 0.666 nested grid (yxw, dan, bmy, 11/6/08)
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 10 Jun 2012 L. Murray Move strat to chemistry menu
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 01 Nov 2012 R. Yantosca Now pass Input_Opt, RC as arguments
- 06 Dec 2012 R. Yantosca Now get TS_DYN from the ESMF environment, if we are connecting to the GEOS-5 GCM
- 11 Dec 2012 R. Yantosca ACCEPT_DATE_TIME_FROM_ESMF has now been renamed to ACCEPT_EXTERNAL_DATE_TIME
- 03 Oct 2013 M. Sulprizio- Removed obsolete option for flux correction. This was used for GEOS-3, which has been retired.
- 23 Jun 2014 R. Yantosca Removed references to logical_mod.F
- 25 Jun 2014 R. Yantosca Removed references to tracer_mod.F
- 20 Sep 2016 R. Yantosca Use "I8" format for write statement

2.2.14 read_convection_menu

Subroutine READ_CONVECTION_MENU reads the CONVECTION MENU section of the GEOS-Chem input file.

INTERFACE:

SUBROUTINE READ_CONVECTION_MENU(am_I_Root, Input_Opt, RC)

USES:

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP

USE FVDAS_CONVECT_MOD, ONLY : INIT_FVDAS_CONVECT

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REVISION HISTORY:

- 20 Jul 2004 R. Yantosca Initial version
- (1) Add option for new non-local PBL scheme. And a check on GEOS-5, LNLPBL turned to false if GEOS-5 is not used (lin, ccc 5/13/09)
- 27 Aug 2010 R. Yantosca Now allow non-local PBL for MERRA met data
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 02 Feb 2012 R. Yantosca Added modifications for MERRA met data
- 13 Apr 2012 R. Yantosca Fixed typo (defined(GEOS_FP) should have been !defined(GEOS_FP))
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 01 Nov 2012 R. Yantosca Now pass Input_Opt, RC as arguments
- 01 Mar 2013 R. Yantosca Now set TS_CONV to the same value as TS_DYN when connecting to the GEOS-5 GCM.
- 12 Aug 2015 R. Yantosca Now allow non-local PBL mixing for MERRA2 met

2.2.15 read_deposition_menu

Subroutine READ_DEPOSITION_MENU reads the DEPOSITION MENU section of the GEOS-Chem input file.

INTERFACE:

SUBROUTINE READ_DEPOSITION_MENU(am_I_Root, Input_Opt, RC)

USES:

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

- 20 Jul 2004 R. Yantosca Initial version
- (1) Now print an informational message for tagged Hg (bmy, 12/15/04)
- (2) We need to call WETDEPID for both wetdep and cloud convection since this sets up the list of soluble tracers (bmy, 3/1/05)

- (3) Remove references to obsolete CO_OH simulation (bmy, 6/24/05)
- (4) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 16 Feb 2011 R. Yantosca Add modifications for APM from G. Luo
- 31 Jul 2012 R. Yantosca Now pass am_I_Root to INIT_DRYDEP
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 01 Nov 2012 R. Yantosca Now pass Input_Opt, RC as arguments
- 26 Feb 2013 R. Yantosca Now call INIT_DUST jere to facilitate connecting to the GEOS-5 GCM
- 23 Jun 2014 R. Yantosca Removed references to logical_mod.F
- 25 Jun 2014 R. Yantosca Removed references to tracer_mod.F
- 25 Jun 2014 R. Yantosca Now set USE_OLSON_2001 = T for GEOS-FP met; this was originally done in INIT_INPUT
- 05 Mar 2015 C. Keller Added PBL_DRYDEP to define if dry deposition rates are calculated over full PBL or 1st model level only.

 Set to .TRUE. (full PBL) if full PBL mixing is used, to false otherwise.

2.2.16 read_gamap_menu

Subroutine READ_GAMAP_MENU reads the GAMAP MENU section of the GEOS-Chem input file.

INTERFACE:

SUBROUTINE READ_GAMAP_MENU(am_I_Root, Input_Opt, RC)

USES:

USE ErrCode_Mod

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

```
25 Apr 2005 - R. Yantosca - Initial version
27 Aug 2010 - R. Yantosca - Added ProTeX headers
30 Jul 2012 - R. Yantosca - Now accept am_I_Root as an argument when running with the traditional driver main.F
01 Nov 2012 - R. Yantosca - Now pass Input_Opt, RC as arguments
```

2.2.17 read_output_menu

Subroutine READ_OUTPUT_MENU reads the OUTPUT MENU section of the GEOS-Chem input file.

INTERFACE:

```
SUBROUTINE READ_OUTPUT_MENU( am_I_Root, Input_Opt, RC )
```

USES:

```
USE CMN_DIAG_MOD ! NJDAY
```

USE CMN_SIZE_MOD ! Size parameters

USE ErrCode_Mod

USE FILE_MOD, ONLY : IOERROR
USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

2.2.18 read_diagnostic_menu

Subroutine READ_DIAGNOSTIC_MENU reads the DIAGNOSTIC MENU section of the GEOS-Chem input file.

INTERFACE:

SUBROUTINE READ_DIAGNOSTIC_MENU(am_I_Root, Input_Opt, RC)

USES:

```
USE BPCH2_MOD,
                   ONLY : OPEN_BPCH2_FOR_WRITE
USE CMN_DIAG_MOD
                        ! NDxx flags, TINDEX, TCOUNT, TMAX
USE CMN_SIZE_MOD
                        ! Size parameters
USE DIAGO3_MOD,
                  ONLY : NDO3,
                                    PD03
USE DIAGO3_MOD,
                  ONLY : PDO3_PL
                                    !eds 9/9/10
USE DIAGO4_MOD,
                  ONLY : NDO4,
                                    PD04,
                                               INIT_DIAGO4
USE DIAG41_MOD,
                  ONLY : ND41,
                                    PD41,
                                               INIT_DIAG41
USE DIAG42_MOD,
                  ONLY: ND42,
                                              INIT_DIAG42
                                    PD42,
USE DIAG53_MOD,
                  ONLY : ND53,
                                               INIT_DIAG53
                                    PD53,
USE DIAG56_MOD,
                  ONLY : ND56,
                                               INIT_DIAG56
                                    PD56,
USE DRYDEP_MOD,
                  ONLY: NUMDEP
USE ErrCode_Mod
USE ERROR_MOD,
                  ONLY : ERROR_STOP
USE FILE_MOD,
                  ONLY : IU_BPCH
USE Input_Opt_Mod, ONLY : OptInput
USE TIME_MOD,
                  ONLY: GET_NYMDb, GET_NHMSb, EXPAND_DATE
```

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

- 20 Jul 2004 R. Yantosca Initial version
- (1) Now reference IU_BPCH from "file_mod.f" and OPEN_BPCH2_FOR_WRITE from "bpch2_mod.f". Now opens the bpch file for output here instead of w/in "main.f" (bmy, 2/3/05)
- (2) Now references "diag03_mod.f" and "diag41_mod.f". Now turn off ND38 when both LWETD=F and LCONV=F. Now calls EXPAND_DATE to replace YYYYMMDD and HHMMSS tokens in the bpch file name with the actual starting date & time of the run. (bmy, 3/25/05)
- (3) Now get diag info for ND09 for HCN/CH3CN sim (bmy, 6/27/05)
- (4) Now references "diag04_mod.f" (bmy, 7/26/05)

- (5) Now make sure all USE statements are USE, ONLY. Also remove reference to DIAG_MOD, it's not needed. (bmy, 10/3/05)
- (6) Now remove reference to NBIOTRCE; Replace w/ NBIOMAX. (bmy, 4/5/06)
- (7) Now reference ND56, PD56, INIT_DIAG56 from "diag56_mod.f" (bmy, 5/10/06)
- (8) Now reference ND42, PD42, INIT_DIAG42 from "diag42_mod.f" (dkh, bmy, 5/22/06)
- (9) Now set max dimension for GFED2 or default biomass (bmy, 9/22/06)
- (10) Bug fix: Should use ND52 in call to SET_TINDEX (cdh, bmy, 2/11/08)
- (11) Remove call to NDXX_SETUP; this is now called in READ_INPUT_FILE. (phs, 11/18/08)
- (12) Now set TINDEX with PD45=NNPAR+1 tracers instead of N_TRACERS. (tmf, 2/10/09)
- (13) NBIOMAX now in CMN_SIZE (fp, 6/2009)
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 26 May 2011 R. Yantosca For ND17, ND18, ND37, ND38, ND39, we need to set N_TMP = N_TRACERS, or else wetdep tracers with indices higher than #32 won't print out.
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 01 Nov 2012 R. Yantosca Now pass Input_Opt, RC as arguments
- 06 Mar 2013 H. Amos merge C. Friedman's POP code
- 08 Nov 2013 M. Sulprizio- Remove HR1_NO, and HR2_NO from ND43 diagnostic.
- 03 Feb 2014 R. Yantosca Remove references to TINDEX, TCOUNT, and TMAX from diag_mod. They are in CMN_SIZE_mod.F.

 Lee Murray reports this causes the compilation to choke on Macintosh platforms.
- 23 Jun 2014 R. Yantosca Now pass Input_Opt, RC to INIT_DIAG_OH
- 24 Jun 2014 R. Yantosca Removed references to logical_mod.F
- 25 Jun 2014 R. Yantosca Removed references to tracer_mod.F
- 15 Dec 2014 M. Sulprizio- Moved radiation diagnostic from ND71 to ND72 to avoid conflicts with hourly max ppbv diagnostic.
- 15 Jan 2015 R. Yantosca Now define Input_Opt%DIAG_COLLECTION
- 22 May 2015 R. Yantosca Remove variables made obsolete by HEMCO
- 23 Jun 2016 R. Yantosca Now call INIT_DIAG_OH from GIGC_Init_Extra
- 20 Jul 2016 R. Yantosca Remove references to NNPAR

2.2.19 set_tindex

Subroutine SET_TINDEX sets the TINDEX and TMAX arrays, which determine how many tracers to print to the punch file.

INTERFACE:

USES:

```
#if defined( TOMAS )
        USE CHARPAK_MOD, ONLY : TXTEXT ! (win, 7/14/09)
#endif
```

USE CMN_DIAG_MOD ! TMAX, TINDEX
USE CMN_SIZE_MOD ! Size parameters

INPUT PARAMETERS:

INTENT(IN) :: am_I_Root ! Is this the root CPU?

REVISION HISTORY:

LOGICAL,

```
20 Jul 2004 - R. Yantosca - Initial version
(1 ) Bug fix: now do not drop the last tracer number if "all" is not
        explicitly specified (tmf, bmy, 11/15/04)
27 Aug 2010 - R. Yantosca - Added ProTeX headers
```

2.2.20 read_planeflight_menu

Subroutine READ_PLANEFLIGHT_MENU reads the PLANEFLIGHT MENU section of the GEOS-Chem input file. This turns on the ND40 flight track diagnostic.

INTERFACE:

```
SUBROUTINE READ_PLANEFLIGHT_MENU( am_I_Root, Input_Opt, RC )
```

USES:

USE CMN_DIAG_MOD ! ND40
USE CMN_SIZE_MOD ! MAXFAM

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP
USE Input_Opt_Mod, ONLY : OptInput

USE PLANEFLIGHT_MOD, ONLY : SET_PLANEFLIGHT

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REVISION HISTORY:

- 20 Jul 2004 R. Yantosca Initial version
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 01 Nov 2012 R. Yantosca Now pass Input_Opt, RC as arguments

2.2.21 read_nd48_menu

Subroutine READ_ND48_MENU reads the ND48 MENU section of the GEOS-Chem input file

INTERFACE:

SUBROUTINE READ_ND48_MENU(am_I_Root, Input_Opt, RC)

USES:

USE DIAG48_MOD, ONLY: INIT_DIAG48, ND48_MAX_STATIONS

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

- 20 Jul 2004 R. Yantosca Initial version
- (1) Bug fix: ND48 stations should now be read correctly. (bmy, 3/6/06)
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 01 Nov 2012 R. Yantosca Now pass Input_Opt, RC as arguments

2.2.22 read_nd49_menu

Subroutine READ_ND49_MENU reads the ND49 MENU section of the GEOS-Chem input file.

INTERFACE:

SUBROUTINE READ_ND49_MENU(am_I_Root, Input_Opt, RC)

USES:

USE CMN_SIZE_MOD

USE DIAG49_MOD, ONLY: INIT_DIAG49

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REVISION HISTORY:

20 Jul 2004 - R. Yantosca - Initial version

27 Aug 2010 - R. Yantosca - Added ProTeX headers

30 Jul 2012 - R. Yantosca - Now accept am_I_Root as an argument when

running with the traditional driver main.F

01 Nov 2012 - R. Yantosca - Now pass Input_Opt, RC as arguments

2.2.23 read_nd50_menu

Subroutine READ_ND50_MENU reads the ND50 MENU section of the GEOS-Chem input file.

INTERFACE:

SUBROUTINE READ_ND50_MENU(am_I_Root, Input_Opt, RC)

USES:

USE DIAG50_MOD, ONLY : INIT_DIAG50

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REVISION HISTORY:

- 20 Jul 2004 R. Yantosca Initial version
- (1) Now include option to save ND51 diagnostic to HDF5 file format (amv, bmy, 12/21/09)
- (2) Increase tracer number to 121. (ccc, 4/20/10)
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 01 Nov 2012 R. Yantosca Now pass Input_Opt, RC as arguments
- 23 Jun 2014 R. Yantosca Removed references to logical_mod.F

2.2.24 read_nd51_menu

Subroutine READ_ND51_MENU reads the ND51 MENU section of the GEOS-Chem input file.

INTERFACE:

SUBROUTINE READ_ND51_MENU(am_I_Root, Input_Opt, RC)

USES:

USE CMN_DIAG_MOD

USE CMN_SIZE_MOD

USE DIAG51_MOD, ONLY : INIT_DIAG51

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REVISION HISTORY:

- 20 Jul 2004 R. Yantosca Initial version
- (1) Now include option to save ND51 diagnostic to HDF5 file format (amv, bmy, 12/21/09)
- (2) Increase # of tracers to 121 (ccc, 4/20/10)
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 01 Nov 2012 R. Yantosca Now pass Input_Opt, RC as arguments
- 23 Jun 2014 R. Yantosca Removed references to logical_mod.F

2.2.25 read_nd51b_menu

Subroutine READ_ND51b_MENU reads the ND51 MENU section of the GEOS-Chem input file.

INTERFACE:

SUBROUTINE READ_ND51b_MENU(am_I_Root, Input_Opt, RC)

USES:

USE CMN_DIAG_MOD

USE CMN_SIZE_MOD

USE DIAG51b_MOD, ONLY : INIT_DIAG51b

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

- 21 Dec 2009 Aaron van D Initial version
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 01 Nov 2012 R. Yantosca Now pass Input_Opt, RC as arguments
- 23 Jun 2014 R. Yantosca Removed references to logical_mod.F

2.2.26 read_nd63_menu

Subroutine READ_ND63_MENU reads the ND63 MENU section of the GEOS-Chem input file. (gvinken, 02/25/11)

INTERFACE:

```
SUBROUTINE READ_ND63_MENU( am_I_Root, Input_Opt, RC )
```

USES:

```
USE CMN_SIZE_MOD
```

USE DIAG63_MOD, ONLY: INIT_DIAG63

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER. INTENT(OUT) :: RC ! Success or failure

REVISION HISTORY:

```
25 Feb 2011 - G. Vinken - Initial version
```

07 Feb 2012 - M. Payer - Added ProTeX headers

24 Feb 2012 - M. Payer - Renamed routine from READ_ND59_MENU to READ_ND63 MENU. ND59 is used by TOMAS.

30 Jul 2012 - R. Yantosca - Now accept am_I_Root as an argument when

running with the traditional driver main.F

01 Nov 2012 - R. Yantosca - Now pass Input_Opt, RC as arguments

20 Sep 2016 - R. Yantosca - Fixed typo (N_ND63 instead of ND63) when

saving to Input_Opt%ND63_TRACERS

2.2.27 read_prod_loss_menu

Subroutine READ_PROD_LOSS_MENU reads the PROD AND LOSS MENU section of the GEOS-Chem input file

INTERFACE:

SUBROUTINE READ_PROD_LOSS_MENU(am_I_Root, Input_Opt, RC)

USES:

USE CMN_DIAG_MOD

USE CMN_SIZE_MOD

USE CHARPAK_MOD, ONLY : ISDIGIT, STRSPLIT

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP

USE gckpp_Parameters, ONLY : NFAM

USE gckpp_Monitor, ONLY : FAM_NAMES
USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REVISION HISTORY:

20 Jul 2004 - R. Yantosca - Initial version

- (1) Bug fixes. Only error check # of prod/loss families for TagOx and TagCO runs if DO_SAVE_PL=T. Also turn off this diagnostic for the offline aerosol run. (bmy, 10/29/04)
- (2) Add error trap is P/L families are asked when using KPP. (ccc, 3/10/10)
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 08 Nov 2012 R. Yantosca Now save fields to the Input_Opt object
- 23 Jun 2014 R. Yantosca Removed references to logical_mod.F
- 25 Jun 2014 R. Yantosca Removed references to tracer_mod.F
- 14 Jan 2016 C. Keller Now refer to Input_Opt%LKPP instead of LKPP

2.2.28 read_unix_cmds_menu

Subroutine READ_UNIX_CMDS_MENU reads the UNIX CMDS MENU section of the GEOS-Chem input file.

INTERFACE:

SUBROUTINE READ_UNIX_CMDS_MENU(am_I_Root, Input_Opt, RC)

USES:

USE CHARPAK_MOD, ONLY : STRSQUEEZE

USE ErrCode_Mod

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REVISION HISTORY:

- 20 Jul 2004 R. Yantosca Initial version
- (1) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 01 Nov 2012 R. Yantosca Now pass Input_Opt, RC as arguments
- 20 Jun 2014 R. Yantosca Remove reference to unix_cmds_mod.F

2.2.29 read_nested_grid_menu

Subroutine READ_NESTED_GRID_MENU reads the NESTED GRID MENU section of the GEOS-CHEM input file.

INTERFACE:

SUBROUTINE READ_NESTED_GRID_MENU(am_I_Root, Input_Opt, RC)

USES:

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

```
20 Jul 2004 - R. Yantosca - Initial version
```

- (1) Now give user the option of saving out nested grid boundary conditions at 2×2.5 resolution for the EU, CH, or NA grids (amv, bmy, 12/18/09)
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 01 Nov 2012 R. Yantosca Now pass Input_Opt, RC as arguments
- 23 Jun 2014 R. Yantosca Removed references to logical_mod.F

2.2.30 read benchmark menu

Subroutine READ_BENCHMARK_MENU reads the BENCHMARK MENU section of the GEOS-Chem input file.

INTERFACE:

SUBROUTINE READ_BENCHMARK_MENU(am_I_Root, Input_Opt, RC)

USES:

USE BENCHMARK_MOD, ONLY: INITIAL_FILE, FINAL_FILE

USE ErrCode_Mod

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

- 20 Jul 2004 R. Yantosca Initial version
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 01 Nov 2012 R. Yantosca Now pass Input_Opt, RC as arguments
- 23 Jun 2014 R. Yantosca Removed references to logical_mod.F

2.2.31 read_mercury_menu

Subroutine READ_MERCURY_MENU reads the BENCHMARK MENU section of the GEOS-Chem input file.

INTERFACE:

```
SUBROUTINE READ_MERCURY_MENU( am_I_Root, Input_Opt, RC )
```

USES:

```
USE ErrCode_Mod
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure
```

REVISION HISTORY:

```
24 Feb 2006 - R. Yantosca - Initial version
```

- (1) Update for Chris Holmes's mercury version. (ccc, 5/6/10)
- (2) Add options to use GTMM for mercury soil emissions (ccc, 9/16/09)
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 01 Nov 2012 R. Yantosca Now pass Input_Opt, RC as arguments
- 23 Jun 2014 R. Yantosca Removed references to logical_mod.F
- 25 Jun 2014 R. Yantosca Removed references to tracer_mod.F
- 25 Apr 2016 R. Yantosca Now init mercury modules from GIGC_INIT_EXTRA
- 27 Jul 2016 M. Sulprizio- Remove IN_HG_RST_FILE and OUT_HG_RST_FILE.

Hg restart fields are now stored in the GEOS-Chem netCDF restart file.

2.2.32 read ch4 menu

Subroutine READ_CH4_MENU reads the CH4 MENU section of the GEOS-Chem input file; this defines emissions options for CH4 tagged simulations.

INTERFACE:

```
SUBROUTINE READ_CH4_MENU( am_I_Root, Input_Opt, RC )
```

USES:

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

03 Aug 2009 - K. Wecht, C. Pickett-Heaps - Initial version

27 Aug 2010 - R. Yantosca - Added ProTeX headers

30 Jul 2012 - R. Yantosca - Now accept am_I_Root as an argument when running with the traditional driver main.F

01 Nov 2012 - R. Yantosca - Now pass Input_Opt, RC as arguments

20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete

19 Feb 2014 - R. Yantosca - Add warning for CH4 budget (which is now

controlled by an #ifdef in global_ch4_mod.F)

23 Jun 2014 - R. Yantosca - Removed references to logical_mod.F

20 Sep 2016 - R. Yantosca - Rewrote IF statement to avoid Gfortran error

2.2.33 read_pops_menu

Subroutine READ_POPS_MENU reads the POPS MENU section of the GEOS-Chem input file; this defines emissions options for POPs simulations.

INTERFACE:

SUBROUTINE READ_POPS_MENU(am_I_Root, Input_Opt, RC)

USES:

USE ErrCode_Mod

USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

```
01 Oct 2012 - C. Friedman - Initial version
26 Nov 2012 - M. Payer - Added ProTeX headers
29 Nov 2012 - M. Payer - Now pass Input_Opt, RC as arguments
26 Mar 2013 - R. Yantosca - Now pass Input_Opt to INIT_POPS
14 Apr 2014 - R. Yantosca - Now echo all POPs parameters to log file
23 Jun 2014 - R. Yantosca - Now use Input_Opt%POP_EMISDIR
25 Aug 2014 - M. Sulprizio- Move call to INIT_POPs to GIGC_Init_Extra
27 Aug 2014 - M. Sulprizio- Remove POP_EMISDIR, emissions are now handled by HEMCO
```

2.2.34 read_passive_tracer_menu

Subroutine READ_PASSIVE_TRACER_MENU reads the passive tracer MENU section of the GEOS-Chem input file; this defines passive tracers to be used for this simulation.

INTERFACE:

SUBROUTINE READ_PASSIVE_TRACER_MENU(am_I_Root, Input_Opt, RC)

USES:

```
USE ErrCode_Mod
```

USE Input_Opt_Mod, ONLY : OptInput

USE PASSIVE_TRACER_MOD, ONLY : INIT_PASSIVE_TRACER USE PASSIVE_TRACER_MOD, ONLY : ADD_PASSIVE_TRACER

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input options

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

04 Sep 2015 - C. Keller - Initial version

2.2.35 validate_directories

Subroutine VALIDATE_DIRECTORIES makes sure that each of the directories that we have read from the GEOS-Chem input file are valid. Also, trailing separator characters will be added.

INTERFACE:

SUBROUTINE VALIDATE_DIRECTORIES(am_I_Root, Input_Opt, RC)

USES:

```
USE ErrCode_Mod
```

USE Input_Opt_Mod, ONLY : OptInput

USE GC_GRID_MOD, ONLY : ITS_A_NESTED_GRID

USE TIME_MOD, ONLY : EXPAND_DATE
USE TIME_MOD, ONLY : GET_NYMDb
USE TIME_MOD, ONLY : GET_NYMDe

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input Options object

OUTPUT PARAMETERS:

INTEGER. INTENT(OUT) :: RC ! Success or failure?

- 20 Jul 2004 R. Yantosca Initial version
- (1) Now make sure all USE statements are USE, ONLY. Now also validate GCAP and GEOS-5 directories. (bmy, 10/3/05)
- (2) Now references DATA_DIR_1x1 from directory_mod.f (bmy, 10/24/05)
- (3) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (4) Now check TPBC_DIR_NA, TPBC_DIR_CH, TPBC_DIR_EU (amv, bmy, 12/18/09)
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 27 Aug 2010 R. Yantosca Now check MERRA directory
- 08 Feb 2012 R. Yantosca Now check GEOS-5.7.x directory
- 09 Feb 2012 R. Yantosca Rewrote USE statements for clarity
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 20 Jun 2014 R. Yantosca Now use fields from Input_Opt
- 05 Mar 2015 R. Yantosca Now also check CHEM_INPUTS_DIR
- 12 Aug 2015 R. Yantosca Now validate Input_Opt%MERRA2_DIR

2.2.36 check_directory

Subroutine CHECK_DIRECTORY makes sure that the given directory is valid. Also a trailing slash character will be added if necessary.

INTERFACE:

```
SUBROUTINE CHECK_DIRECTORY( Input_Opt, DIR )
```

USES:

```
USE ERROR_MOD, ONLY : ERROR_STOP
USE FILE_MOD, ONLY : FILE_EXISTS
USE Input_Opt_Mod, ONLY : OptInput
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(OptInput), INTENT(INOUT) :: Input_Opt  ! Input Options object
CHARACTER(LEN=*), INTENT(INOUT) :: DIR     ! Dir to be checked
```

REVISION HISTORY:

```
20 Mar 2003 - R. Yantosca - Initial version
(1 ) Now references FILE_EXISTS from "file_mod.f" (bmy, 3/23/05)
27 Aug 2010 - R. Yantosca - Added ProTeX headers
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
20 Jun 2014 - R. Yantosca - Now added Input_Opt object via arg list
```

2.2.37 check_time_steps

Subroutine CHECK_TIME_STEPS computes the smallest dynamic time step for the model, based on which operation are turned on. This is called from routine READ_INPUT_FILE, after all of the timesteps and logical flags have been read from "input.geos".

INTERFACE:

```
SUBROUTINE CHECK_TIME_STEPS( am_I_Root, Input_Opt, RC )
```

USES:

```
USE ERROR_MOD, ONLY : GEOS_CHEM_STOP
USE Input_Opt_Mod, ONLY : OptInput
USE TIME_MOD, ONLY : SET_TIMESTEPS
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

- 20 Jul 2004 R. Yantosca Initial version
- (1) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (2) Add TS_DIAG, the largest time steps used for diagnostics. And test that all time steps are multiple of the smallest one. (ccc, 5/13/09)
- (3) Corrected typos -99999 instead of -999999 (phs, bmy, 8/21/09)
- (4) Now compute TS_SUN_2 which is 1/2 of the chemistry timestep (or smallest timestep if LCHEM=LEMIS=LDRYD=F). This is used to compute SUNCOS at the midpoint of the timestep instead of the beginning. (bmy, 4/27/10)
- 27 Aug 2010 R. Yantosca Added ProTeX headers
- 07 Oct 2011 R. Yantosca Add extra error checks for centralizing chemistry timestep algorithm
- 07 Oct 2011 R. Yantosca Remove TS_SUN_2 from call to SET_TIMESTEPS
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 23 Jun 2014 R. Yantosca Removed references to logical_mod.F

2.2.38 is_last_day_good

Suborutine IS_LAST_DAY_GOOD tests to see if there is output scheduled on the last day of the run.

INTERFACE:

SUBROUTINE IS_LAST_DAY_GOOD

USES:

USE CMN_DIAG_MOD

USE CMN_SIZE_MOD

USE ERROR_MOD, ONLY : ERROR_STOP USE JULDAY_MOD, ONLY : JULDAY

USE TIME_MOD, ONLY: GET_NYMDe, ITS_A_LEAPYEAR, YMD_EXTRACT

- 20 Jul 2004 R. Yantosca Initial version
- (1) Moved to "input_mod.f" from "main.f" (bmy, 1/11/05)
- (2) Now call ITS_A_LEAPYEAR with FORCE=.TRUE. to always return whether the year Y would be a leap year, regardless of met field type. (swu, bmy, 4/24/06)
- 27 Aug 2010 R. Yantosca Added ProTeX headers

2.2.39 gc_init_extra

Suborutine GC_INIT_EXTRA initializes other GEOS-Chem modules that have not been initialized in either GC_Allocate_All or GC_Init_all.

INTERFACE:

SUBROUTINE GC_Init_Extra(am_I_Root, Input_Opt, State_Chm, RC)

USES:

```
USE Aerosol_Mod,
                        ONLY : Init_Aerosol
USE Carbon_Mod,
                        ONLY : Init_Carbon
USE CO2_Mod,
                        ONLY : Init_CO2
USE C2H6_Mod,
                       ONLY: Init_C2H6
USE Chemgrid_Mod,
                        ONLY : Init_Chemgrid
USE Depo_Mercury_Mod,
                        ONLY : Init_Depo_Mercury
USE Diag03_Mod,
                        ONLY: Init_Diag03
                        ONLY : Init_Diag20
USE Diag20_Mod,
USE Diag_OH_Mod,
                        ONLY : Init_Diag_OH
USE Drydep_Mod,
                        ONLY : Init_Drydep
                        ONLY : Init_Dust
USE Dust_Mod,
USE ErrCode_Mod
USE Error_Mod,
                        ONLY : Debug_Msg
USE Gamap_Mod,
                        ONLY : Do_Gamap
                        ONLY : Init_Get_Ndep
USE Get_Ndep_Mod,
USE Global_CH4_Mod,
                        ONLY : Init_Global_CH4
USE Input_Opt_Mod,
                        ONLY : OptInput
USE Linoz_Mod,
                        ONLY : Init_Linoz
USE Land_Mercury_Mod,
                        ONLY : Init_Land_Mercury
USE Mercury_Mod,
                        ONLY : Init_Mercury
                        ONLY : Init_Modis_Lai
USE Modis_Lai_Mod,
USE Ocean_Mercury_Mod, ONLY : Init_Ocean_Mercury
                        ONLY : Init_POPs
USE POPs_Mod,
USE Seasalt_Mod,
                        ONLY : Init_SeaSalt
USE State_Chm_Mod,
                        ONLY : ChmState
USE Sulfate_Mod,
                        ONLY : Init_Sulfate
USE Tagged_CO_Mod,
                        ONLY: Init_Tagged_CO
USE Tagged_03_Mod,
                        ONLY : Init_Tagged_03
USE Toms_Mod,
                        ONLY : Init_Toms
USE TPCORE_BC_Mod,
                        ONLY : Init_TPCORE_BC
USE Vdiff_Pre_Mod,
                        ONLY : Set_Vdiff_Values
USE WetScav_Mod,
                        ONLY : Init_WetScav
```

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

INPUT/OUTPUT PARAMETERS:

```
TYPE(OptInput), INTENT(INOUT) :: Input_Opt   ! Input Options object
TYPE(ChmState), INTENT(INOUT) :: State_Chm   ! Chemistry state object
```

INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

Several of the INIT routines now called within GC_Init_Extra had originally been called from the Run method. We now gather these INIT routines here so that they may be called from the Initialization method. This is necessary when connecting GEOS-Chem to the GEOS-5 GCM via ESMF.

GC_Init_Extra should be called after the call to DO_DRYDEP, since these routines depend on dry deposition parameters being set up first.

REVISION HISTORY:

```
04 Mar 2013 - R. Yantosca - Initial revision
05 Mar 2013 - R. Yantosca - Now call INIT_AEROSOL (GeosCore/aerosol_mod.F)
15 Mar 2013 - R. Yantosca - Now call INIT_LINOZ (GeosCore/linoz_mod.F)
29 Mar 2013 - R. Yantosca - Now call INIT_TROPOPAUSE (so that we can pass
                            a LVARTROP from Input_Opt and not logical_mod.F)
10 Apr 2014 - R. Yantosca - Now call INIT_TAGGED_CO
10 Apr 2014 - R. Yantosca - Now call INIT_TAGGED_OX and INIT_GLOBAL_CH4 \,
11 Apr 2014 - R. Yantosca - Now call INIT_C2H6 and INIT_HCN_CH3CN
14 Apr 2014 - R. Yantosca - Also call INIT_C2H6 if it's a fullchem sim
                            since we read C2H6 emissions from c2h6_mod.F
25 Jun 2014 - R. Yantosca - Now call INIT_MODIS_LAI
25 Jun 2014 - R. Yantosca - Now call SET_VDIFF_VALUES (vdiff_pre_mod.F90)
25 Aug 2014 - M. Sulprizio- Now call INIT_POPS
16 Mar 2015 - R. Yantosca - Now call INIT_TOMS here
28 Aug 2015 - R. Yantosca - Now initialize drydep & wetdep here, so that
                            we can take advantage of the species database
03 Sep 2015 - R. Yantosca - Now call INIT_WETSCAV instead of WETDEPID
21 Sep 2015 - R. Yantosca - Now pass State_Chm to INIT_POPS
22 Sep 2015 - R. Yantosca - Bug fix: only call INIT_WETSCAV if convection,
                            wetdep, or chemistry ist turned on.
                            replicates the prior behavior,
23 Sep 2015 - R. Yantosca - Now pass State_Chm to INIT_SEASALT
23 Sep 2015 - R. Yantosca - Now pass State_Chm to INIT_SULFATE
25 Apr 2016 - R. Yantosca - Now call INIT_DIAGO3 here
25 Apr 2016 - R. Yantosca - Now initialize all mercury modules from here
23 Jun 2016 - R. Yantosca - Now call INIT_DIAG_OH from here
16 Aug 2016 - M. Sulprizio- Rename from GIGC_Init_Extra to GC_Init_Extra.
                            The "gigc" nomenclature is no longer used.
```

2.2.40 do_error_checks

Makes sure that certain species are defined in order to proceed with a certain option. Halts the simulation with an error message if incorrect inputs would have caused a simulation to crash.

INTERFACE:

SUBROUTINE Do_Error_Checks(am_I_root, Input_Opt, RC)

USES:

USE ErrCode_Mod

USE Error_Mod, ONLY : Error_Stop
USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : Ind_

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC

REMARKS:

These error checks were originally called when the various menus were read in from disk. However, in order to use the Ind_() function to look up given species indices, we need to call this after the Species Database (which is in State_Chm) is initialized. Therefore, we have now moved these error checks to this routine, which is now called from GC_Init_Extra.

The Ind_() function now defines all species ID's. It returns -1 if a species cannot be found. The prior behavior was to return 0 if a species wasn't found. Therefore, in order to preserve the logic of the error checks, we must force any -1's returned by Ind_() to 0's in this subroutine.

REVISION HISTORY:

22 Jun 2016 - R. Yantosca - Initial version

$2.3 \quad Fortran: \ Module \ Interface \ gc_environment_mod.F90$

Module GC_ENVIRONMENT_MOD establishes the runtime environment for the GEOS-Chem. It is designed to receive model parameter and geophysical environment information and allocate memory based upon it.

It provides routines to do the following:

• Allocate geo-spatial arrays

- Initialize met. field derived type.
- Initialize Chemistry, Metorology, Emissions, and Physics States

INTERFACE:

```
MODULE GC_Environment_Mod
!USES

IMPLICIT NONE
PRIVATE
```

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: GC_Allocate_All
PUBLIC :: GC_Init_All

REMARKS:

For consistency, we should probably move the met state initialization to the same module where the met state derived type is contained.

REVISION HISTORY:

```
26 Jan 2012 - M. Long - Created module file

13 Aug 2012 - R. Yantosca - Added ProTeX headers

19 Oct 2012 - R. Yantosca - Removed routine INIT_LOCAL_MET, this is now handled in Headers/gigc_state_met_mod.F90

22 Oct 2012 - R. Yantosca - Renamed to gigc_environment_mod.F90

20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete

28 Aug 2015 - R. Yantosca - Remove Get_nSchm_nSchmBry; stratospheric chemistry fields are now read by HEMCO

16 Aug 2016 - M. Sulprizio- Rename from gigc_environment_mod.F90 to gc_environment_mod.F90. The "gigc" nomenclature is no longer used.
```

2.3.1 gc_allocate_all

Subroutine GC_ALLOCATE_ALL allocates all LAT/LON ALLOCATABLE arrays for global use by the GEOS-Chem either as a standalone program or module.

INTERFACE:

USES:

USE CMN_DIAG_Mod, ONLY : Init_CMN_DIAG
USE CMN_FJX_MOD, ONLY : Init_CMN_FJX
USE CMN_03_Mod, ONLY : Init_CMN_03
USE CMN_SIZE_Mod, ONLY : Init_CMN_SIZE

USE ErrCode_Mod

USE Input_Opt_Mod

IMPLICIT NONE

INPUT PARAMETERS:

LOGICAL,	INTENT(IN)	:: am_I_Root	! Are we on the root CPU?
INTEGER,	OPTIONAL	:: value_I_LO	! Min local lon index
INTEGER,	OPTIONAL	:: value_J_LO	! Min local lat index
INTEGER,	OPTIONAL	:: value_I_HI	! Max local lon index
INTEGER,	OPTIONAL	:: value_J_HI	! Max local lat index
INTEGER,	OPTIONAL	:: value_IM	! Local # of lons
INTEGER,	OPTIONAL	:: value_JM	! Local # of lats
INTEGER,	OPTIONAL	:: value_LM	! Local # of levels
INTEGER,	OPTIONAL	:: value_IM_WORLD	! Global # of lons
INTEGER,	OPTIONAL	:: value_JM_WORLD	! Global # of lats
INTEGER,	OPTIONAL	:: value_LM_WORLD	! Global # of levels

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input Options object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

For error checking, return up to the main routine w/ an error code. This can be improved upon later.

REVISION HISTORY:

```
26 Jan 2012 - M. Long - Initial version

13 Aug 2012 - R. Yantosca - Added ProTeX headers

17 Oct 2012 - R. Yantosca - Add am_I_Root, RC as arguments

22 Oct 2012 - R. Yantosca - Renamed to GIGC_Allocate_All

30 Oct 2012 - R. Yantosca - Now pass am_I_Root, RC to SET_COMMSOIL_MOD

01 Nov 2012 - R. Yantosca - Now zero the fields of the Input Options object

16 Nov 2012 - R. Yantosca - Remove this routine from the #ifdef DEVEL block

27 Nov 2012 - R. Yantosca - Now pass Input_Opt to INIT_COMODE_LOOP

03 Dec 2012 - R. Yantosca - Now pass am_I_Root, RC to INIT_CMN_SIZE

03 Dec 2012 - R. Yantosca - Add optional arguments to accept dimension
```

size information from the ESMF interface

```
13 Dec 2012 - R. Yantosca - Remove reference to obsolete CMN_DEP_mod.F

13 Dec 2012 - R. Yantosca - Remove reference to obsolete CMN_mod.F

23 Jul 2014 - R. Yantosca - Remove reference to obsolete CMN_NOX_mod.F

25 Jul 2014 - R. Yantosca - Remove reference to obsolete commsoil_mod.F90

25 Jul 2014 - R. Yantosca - Now call INIT_GET_NDEP (GeosCore/get_ndep_mod.F)

04 Aug 2015 - C. Keller - Now pass LLTROP and LLSTRAT to INIT_CMN_SIZE.

17 Jun 2016 - R. Yantosca - Move call to INIT_GET_NDEP to GIGC_INIT_EXTRA

which is called after species database init

30 Jun 2016 - M. Sulprizio- Remove call to INIT_COMODE_LOOP; it's obsolete
```

2.3.2 gc_init_all

Subroutine GC_INIT_ALL initializes the top-level data structures that are either passed to/from GC or between GC components (emis-; transport-; chem-; etc)

INTERFACE:

```
SUBROUTINE GC_Init_All( am_I_Root, Input_Opt, State_Chm, State_Met, RC )
```

USES:

```
USE CMN_Size_Mod, ONLY : IIPAR, JJPAR, LLPAR
USE CMN_SIZE_Mod, ONLY : NDUST, NAER
USE ErrCode_Mod
USE Input_Opt_Mod
USE State_Chm_Mod
USE State_Met_Mod
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(OptInput), INTENT(INOUT) :: Input_Opt   ! Input Options object
TYPE(MetState), INTENT(INOUT) :: State_Met   ! Meteorology State object
TYPE(ChmState), INTENT(INOUT) :: State_Chm   ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure
```

REMARKS:

Need to add better error checking, currently we just return upon error.

```
26 Jan 2012 - M. Long - Initial version
13 Aug 2012 - R. Yantosca - Added ProTeX headers
16 Oct 2012 - R. Yantosca - Renamed LOCAL_MET argument to State_Met
16 Oct 2012 - R. Yantosca - Renamed GC_STATE argument to State_Chm
```

```
16 Oct 2012 - R. Yantosca - Call Init_Chemistry_State (in gc_type2_mod.F90,
                            which was renamed from INIT_CHEMSTATE)
19 Oct 2012 - R. Yantosca - Now reference gigc_state_met_mod.F90
19 Oct 2012 - R. Yantosca - Now reference gigc_state_chm_mod.F90
19 Oct 2012 - R. Yantosca - Now reference gigc_errcode_mod.F90
19 Oct 2012 - R. Yantosca - Now reference IGAS in Headers/comode_loop_mod.F
22 Oct 2012 - R. Yantosca - Renamed to GIGC_Init_All
26 Oct 2012 - R. Yantosca - Now call Get_nSchm, nSchmBry to find out the
                            number of strat chem species and Bry species
01 Nov 2012 - R. Yantosca - Now use LSCHEM from logical_mod.F
09 Nov 2012 - R. Yantosca - Now pass Input Options object for GIGC
26 Feb 2013 - R. Yantosca - Now pass Input_Opt to Init_GIGC_State_Chm
28 Aug 2015 - R. Yantosca - Remove strat-chem options from call to
                            Init_GIGC_State_Chm; this is done by HEMCO
25 Jan 2016 - R. Yantosca - Bug fix: Declare Input_Opt as INTENT(INOUT),
                            to match the declaration in INIT_GIGC_STATE_CHM
28 Jan 2016 - M. Sulprizio- Remove NBIOMAX from call to Init_GIGC_State_Chm
30 Jun 2016 - M. Sulprizio- Remove nSpecies from call to Init_GIGC_State_Chm
```

2.4 Fortran: Module Interface restart_mod.F

Module RESTART_MOD contains variables and routines which are used to read and write restart files for GEOS-Chem species in units of [v/v] dry mixing ratio, which represents mol species per mol dry air.

INTERFACE:

MODULE RESTART_MOD

USES:

```
USE CMN_SIZE_MOD
   USE ErrCode_Mod
   USE ERROR_MOD
   USE HCO_INTERFACE_MOD, ONLY : HcoState
   USE inquireMod,
                      ONLY : findFreeLUN
   USE PhysConstants
   USE Precision_Mod
   USE UnitConv_Mod
   IMPLICIT NONE
   PRIVATE
!PUBLIC MEMBER FUNCTIONS
   PUBLIC :: READ_GC_RESTART
   PUBLIC :: WRITE_GC_RESTART
   PUBLIC :: INIT_GC_RESTART
   PUBLIC :: COMPARE_TRC_SPC ! temporary for tracer removal debugging
```

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: CHECK_RST_DIMENSIONS

DEFINED PARAMETERS:

REVISION HISTORY:

- 25 Jun 2002 R. Yantosca Initial version
- (1) Moved routines "make_restart_file.f"" and "read_restart_file.f" into this module. Also now internal routines to "read_restart_file.f" are now a part of this module. Now reference "file_mod.f" to get file unit numbers and error checking routines. (bmy, 6/25/02)
- (2) Now reference AD from "dao_mod.f". Now reference "error_mod.f".

 Also added minor bug fix for ALPHA platform. (bmy, 10/15/02)
- (3) Now references "grid_mod.f" and the new "time_mod.f" (bmy, 2/11/03)
- (4) Added error-check and cosmetic changes (bmy, 4/29/03)
- (5) Removed call to COPY_STT_FOR_OX, it's obsolete (bmy, 8/18/03)
- (6) Add fancy output (bmy, 4/26/04)
- (7) Added routine SET_RESTART. Now reference "logical_mod.f" and "tracer_mod.f" (bmy, 7/20/04)
- (8) Removed obsolete routines TRUE_TRACER_INDEX and COPY_DATA_FOR_CO_OH (bmy, 6/28/05)
- (9) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (10) Now pass TAU via the arg list in MAKE_RESTART_FILE (bmy, 12/15/05)
- (11) Add MAKE_CSPEC_FILE and READ_CSPEC_FILE routines to save and read CSPEC_FULL restart files (dkh, 02/12/09)
- 11 Jul 2011 R. Yantosca Corrected mis-indexing problem w/ the CSPEC restart file
- 21 Jul 2011 M. Long Now include F77_CMN_SIZE instead of CMN_SIZE
- 03 Aug 2012 R. Yantosca Move calls to findFreeLUN out of DEVEL block
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 19 Nov 2014 M. Yannetti Added PRECISION_MOD
- 09 Feb 2016 E. Lundgren Add NetCDF restart file routines
- 11 Jul 2016 E. Lundgren Store only species in restart files
- 12 Jul 2016 E. Lundgren Remove bpch restart file format option and associated routines
- 09 Aug 2016 E. Lundgren Remove obsolete routines convert_tracer_to_vv and set_restart and associated module vars; replace all tracer language to species; rename OUTPUT_RESTART_FILE to OUTPUT_GC_RST_PREFIX
- 29 Nov 2016 R. Yantosca grid_mod.F90 is now gc_grid_mod.F90

2.4.1 init_gc_restart

Subroutine INIT_GC_RESTART initializes the GEOS-Chem restart file collection and populates it with containers. This collection includes restart concentrations for each species as

well as additional data if running the mercury simulation.

INTERFACE:

```
SUBROUTINE INIT_GC_RESTART( am_I_Root, Input_Opt, & State_Chm, RC )
```

USES:

```
USE GC_GRID_MOD, ONLY : AREA_M2
USE HCO_Error_Mod
```

USE HCO_Diagn_Mod

USE Input_Opt_Mod, ONLY : OptInput
USE Species_Mod, ONLY : Species
USE State_Chm_Mod, ONLY : ChmState
USE TIME_MOD, ONLY : GET_TS_CHEM

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
```

INPUT/OUTPUT PARAMETERS:

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REVISION HISTORY:

2.4.2 read_gc_restart

Subroutine READ_GC_RESTART reads species concentrations [mol/mol] from the GEOS-Chem restart file and uses them to initialize species concentrations in [kg/kg dry]. If species data are missing from the restart file, pre-configured background values are used. If using the mercury simulation, additional restart data are read from file.

INTERFACE:

```
SUBROUTINE READ_GC_RESTART( am_I_Root, YYYYMMDD, HHMMSS,
& Input_Opt, State_Met, State_Chm, RC )
```

USES:

USE m_netcdf_io_open ! netCDF file open USE m_netcdf_io_read ! netCDF read USE m_netcdf_io_readattr ! netCDF attribute reads USE m_netcdf_io_get_dimlen ! netCDF get dimensions ! netCDF file close USE m_netcdf_io_close USE PHYSCONSTANTS, ONLY : BOLTZ USE CHEMGRID_MOD, ONLY : ITS_IN_THE_TROP
USE Input_Opt_Mod, ONLY : OptInput
USE Species_Mod, ONLY : Species USE State_Chm_Mod, ONLY : ChmState USE State_Met_Mod, ONLY : MetState USE TIME_MOD, ONLY : EXPAND_DATE ! For Hg simulation restart file USE OCEAN_MERCURY_MOD, ONLY: HgOaq, Hg2aq, HgPaq, Hgaq_tot USE OCEAN_MERCURY_MOD, ONLY : CHECK_OCEAN_MERCURY USE DEPO_MERCURY_MOD, ONLY : SNOW_HG_OC, SNOW_HG_STORED_OC USE DEPO_MERCURY_MOD, ONLY : SNOW_HG_LN, SNOW_HG_STORED_LN

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

INTEGER, INTENT(IN) :: YYYYMMDD ! YYYY/MM/DD GMT date

INTEGER, INTENT(IN) :: HHMMSS ! hh:mm:ss GMT time

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

include "netcdf.inc"

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

```
09 Feb 2016 - E. Lundgren - Initial version
20 Apr 2016 - E. Lundgren - Implement ocean and snow Hg variables
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
31 May 2016 - E. Lundgren - Replace Input_Opt%TRACER_MW_G with species
database field emMW_g (emitted species g/mol)
06 Jun 2016 - M. Sulprizio- Replace NTSPEC with State_Chm%nSpecies and
NAMEGAS with SpcInfo%Name from species database
22 Jun 2016 - R. Yantosca - Now refer to HgO_Id_List, Hg2_Id_List, and
HgP_Id_List fields of State_Chm
11 Jul 2016 - E. Lundgren - Remove tracers and read only species
12 Jul 2016 - E. Lundgren - Rename from read_gc_restart_nc
```

```
18 Jul 2016 - M. Sulprizio- Remove special handling of ISOPN, MMN, CFCX, and
HCFCX. Family tracers have been eliminated.

25 Jul 2016 - E. Lundgren - Store whether species in rst file in species db
rather than module-level variable

03 Aug 2016 - E. Lundgren - Remove tracers; now only use species

11 Aug 2016 - E. Lundgren - Move source of background values to spc database
```

2.4.3 write_gc_restart

Subroutine WRITE_GC_RESTART writes species concentrations [mol/mol] to the GEOS-Chem restart file in NetCDF format. If using the mercury simulation, additional data such as ocean mercury values are written to the restart file.

INTERFACE:

```
SUBROUTINE WRITE_GC_RESTART( am_I_Root, YYYYMMDD, HHMMSS, & Input_Opt, State_Chm, State_Met, & RC )
```

USES:

```
USE Input_Opt_Mod,
                        ONLY : OptInput
USE Species_Mod,
                        ONLY : Species
USE State_Chm_Mod,
                        ONLY : ChmState
USE State_Met_Mod,
                        ONLY : MetState
USE TIME_MOD,
                        ONLY : EXPAND_DATE
! HEMCO
USE HCO_Error_Mod
USE HCO_Diagn_Mod,
                        ONLY : Diagn_Update
USE HCOIO_Diagn_Mod,
                        ONLY : HCOIO_Diagn_WriteOut
! For Hg simulation
USE OCEAN_MERCURY_MOD,
                        ONLY: HgOaq, Hg2aq, HgPaq, Hgaq_tot
USE OCEAN_MERCURY_MOD,
                        ONLY : CHECK_OCEAN_MERCURY
USE DEPO_MERCURY_MOD,
                        ONLY : SNOW_HG_OC, SNOW_HG_STORED_OC
```

INPUT PARAMETERS:

```
LOGICAL,
                INTENT(IN)
                              :: am_I_Root
                                             ! Are we on the root CPU?
INTEGER,
                              :: YYYYMMDD
                                             ! YYYY/MM/DD GMT date
               INTENT(IN)
                              :: HHMMSS
                                             ! hh:mm:ss GMT time
INTEGER,
               INTENT(IN)
                              :: Input_Opt
TYPE(OptInput), INTENT(IN)
                                             ! Input Options object
TYPE(MetState), INTENT(IN)
                              :: State_Met
                                             ! Meteorology State object
```

ONLY: SNOW_HG_LN, SNOW_HG_STORED_LN

INPUT/OUTPUT PARAMETERS:

USE DEPO_MERCURY_MOD,

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

2.4.4 check_rst_dimensions

Subroutine CHECK_RST_DIMENSIONS checks to see if dimensions read from the netCDF file match the defined GEOS-Chem dimensions. If not, then it will stop the GEOS-Chem simulation with an error message.

INTERFACE:

INPUT PARAMETERS:

```
OPTIONAL, INTENT(IN) :: lon
                                                      ! Lon dimension
INTEGER,
INTEGER,
                OPTIONAL, INTENT(IN) :: lat
                                                      ! Lat dimension
                OPTIONAL, INTENT(IN) :: lev
                                                      ! Alt dimension
INTEGER,
                OPTIONAL, INTENT(IN) :: time
                                                      ! Time dimension
INTEGER,
INTEGER,
                OPTIONAL, INTENT(IN) :: time_expected ! Expected # of
                                                      ! time slots
CHARACTER(LEN=*), INTENT(IN)
                            :: LOC
                                                     ! Caller location
```

REMARKS:

REVISION HISTORY:

```
(1 ) Added to "restart_mod.f". Now no longer allow initialization with less than a globally-sized data block. (bmy, 6/25/02)
```

(2) Now reference GEOS_CHEM_STOP from "error_mod.f", which frees all allocated memory before stopping the run. (bmy, 10/15/02)

```
11 Jul 2011 - R. Yantosca - Added ProTeX headers
```

21 Jul 2011 - M. Long - Now include F77_CMN_SIZE instead of CMN_SIZE

09 Feb 2016 - E. Lundgren - Add args and all args optional except location

01 Apr 2016 - E. Lundgren - Rename this subroutine from check_dimensions to

check_rst_dimensions for global clarity

2.4.5 compare_trc_spc

Subroutine COMPARE_TRC_SPC prints out species values to log in kg/kg dry for advected species, and prints out non-advected species molec/cm3. This can only be used where tracers were kg/kg dry.

INTERFACE:

```
SUBROUTINE COMPARE_TRC_SPC( am_I_Root, Input_Opt,
& State_Met, State_Chm, LOC, RC )
```

USES:

```
USE Input_Opt_Mod, ONLY : OptInput
USE Species_Mod, ONLY : Species
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

CHARACTER(LEN=*), INTENT(IN) :: LOC

include "netcdf.inc"
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

```
08 Aug 2016 - E. Lundgren - Initial version
```

2.5 Fortran: Module Interface cleanup.F

Subroutine CLEANUP deallocates the memory assigned to dynamically allocatable arrays just before exiting a GEOS-Chem simulation.

INTERFACE:

SUBROUTINE CLEANUP(am_I_Root, ERROR, RC)

USES:

```
USE AEROSOL_MOD,
                             ONLY : CLEANUP_AEROSOL
USE C2H6_MOD,
                             ONLY: CLEANUP_C2H6
USE CARBON_MOD,
                             ONLY : CLEANUP_CARBON
USE CHEMGRID_MOD,
                             ONLY: CLEANUP_CHEMGRID
                             ONLY : CLEANUP_CO2
USE CO2_MOD,
USE CMN_FJX_Mod,
                             ONLY : Cleanup_CMN_FJX
                             ONLY: Cleanup_CMN_03
USE CMN_O3_Mod,
USE CMN_SIZE_Mod,
                             ONLY : Cleanup_CMN_SIZE
                             ONLY : CLEANUP_DIAG
USE DIAG_MOD,
USE DIAGO3_MOD,
                             ONLY : CLEANUP_DIAGO3
USE DIAGO4_MOD,
                             ONLY: CLEANUP_DIAGO4
USE DIAG20_MOD,
                             ONLY: CLEANUP_DIAG20
USE DIAG41_MOD,
                             ONLY: CLEANUP_DIAG41
USE DIAG50_MOD,
                             ONLY: CLEANUP_DIAG50
USE DIAG51_MOD,
                             ONLY : CLEANUP_DIAG51
USE DIAG53_MOD,
                             ONLY : CLEANUP_DIAG53 !(clf, 3/11/11)
USE DIAG_OH_MOD,
                             ONLY : CLEANUP_DIAG_OH
                             ONLY : CLEANUP_DRYDEP
USE DRYDEP_MOD,
USE DUST_MOD,
                             ONLY : CLEANUP_DUST
                             ONLY : DEBUG_MSG
USE ERROR_MOD,
                             ONLY : CLEANUP_FLEXCHEM
USE FLEXCHEM_MOD,
USE GEOSFP_READ_MOD,
                             ONLY : CLEANUP_GEOSFP_READ
USE GET_NDEP_MOD,
                             ONLY : CLEANUP_GET_NDEP
USE GLOBAL_CH4_MOD,
                             ONLY: CLEANUP_GLOBAL_CH4
USE GC_GRID_MOD,
                             ONLY : CLEANUP_GRID
USE HDF_MOD,
                             ONLY : CLEANUP_HDF
USE Input_Opt_Mod,
                             ONLY : OptInput
USE ISOROPIAII_MOD,
                             ONLY : CLEANUP_ISOROPIAII
USE LINOZ_MOD,
                             ONLY : CLEANUP_LINOZ
USE MERCURY_MOD,
                             ONLY : CLEANUP_MERCURY
                             ONLY : CLEANUP_MODIS_LAI
USE MODIS_LAI_MOD,
USE OCEAN_MERCURY_MOD,
                             ONLY : CLEANUP_OCEAN_MERCURY
USE DEPO_MERCURY_MOD,
                             ONLY : CLEANUP_DEPO_MERCURY
USE LAND_MERCURY_MOD,
                             ONLY : CLEANUP_LAND_MERCURY
USE MERRA2_READ_MOD,
                             ONLY: CLEANUP_MERRA2_READ
USE PBL_MIX_MOD,
                             ONLY : CLEANUP_PBL_MIX
                             ONLY : CLEANUP_PJC_PFIX
USE PJC_PFIX_MOD,
USE PLANEFLIGHT_MOD,
                             ONLY : CLEANUP_PLANEFLIGHT
                             ONLY : CLEANUP_PRESSURE
USE PRESSURE_MOD,
```

USE Regrid_A2A_Mod, ONLY : Cleanup_Map_A2a USE SEASALT_MOD, ONLY : CLEANUP_SEASALT USE SULFATE_MOD, ONLY : CLEANUP_SULFATE USE STRAT_CHEM_MOD, ONLY : CLEANUP_STRAT_CHEM USE TAGGED_CO_MOD, ONLY : CLEANUP_TAGGED_CO defined(TOMAS) #if USE TOMAS_MOD, ONLY: CLEANUP_TOMAS !sfarina, 1/16/13 #endif USE TOMS_MOD, ONLY : CLEANUP_TOMS USE TPCORE_FVDAS_MOD, ONLY : EXIT_TPCORE ONLY : EXIT_TPCORE_WINDOW USE TPCORE_WINDOW_MOD, #if ! defined(ESMF_) USE TRANSPORT_MOD, ONLY : CLEANUP_TRANSPORT #endif USE UCX_MOD, ONLY : CLEANUP_UCX USE VDIFF_PRE_Mod, ONLY : Cleanup_VDIFF_PRE USE PASSIVE_TRACEr_MOD, ONLY : Cleanup_Passive_Tracer USE WETSCAV_MOD, ONLY : CLEANUP_WETSCAV ! HEMCO #if !defined(ESMF_) USE EMISSIONS_MOD, ONLY : EMISSIONS_FINAL #endif #if defined(NC_DIAG) ! Cleanup routine for netCDF diagnostics structure USE DIAGNOSTICS_MOD, ONLY : DIAGNOSTICS_FINAL #endif #if defined(RRTMG) USE RRTMG_RAD_TRANSFER_MOD, ONLY : CLEANUP_SURFACE_RAD USE RRTMG_RAD_TRANSFER_MOD, ONLY : CLEANUP_STRAT_CLIM USE RRTMG_RAD_TRANSFER_MOD, ONLY : CLEANUP_MCICA_CLOUDS #endif

IMPLICIT NONE

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
LOGICAL, INTENT(IN) :: ERROR ! Cleanup after error?

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REVISION HISTORY:

29 Nov 1999 - R. Yantosca - Initial version

- (1) CLEANUP is written in Fixed-Format F90.
- (2) Now calls CLEANUP_WETSCAV, which deallocates arrays from "wetscav_mod.f". (bmy, 3/9/00)
- (3) Add call to CLEANUP_SULFATE, which deallocates arrays from "sulfate_mod.f". Also now deallocate ND32 arrays. (bmy, 6/6/00)
- (4) Add call to CLEANUP_DAO, which deallocates arrays from "dao_mod.f". (bmy, 6/26/00)
- (5) Add call to CLEANUP_TAGGED_CO and CLEANUP_COMODE, which deallocates arrays from and "comode_mod.f". (bmy, 7/19/00)
- (6) Add call to CLEANUP_GLOBAL_OH and CLEANUP_COMODE, which deallocates arrays from "global_oh_mod.f". (bmy, 7/28/00)
- (7) Add calls to CLEANUP_BIOMASS and CLEANUP_BIOFUEL, which deallocates arrays from "biomass_mod.f" and "biofuel_mod.f". Also deallocate the AD32_bf array for the biofuel NOx diagnostic. (bmy, 9/12/00)
- (8) Add call to CLEANUP_DIAG51, to deallocate module arrays from "diag51_mod.f" (bmy, 11/29/00)
- (9) Removed obsolete code from 11/29/00 (bmy, 12/21/00)
- (10) Add call to CLEANUP_CH4, to deallocate module arrays from "global_ch4_mod.f" (bmy, 1/16/01)
- (11) Now deallocate the AD34 array. Also updated comments and made some cosmetic changes. (bmy, 3/15/01)
- (12) Now deallocate the AD12 array (bdf, bmy, 6/15/01)
- (13) Add call to CLEANUP_ACETONE, to deallocate module arrays from "acetone_mod.f" Also deallocate AD11 array. Also deallocate variables from dao_mod.f last, to try to avoid bus error on SGI (bmy, 8/3/01)
- (14) Added call to CLEANUP_UVALBEDO from "uvalbedo_mod.f". Also removed obsolete code from 9/01. Also only include references to CLEANUP_* subroutines in other modules for clarity. (bmy, 1/15/02)
- (15) Added call to CLEANUP_C2H6 from "c2h6_mod.f" (bmy, 1/25/02)
- (17) Now deallocate CTNO2, CTHO2, LTNO2, LTHO2 arrays (rvm, bmy, 2/27/02)
- (18) Now reference CLEANUP_PLANEFLIGHT from "planeflight_mod.f".

 Now also deallocate ADO1 and ADO2 arrays. (mje, bmy, 8/7/02)
- (20) Now reference cleanup routine from "transport_mod.f" (bmy, 2/10/03)
- (21) Now reference cleanup routine from "pjc_pfix_mod.f" and "tpcore_fvdas_mod.f90". (bmy, 5/9/03)
- (22) Now reference cleanup routine from "toms_mod.f" (bmy, 7/14/03)
- (23) Now reference cleanup routine from "carbon_mod.f", "dust_mod.f", and "dust_dead_mod.f". (bmy, 7/14/03)
- (23) Now references cleanup routine from "lightning__nox_mod.f" (bmy, 4/14/04)
- (24) Now references cleanup routine from "seasalt_mod.f" (bmy, 4/26/04)
- (25) Now references cleanup routines from new modules (bmy, 7/20/04)

- (26) Now calls cleanup routine from "epa_nei_mod.f" (bmy, 11/5/04)
- (27) Now call CLEANUP_MERCURY from "mercury_mod.f" (eck, bmy, 12/7/04)
- (28) Now call CLEANUP_OCEAN_MERCURY from "ocean_mercury_mod.f". Also reordered the calling sequence. (sas, bmy, 1/21/05)
- (29) Now call CLEANUP_PBL_MIX from "pbl_mix_mod.f". Now call CLEANUP_DIAG41 from "diag41_mod.f". (bmy, 2/17/05)
- (30) Now calls CLEANUP_HCN_CH3CN from "hcn_ch3cn_mod.f (bmy, 6/23/05)
- (31) Now calls CLEANUP_DIAGO4, CLEANUP_CO2, and CLEANUP_TROPOPAUSE (bmy, 8/15/05)
- (32) Now calls CLEANUP_LAI from "lai_mod.f", CLEANUP_MEGAN from "megan_mod.f" and CLEANUP_REGRID_1x1 from "regrid_1x1_mod.f" (tmf, bdf, bmy, 10/24/05)
- (33) Now calls CLEANUP_EMEP from "emep_mod.f" (bdf, bmy, 11/1/05)
- (34) Now calls CLEANUP_GC_BIOMASS and CLEANUP_GFED2_BIOMASS (bmy, 4/5/06)
- (35) Now calls CLEANUP_DIAG56 from "diag56_mod.f" and CLEANUP_LIGHTNING_NOX_NL from "lightning_nox_nl_mod.f" (ltm, bmy, 5/5/06)
- (36) Now references CLEANUP_BRAVO from "bravo_mod.f" and CLEANUP_EDGAR from "edgar_mod.f" (bmy, 7/6/06)
- (37) Now calls CLEANUP_H2_HD from "h2_hd_mod.f" and CLEANUP_GLOBAL_O1D from "global_o1d_mod.f". Remove call to CLEANUP_LIGHTNING_NOx_NL from "lightning_nox_nl_mod.f (hup, phs, bmy, 10/2/07)
- (38) Now calls GEOS5_EXIT_TPCORE_WINDOW to finalize the TPCORE for GEOS-5 nested window simulations (yxw, dan, bmy, 11/6/08)
- (39) Now references CLEANUP_CAC_ANTHRO (amv, phs, 3/10/08)
- (40) Now references CLEANUP_ARCTAS_SHIP (phs, 3/10/08)
- (41) Now references CLEANUP_VISTAS_ANTHRO (phs, 3/10/08)
- (41) Now references CLEANUP_LINOZ (phs, 10/16/09)
- (42) Now references CLEANUP_HDF (amv, bmy, 12/21/09)
- (43) Now references CLEANUP_ISOROPIAII (ccc, bmy, 1/29/09)
- (44) Now references CLEANUP_DEPO_MERCURY and CLEANUP_LAND_MERCURY (ccc, 5/6/10)
- (45) Added call to CLEANUP_GLOBAL_OC, which deallocates arrays from "global_oc_mod.f" (clf, 2/28/2011)
- (46) Added call to CLEANUP_GLOBAL_BC, which deallocates arrays from "global_bc_mod.f" (clf, 2/28/2011)
- 13 Aug 2010 R. Yantosca Added ProTeX headers
- 28 Feb 2011 C. Friedman Added call to CLEANUP_GLOBAL_OC, which deallocates arrays from "global_oc_mod.f"
- 22 Aug 2011 R. Yantosca Add modifications for APM microphysics (G. Luo)
- 07 Sep 2011 P. Kasibhatla Add modifications for GFED3
- 19 Mar 2012 M. Payer Remove call to CLEANUP_ACETONE. It is no longer needed after removal of JO1D and RESP routines.
- 05 Apr 2012 R. Yantosca Now call CLEANUP_MODIS_LAI
- 11 Apr 2012 R. Yantosca Remove reference to obsolete lai_mod.F
- 01 May 2012 M. Payer Added calls for CLEANUP_GLOBAL_GRID and CLEANUP_GRID
- 19 Nov 2012 R. Yantosca Add cleanup calls for modules in Headers;

```
these were omitted during development
28 Nov 2012 - R. Yantosca - Remove reference to CLEANUP_DAO; we have now
                            removed all allocatable arrays from dao_mod.F
03 Dec 2012 - R. Yantosca - Now call Cleanup_CMN_SIZE
13 Dec 2012 - R. Yantosca - Remove reference to obsolete CMN_DEP_mod.F
06 Mar 2013 - H. Amos
                         - Merge C. Friedman's PAH code
14 Mar 2013 - M. Payer
                          - Restore reference to CLEANUP_DAO. Some arrays
                            have been restored to dao_mod.F for use in
                            the vertical regridding of OH for offline
                            simulations.
24 Mar 2013 - S.D. Eastham- Switched TROPOPAUSE_MOD to CHEMGRID_MOD
04 Apr 2013 - S.D. Eastham- Added call for CLEANUP_UCX
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
26 Sep 2013 - R. Yantosca - Renamed GEOS_57 Cpp switch to GEOS_FP
26 Sep 2013 - R. Yantosca - Now reference EXIT_GEOSFP_TPCORE_WINDOW
29 Oct 2013 - R. Yantosca - Now call CLEANUP_DAO for all simulations (if
                            arrays are not allocated it'll exit gracefully)
03 Jun 2014 - R. Yantosca - Don't finalize HEMCO if emissions are turned
                            off. This prevents a seg fault error.
03 Jun 2014 - R. Yantosca - Now pass Input_Opt via the argument list
03 Jun 2014 - R. Yantosca - Remove references to emissions modules that
                            HEMCO renders obsolete
24 Jun 2014 - R. Yantosca - Remove CLEANUP_BROMOCARB; HEMCO replaces this
25 Jun 2014 - R. Yantosca - Remove reference to tracer_mod.F
21 Jul 2014 - R. Yantosca - Remove reference to regrid_1x1_mod.F
23 Jul 2014 - R. Yantosca - Remove reference to obsolete CMN_mod.F
23 Jul 2014 - R. Yantosca - Remove reference to obsolete global_grid_mod.F
23 Jul 2014 - R. Yantosca - Remove reference to obsolete CMN_NOX_mod.F
25 Jul 2014 - R. Yantosca - Remove reference to commsoil_mod.F90
25 Jul 2014 - R. Yantosca - Now call CLEANUP_GET_NDEP
15 Aug 2014 - R. Yantosca - Remove reference to biofuel_mod.F
15 Aug 2014 - R. Yantosca - Remove reference to biomass_mod.F
10 Sep 2014 - M. Sulprizio- Remove references to global_oc_mod.F and
                            global_bc_mod.F
23 Sep 2014 - M. Sulprizio- Remove references to global_hno3_mod.F and
                            global_no3_mod.F
12 Jan 2015 - R. Yantosca - Remove CLEANUP_UVALBEDO routine
11 Mar 2015 - R. Yantosca - Remove call to CLEANUP_GLOBAL_OH
11 Mar 2015 - R. Yantosca - Remove call to CLEANUP_GLOBAL_NOX
16 Mar 2015 - R. Yantosca - Remove call to CLEANUP_HCN_CH3CN
25 Mar 2015 - C. Keller - Now cleanup UCX before emissisions.
16 Apr 2015 - R. Yantosca - Remove call to CLEANUP_DAO; it's obsolete
24 Mar 2016 - C. Keller
                         - Remove input arg Input_Opt; this is cleaned
                            up before routine CLEANUP is called.
18 May 2016 - M. Sulprizio- Remove call to CLEANUP_COMODE; it's obsolete
30 Jun 2016 - M. Sulprizio- Remove call to CLEANUP_COMODE_LOOP; it's obsolete
29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90
```

3 Transport modules

These modules contain routines to advect GEOS-Chem speecies using assimilated meteorology fields.

3.1 Fortran: Module Interface transport_mod.F

Module TRANSPORT_MOD is used to call the proper version of the TPCORE advection scheme for GCAP, GEOS-4, GEOS-5, or GEOS-5.7 nested-grid or global simulations.

INTERFACE:

MODULE TRANSPORT_MOD

USES:

USE PRECISION_MOD ! For GEOS-Chem Precision (fp)
USE PRESSURE_MOD

IMPLICIT NONE PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: CLEANUP_TRANSPORT

PUBLIC :: DO_TRANSPORT
PUBLIC :: INIT_TRANSPORT

PUBLIC :: INIT_WINDOW_TRANSPORT

PUBLIC :: SET_TRANSPORT

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: GEOS4_GEOS5_GLOBAL_ADV

PRIVATE :: GCAP_GLOBAL_ADV
PRIVATE :: DO_WINDOW_TRANSPORT

- 10 Mar 2003 Y. Wang, R. Yantosca Initial version
- (1) Now can select transport scheme for GEOS-3 winds. Added code for PJC pressure fixer. (bdf, bmy, 5/8/03)
- (2) Now delete DSIG array, it's obsolete. Also added new PRIVATE function GET_AIR_MASS to compute air masses from the input/output pressures from the new GEOS-4/fvDAS TPCORE. (bmy, 6/24/03)
- (3) Now references DEBUG_MSG from "error_mod.f". (bmy, 8/7/03)
- (4) Bug fix in DO_GLOBAL_TRANSPORT (bmy, 10/21/03)
- (5) IORD, JORD, KORD are now module variables. Now references "logical_mod.f" and "tracer_mod.f" (bmy, 7/20/04)
- (6) Add mass-flux diagnostics to TPCORE_FVDAS (bdf, bmy, 9/28/04)
- (7) Now references "diag_mod.f" (bmy, 9/28/04)

- (8) Now modified for GEOS-5 and GCAP met fields (swu, bmy, 5/25/05)
- (9) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (10) Now flip arrays in call to TPCORE_FVDAS (bmy, 6/16/06)
- (11) Added modifications for SUN compiler (bmy, 7/12/06)
- (12) Bug fixes in DO_GLOBAL_TRANSPORT (bmy, 11/29/06)
- (13) Split off GCAP, GEOS-3, GEOS-4/GEOS-5 specific calling sequences into separate subroutines. Also removed some obsolete module variables. (bmy, 10/30/07)
- (14) Modifications for GEOS-5 nested grid (yxw, dan, bmy, 11/6/08)
- (15) Bug fix in mass balance in GCAP_GLOBAL_ADV and GEOS4_GEOS5_GLOBAL_ADV. (ccc, 2/17/09)
- 26 Feb 2010 R. Yantosca Removed references to obsolete LEMBED switch
- 26 Feb 2010 R. Yantosca Added ProTex Headers
- 08 Mar 2010 C. Carouge Modify call to tpcore_fvdas. We do not re-order mass fluxes diagnostics anymore.
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 01 Mar 2012 R. Yantosca Now reference new grid_mod.F90
- 21 Jun 2012 R. Yantosca Now use pointers to flip arrays in vertical
- 21 Jun 2012 R. Yantosca Comment out GEOS-3 window subroutine
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 26 Sep 2013 R. Yantosca Renamed "GEOS57" to "GEOSFP" in routine names
- 24 Nov 2014 M. Yannetti Added PRECISION_MOD
- 12 Feb 2015 E. Lundgren Added functionality for writing diags to netcdf
- 15 Apr 2015 R. Yantosca Add TARGET spec to A_M2 array
- 24 Jun 2015 E. Lundgren Now use kg/kg total air as tracer units (previously v/v) for advection
- 24 Jun 2015 E. Lundgren Remove post-advection residual mass correction and GET_AIR_MASS function since no longer needed when using kg/kg total air in advection
- 13 Aug 2015 E. Lundgren Tracer units are now input as kg/kg dry air (previously v/v)
- 19 Jan 2016 E. Lundgren Move DiagnUpdate_Transport to diagnostics_mod and consolidate netcdf and bpch diagnostic code
- 23 Jun 2016 R. Yantosca Remove references to APM code; it is no longer compatible with the FlexChem implementation
- 29 Nov 2016 R. Yantosca grid_mod.F90 is now gc_grid_mod.F90

3.1.1 do_transport

Subroutine DO_TRANSPORT is the driver routine for the proper TPCORE program for GEOS-3, GEOS-4/GEOS-5, or window simulations.

INTERFACE:

```
SUBROUTINE DO_TRANSPORT( am_I_Root, Input_Opt, & State_Met, State_Chm, RC )
```

USES:

```
USE CMN_SIZE_MOD
     USE ErrCode_Mod
     USE GC_GRID_MOD,
                              ONLY : ITS_A_NESTED_GRID
     USE Input_Opt_Mod,
                              ONLY : OptInput
     USE State_Chm_Mod,
                              ONLY : ChmState
     USE State_Met_Mod,
                              ONLY : MetState
     USE TPCORE_BC_MOD,
                              ONLY : INIT_TPCORE_BC
     USE TIME_MOD,
                              ONLY : GET_TS_DYN
#if defined( USE_TEND )
      USE TENDENCIES_MOD
#endif
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REVISION HISTORY:

- 10 Mar 2003 R. Yantosca Initial version
- (1) Removed IORD, JORD, KORD from the arg list. Also now removed reference to CMN, it's not needed. (bmy, 7/20/04)
- (2) Now call separate routines for different met fields. (bmy, 10/30/07)
- (3) Now references subroutine INIT_TPCORE_BC from tpcore_bc_mod.f and DO_GEOS5_FVDAS_WINDOW_TRANSPORT from

```
"tpcore_geos5_fvdas_window_mod.f90". (yxw, dan, bmy, 11/6/08)
```

- 26 Feb 2010 R. Yantosca Removed references to obsolete LEMBED switch
- 26 Feb 2010 R. Yantosca Added ProTeX headers
- 06 Oct 2010 R. Yantosca Treat MERRA in the same way as GEOS-5.
- 28 Feb 2012 R. Yantosca Treat GEOS-5.7 in the same way as MERRA
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 25 Mar 2013 R. Yantosca Now accept am_I_Root, Input_Opt, State_Chm, RC
- 31 Mar 2015 E. Lundgren Make State_Met INTENT(INOUT) for AIRQNT calls
- 19 Jul 2016 R. Yantosca Now bracket DO_TEND calls with #ifdef USE_TEND

3.1.2 geos4_geos5_global_adv

Subroutine GEOS4_GEOS5_GLOBAL_ADV is the driver routine for TPCORE with the GMAO GEOS-4 or GEOS-5 met fields.

INTERFACE:

```
SUBROUTINE GEOS4_GEOS5_GLOBAL_ADV( am_I_Root, Input_Opt,
                                   State_Met, State_Chm, RC )
```

USES:

USE CMN_DIAG_MOD ! NDxx flags USE CMN_SIZE_MOD ! Size parameters USE DAO_MOD, ONLY : AIRQNT

#if defined(BPCH_DIAG)

USE DIAG_MOD, ONLY: MASSFLEW, MASSFLNS, MASSFLUP

#elif defined(NC_DIAG)

USE DIAGNOSTICS_MOD, ONLY : DIAGNUPDATE_TRANSPORT_FLUX

#endif

USE ErrCode_Mod

USE ERROR_MOD

USE Input_Opt_Mod, ONLY: OptInput USE State_Chm_Mod, ONLY : ChmState USE State_Met_Mod, ONLY : MetState USE State_Met_Mod, ONLY : MetState

USE PhysConstants ! Physical constants

USE PJC_PFIX_MOD, ONLY : DO_PJC_PFIX USE TIME_MOD, ONLY : GET_TS_DYN USE TPCORE_FVDAS_MOD, ONLY : TPCORE_FVDAS

USE UnitConv_Mod

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object

OUTPUT PARAMETERS:

INTENT(OUT) :: RC ! Success or failure? INTEGER,

REMARKS:

As of July 2016, we assume that all of the advected species are listed first in the species database. This is the easiest way to pass a slab to the TPCORE routine. This may change in the future. (bmy, 7/13/16)

Note: the mass flux diagnostic arrays (MASSFLEW, MASSFLNS and MASSFLUP) are incremented upside-down (level 1 = top of the atmosphere). The levels order is reversed only when written out to diagnostic output.

```
30 Oct 2007 - R. Yantosca - Initial version
(1 ) Split off the GEOS-4 & GEOS-5 relevant parts from the previous
      routine DO_GLOBAL_TRANSPORT (bmy, 10/30/07)
(2) Activate the call to SAVE_GLOBAL_TPCORE_BC (yxw, dan, bmy, 11/6/08)
(3) Bug fix in mass balance: only account for cells of STT with non-zero
      concentrations when doing the computation (ccc, bmy, 2/17/09)
26 Feb 2010 - R. Yantosca - Removed references to obsolete LEMBED switch
26 Feb 2010 - R. Yantosca - Added ProTeX headers
16 Feb 2011 - R. Yantosca - Add modifications for APM microphysics (G. Luo)
21 Jun 2012 - R. Yantosca - Now use pointers to flip indices in vertical
09 Nov 2012 - M. Payer
                         - Replaced all met field arrays with State_Met
                            derived type object
25 Mar 2013 - R. Yantosca - Now accept am_I_Root, Input_Opt, State_Chm, RC
04 Jun 2013 - R. Yantosca - Replace pointer STT with State_Chm%Tracers
26 Feb 2015 - E. Lundgren - Replace GET_PEDGE with State_Met%PEDGE.
31 Mar 2015 - E. Lundgren - Move AIRQNT call from main to within transport
09 Jun 2015 - E. Lundgren - Remove dependency on tpcore_bc_mod since not used
15 Jun 2015 - E. Lundgren - Tracer units in advection are now kg/kg total air
                            (previously v/v)
15 Jun 2015 - E. Lundgren - Remove mass residual adjustment to tracer
                            concentration following advection
13 Aug 2015 - E. lundgren - Remove v/v <-> kg/kg conversion
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected
                            species ID from State_Chm%Map_Advect.
20 Jul 2016 - R. Yantosca - Add minor bug fixes for netCDF diagnostics
20 Jul 2016 - R. Yantosca - Now replace NNPAR with State_Chm%nAdvect
20 Jul 2016 - R. Yantosca - Now pass State_Chm to DiagnUpdate_Transport_Flux
03 Aug 2016 - R. Yantosca - Removed temporary tracer-removal code
```

3.1.3 gcap_global_adv

Subroutine GCAP_GLOBAL_ADV is the driver routine for TPCORE with the GCAP/GISS met fields.

INTERFACE:

USE DIAGNOSTICS_MOD, ONLY : DIAGNUPDATE_TRANSPORT_FLUX

#endif

USE ErrCode_Mod

USE ERROR_MOD

USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState

USE PhysConstants ! Physical constants

USE PJC_PFIX_MOD, ONLY: DO_PJC_PFIX
USE TIME_MOD, ONLY: GET_TS_DYN
USE TPCORE_FVDAS_MOD, ONLY: TPCORE_FVDAS

USE UnitConv_Mod

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

As of July 2016, we assume that all of the advected species are listed first in the species database. This is the easiest way to pass a slab to the TPCORE routine. This may change in the future. (bmy, 7/13/16) Note: the mass flux diagnostic arrays (MASSFLEW, MASSFLNS and MASSFLUP) are incremented upside-down (level 1 = top of the atmosphere). The levels order is reversed only when written out to diagnostic output.

- 30 Oct 2007 R. Yantosca Initial version
- (1) Split off the GCAP relevant parts from the previous routine DO_GLOBAL_TRANSPORT (bmy, 10/30/07)
- (2) Bug fix in mass balance: only account for cells of STT with non-zero concentrations when doing the computation (ccc, bmy, 2/17/09)
- 26 Feb 2010 R. Yantosca Removed references to obsolete LEMBED switch
- 26 Feb 2010 R. Yantosca Added ProTeX headers
- 16 Feb 2011 R. Yantosca Add modifications for APM microphysics (G. Luo)
- 21 Jun 2012 R. Yantosca Now use pointers to flip arrays in the vertical
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 25 Mar 2013 R. Yantosca Now accept am_I_Root, Input_Opt, State_Chm, RC
- 04 Jun 2013 R. Yantosca Replace pointer STT with State_Chm%Tracers
- 04 Sep 2014 R. Yantosca Avoid div-by-zero errors in division w/ SUMADA

```
26 Feb 2015 - E. Lundgren - Replace GET_PEDGE with State_Met%PEDGE.

31 Mar 2015 - E. Lundgren - Move AIRQNT call from main to within transport

09 Jun 2015 - E. Lundgren - Remove dependency on tpcore_bc_mod since not used

15 Jun 2015 - E. Lundgren - Tracer units in advection are now kg/kg total air

(previously v/v)

15 Jun 2015 - E. Lundgren - Remove mass residual adjustment to tracer

concentration following advection

13 Aug 2015 - E. lundgren - Remove v/v <-> kg/kg conversion

29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts

30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

20 Jul 2016 - R. Yantosca - Add minor bug fixes for netCDF diagnostics

20 Jul 2016 - R. Yantosca - Now replace NNPAR with State_Chm%nAdvect

20 Jul 2016 - R. Yantosca - Now pass State_Chm to DiagnUpdate_Transport_Flux

03 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code
```

3.1.4 do_window_transport

USE TPCORE_BC_MOD,

Subroutine DO_WINDOW_TRANSPORT is the driver program for the proper TPCORE program for the GEOS-5/GEOS-FP/MERRA2 nested-grid simulations.

INTERFACE:

```
SUBROUTINE DO_WINDOW_TRANSPORT( am_I_Root, Input_Opt,
                                       State_Met, State_Chm, RC )
USES:
       USE CMN_DIAG_MOD
                                      ! NDxx flags
       USE CMN_SIZE_MOD
                                      ! Size parameters
      USE DAO_MOD,
                                 ONLY : AIRQNT
 #if defined( BPCH_DIAG )
      USE DIAG_MOD,
                                 ONLY: MASSFLEW, MASSFLNS, MASSFLUP
 #elif defined( NC_DIAG )
       USE DIAGNOSTICS_MOD,
                                 ONLY : DIAGNUPDATE_TRANSPORT_FLUX
 #endif
       USE ErrCode_Mod
       USE ERROR_MOD
       USE GC_GRID_MOD,
                                 ONLY : GET_XOFFSET,
                                                       GET_YOFFSET
      USE Input_Opt_Mod,
                                 ONLY: OptInput
       USE State_Chm_Mod,
                                 ONLY : ChmState
      USE State_Met_Mod,
                                 ONLY : MetState
      USE PhysConstants
                                      ! Physical constants
      USE PJC_PFIX_WINDOW_MOD,
                                 ONLY : DO_PJC_PFIX_WINDOW
      USE TIME_MOD,
                                 ONLY : GET_TS_DYN
      USE TPCORE_BC_MOD,
                                 ONLY : IO_W, JO_W, I1_W, J1_W
      USE TPCORE_BC_MOD,
                                 ONLY: I2_W, J2_W, IM_W, JM_W, IGZD
```

ONLY : DO_WINDOW_TPCORE_BC

```
USE TPCORE_WINDOW_MOD, ONLY : TPCORE_WINDOW USE UnitConv_Mod
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

As of July 2016, we assume that all of the advected species are listed first in the species database. This is the easiest way to pass a slab to the TPCORE routine. This may change in the future. (bmy, 7/13/16)

Note: the mass flux diagnostic arrays (MASSFLEW, MASSFLNS and MASSFLUP) are incremented upside-down (level $1 = top \ of \ the \ atmosphere$). The levels order is reversed only when written out to diagnostic output.

- 10 Mar 2003 R. Yantosca Initial version 26 Feb 2010 - R. Yantosca - Removed references to obsolete LEMBED switch
- 26 Feb 2010 R. Yantosca Added ProTeX headers
- 16 Feb 2011 R. Yantosca Add modifications for APM from G. Luo 21 Jun 2012 R. Yantosca Now use pointers to flip arrays in the vertical
- 04 Jun 2013 R. Yantosca Replace pointer STT with State_Chm%Tracers
- 26 Feb 2015 E. Lundgren Replace GET_PEDGE with State_Met%PEDGE.
- 31 Mar 2015 E. Lundgren Move AIRQNT call from main to within transport
- 01 Apr 2015 L. Zhang Add updates to skip the window region
- 15 Apr 2015 R. Yantosca Add more pointers to avoid array temporaries
- 15 Jun 2015 E. Lundgren Tracer units in advection are now kg/kg total air (previously v/v)
- 15 Jun 2015 E. Lundgren Remove mass residual adjustment to tracer concentration prior to advection
- 13 Aug 2015 E. lundgren Remove v/v <-> kg/kg conversion
- 04 Nov 2015 M. Sulprizio- Rename from DO_GEOSFP_WINDOW_TRANSPORT to DO_WINDOW_TRANSPORT for use with all nested grids
- 29 Apr 2016 R. Yantosca Don't initialize pointers in declaration stmts
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.
- 20 Jul 2016 R. Yantosca Add minor bug fixes for netCDF diagnostics
- 20 Jul 2016 R. Yantosca Now replace NNPAR with State_Chm%nAdvect
- 20 Jul 2016 R. Yantosca Now pass State_Chm to DiagnUpdate_Transport_Flux
- 03 Aug 2016 R. Yantosca Removed temporary tracer-removal code

3.1.5 set_transport

Subroutine SET_TRANSPORT passes IORD, JORD, KORD values from "input_mod.f".

INTERFACE:

```
SUBROUTINE SET_TRANSPORT( I_ORD, J_ORD, K_ORD )
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I_ORD ! IORD option for E/W advection
INTEGER, INTENT(IN) :: J_ORD ! JORD option for N/S advection
INTEGER, INTENT(IN) :: K_ORD ! KORD option for vertical diffusion
```

REVISION HISTORY:

```
20 Jul 2004 - R. Yantosca - Initial version
26 Feb 2010 - R. Yantosca - Added ProTeX headers
```

3.1.6 init_transport

Subroutine INIT_TRANSPORT initializes all module variables and arrays.

INTERFACE:

```
SUBROUTINE INIT_TRANSPORT( am_I_Root, Input_Opt, RC )
```

USES:

```
USE CMN_SIZE_MOD
                           ! Size parameters
USE ErrCode_Mod
```

USE ERTCOde_Mod

USE ERROR_MOD, ONLY : ALLOC_ERR

USE GC_GRID_MOD, ONLY : GET_AREA_M2, GET_YMID_R

USE Input_Opt_Mod, ONLY : OptInput

USE PhysConstants ! Re

USE TIME_MOD, ONLY : GET_TS_DYN

USE TPCORE_FVDAS_MOD, ONLY : INIT_TPCORE

INPUT PARAMETERS:

```
INTENT(IN) :: am_I_Root ! Are we on the root CPU?
LOGICAL,
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

- 10 Mar 2003 R. Yantosca Initial version
- (1) Now references GET_TS_DYN from "time_mod.f", INIT_TPCORE_FVDAS from "tpcore_fvdas_mod.f90", and GET_YMID_R from "grid_mod.f". Now also include "CMN_SETUP". (bdf, bmy, 4/28/03)
- (2) Remove reference to DSIG, it's obsolete. (bmy, 6/24/03)
- (3) Now references LEMBED & LTPFV from "logical_mod.f". Now references N_TRACERS from "tracer_mod.f". (bmy, 7/20/04)
- (4) Now modified for GEOS-5 and GCAP met fields (swu, bmy, 5/25/05)
- (5) Removed reference to USE_GEOS_4_TRANSPORT, STT_I1, STT_I2, STT_J1, STT_J2, variables (bmy, 10/30/07)
- (6) Deleted reference to CMN, it's not needed anymore (bmy, 11/6/08)
- 26 Feb 2010 R. Yantosca Removed references to obsolete LEMBED switch
- 26 Feb 2010 R. Yantosca Added ProTeX headers
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 01 Mar 2012 R. Yantosca Now use GET_AREA_M2(I,J,L) from grid_mod.F90
- 01 Mar 2012 R. Yantosca Now use GET_YMID_R_W(I,J,L) from grid_mod.F90
- 25 Mar 2013 R. Yantosca Now accept am_I_Root, Input_Opt, RC
- 05 Dec 2014 M. Yannetti Added REAL_N_DYN

3.1.7 init_window_transport

Subroutine INIT_WINDOW_TRANSPORT initializes all module variables and arrays for the GEOS-5/GEOS-FP/MERRA2 nested grid simulation.

INTERFACE:

SUBROUTINE INIT_WINDOW_TRANSPORT(am_I_Root,Input_Opt,RC)

USES:

USE CMN_SIZE_MOD ! Size parameters
USE ErrCode_Mod

USE ERROR_MOD, ONLY : ALLOC_ERR, GC_Error USE GC_GRID_MOD, ONLY : GET_AREA_M2

USE GC_GRID_MOD, ONLY : GET_YMID_R_W

USE PhysConstants ! Re

USE TIME_MOD, ONLY : GET_TS_DYN USE TPCORE_FVDAS_MOD, ONLY : INIT_TPCORE

USE TPCORE_BC_MOD, ONLY : IO_W, JO_W, I1_W, J1_W
USE TPCORE_BC_MOD, ONLY : I2_W, J2_W, IM_W, JM_W
USE TPCORE_BC_MOD, ONLY : IGZD, INIT_TPCORE_BC

USE TPCORE_WINDOW_MOD, ONLY : INIT_WINDOW

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

```
06 Jun 2008 - D. Chen & R. Yantosca - Initial version
26 Feb 2010 - R. Yantosca - Removed references to obsolete LEMBED switch
26 Feb 2010 - R. Yantosca - Added ProTeX headers
01 Mar 2012 - R. Yantosca - Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
01 Mar 2012 - R. Yantosca - Now use GET_YMID_R_W(I,J,L) from grid_mod.F90
25 Mar 2013 - R. Yantosca - Now accept am_I_Root, Input_Opt, State_Chm, RC
26 Sep 2013 - R. Yantosca - Renamed to INIT_GEOSFP_WINDOW_TRANSPORT
05 Dec 2014 - M. Yannetti - Added REAL_N_DYN
04 Nov 2015 - M. Sulprizio- Renamed from INIT_GEOSFP_WINDOW_TRANSPORT to
INIT_WINDOW_TRANSPORT for use with all nested
```

3.1.8 cleanup_transport

Subroutine CLEANUP_TRANSPORT deallocates all module arrays.

grids

INTERFACE:

SUBROUTINE CLEANUP_TRANSPORT

REVISION HISTORY:

```
10 Mar 2003 - R. Yantosca - Initial version
(1 ) Remove reference to DSIG, it's obsolete. (bmy, 6/24/03)
(2 ) Remove obsolete embedded chemistry arrays (bmy, 10/30/07)
26 Feb 2010 - R. Yantosca - Added ProTeX headers
12 Feb 2015 - E. Lundgren - Added new diagnostics arrays for netcdf output
```

3.2 Fortran: Module Interface pjc_pfix_mod.F

Module Pjc_Pfix_Mod contains routines which implements the Philip Cameron-Smith pressure fixer for the new fvDAS transport scheme. (bdf, bmy, 5/8/03, 10/27/03)

INTERFACE:

```
MODULE Pjc_Pfix_Mod
```

USES:

```
USE PRECISION_MOD ! For GEOS-Chem Precision (fp)
```

IMPLICIT NONE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: Do_Pjc_Pfix
PUBLIC :: Cleanup_Pjc_Pfix

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: Calc_Pressure

PRIVATE :: Calc_Advection_Factors

PRIVATE :: Adjust_Press
PRIVATE :: Init_Press_Fix
PRIVATE :: Do_Press_Fix_LLNL
PRIVATE :: Average_Press_Poles

PRIVATE :: Convert_Winds

PRIVATE :: Calc_Horiz_Mass_Flux
PRIVATE :: Calc_Divergence
PRIVATE :: Set_Press_Terms

PRIVATE :: Do_Divergence_Pole_Sum

PRIVATE :: Xpavg

PRIVATE :: Init_Pjc_Pfix

AUTHOR:

Philip Cameron-Smith and John Tannahill, GMI project @ LLNL (2003) Brendan Field and Bob Yantosca (5/8/03) Modified for new GMI TPCORE by Claire Carouge (ccarouge@seas.harvard.edu)

REVISION HISTORY:

- (1) Bug fix for Linux/PGI compiler in routines ADJUST_PRESS and INIT_PRESS_FIX. (bmy, 6/23/03)
- (2) Now make P1, P2 true surface pressure in D0_PJC_PFIX (bmy, 10/27/03)
- 01 Mar 2012 R. Yantosca Now reference new grid_mod.F90
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 19 Nov 2014 M. Yannetti Added PRECISION_MOD
- 29 Nov 2016 R. Yantosca grid_mod.F90 is now gc_grid_mod.F90

3.2.1 Do_Pjc_Pfix

Subroutine Do_Pjc_Pfix is the driver routine for the Philip Cameron-Smith pressure fixer for the fvDAS transport scheme. (bdf, bmy, 5/8/03, 3/5/07)

We assume that the winds are on the A-GRID, since this is the input that the fvDAS transport scheme takes. (bdf, bmy, 5/8/03)

INTERFACE:

SUBROUTINE Do_Pjc_Pfix(D_DYN, P1, P2, UWND, VWND, XMASS, YMASS)

USES:

```
USE CMN_SIZE_MOD   ! Size parameters
USE PhysConstants   ! Physical constants
```

INPUT PARAMETERS:

```
! Dynamic timestep [s]
REAL(fp), INTENT(IN) :: D_DYN

! True PSurface at middle of dynamic timestep [hPa]
REAL(fp), INTENT(IN) :: P1(:,:)

! True PSurface at end of dynamic timestep [hPa]
REAL(fp), INTENT(IN) :: P2(:,:)

! Zonal (E-W) wind [m/s]
REAL(fp), INTENT(IN) :: UWND(IIPAR, JJPAR, LLPAR)

! Meridional (N-S) wind [m/s]
REAL(fp), INTENT(IN) :: VWND(IIPAR, JJPAR, LLPAR)
```

OUTPUT PARAMETERS:

```
! E-W mass fluxes [mixing ratio]
REAL(fp), INTENT(OUT) :: XMASS(IIPAR,JJPAR,LLPAR)
! N-S mass fluxes [mixing ratio]
REAL(fp), INTENT(OUT) :: YMASS(IIPAR,JJPAR,LLPAR)
```

AUTHOR:

Brendan Field and Bob Yantosca (5/8/03)

REMARKS:

- (1) Now P1 and P2 are "true" surface pressures, and not PS-PTOP. If using this P-fixer w/ GEOS-3 winds, pass true surface pressure to this routine. (bmy, 10/27/03)
- (2) Now define P2_TMP array for passing to ADJUST_PRESS (yxw, bmy, 3/5/07)

REVISION HISTORY:

```
02 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Declare all REAL variables as REAL(fp).

04 Nov 2013 - M. Sulprizio- Eliminate array temporaries by accepting assumed-shape dummy arguments
```

3.2.2 Calc_Pressure

Subroutine Calc_Pressure recalculates the new surface pressure from the adjusted air masses XMASS and YMASS. This is useful for debugging purposes. (bdf, bmy, 5/8/03)

INTERFACE:

```
SUBROUTINE Calc_Pressure( XMASS, YMASS, RGW_FV, PS_NOW, PS_AFTER )
```

USES:

```
USE CMN_SIZE_MOD ! Size parameters
```

INPUT PARAMETERS:

```
! E-W mass flux from pressure fixer
REAL(fp), INTENT(IN) :: XMASS(IIPAR, JJPAR, LLPAR)
! N-S mass flux from pressure fixer
REAL(fp), INTENT(IN) :: YMASS(IIPAR, JJPAR, LLPAR)
! Surface pressure - PTOP at current time
REAL(fp), INTENT(IN) :: PS_NOW(IIPAR, JJPAR)
! 1 / (SINE(J+1) - SINE(J)) -- latitude factor
REAL(fp), INTENT(IN) :: RGW_FV(JJPAR)
```

OUTPUT PARAMETERS:

```
! Surface pressure - PTOP adjusted by P-fixer
REAL(fp), INTENT(OUT) :: PS_AFTER(IIPAR,JJPAR)
```

AUTHOR:

Brendan Field and Bob Yantosca (5/8/03)

REVISION HISTORY:

```
02 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Declare all REAL variables as REAL(fp).

23 Jul 2014 - R. Yantosca - Removed reference to obsolete CMN_mod.F
```

3.2.3 Calc_Advection_Factors

Subroutine Calc_Advection_Factors calculates the relative area of each grid box, and the geometrical factors used by this modified version of TPCORE. These geomoetrical DO assume that the space is regularly gridded, but do not assume any link between the surface area and the linear dimensions.

INTERFACE:

```
SUBROUTINE Calc_Advection_Factors
& (mcor, rel_area, geofac, geofac_pc)
```

USES:

```
USE CMN_SIZE_MOD   ! Size parameters
USE PhysConstants  ! Physical constants
```

INPUT PARAMETERS:

```
! Area of grid box (m^2)
REAL(fp), INTENT(IN) :: mcor(i1_gl :i2_gl, ju1_gl:j2_gl)
```

OUTPUT PARAMETERS:

```
! relative surface area of grid box (fraction)
REAL(fp), INTENT(OUT) :: rel_area(i1_gl :i2_gl, ju1_gl:j2_gl)
! Geometrical factor for meridional advection; geofac uses
! correct spherical geometry, and replaces acosp as the
! meridional geometrical factor in tpcore
REAL(fp), INTENT(OUT) :: geofac(ju1_gl:j2_gl)
! Special geometrical factor (geofac) for Polar cap
REAL(fp), INTENT(OUT) :: geofac_pc
```

AUTHOR:

Philip Cameron-Smith and John Tannahill, GMI project @ LLNL (2003)

REMARKS:

Now reference PI from "CMN_GCTM" for consistency. Also force double-precision with the "D" exponent. (bmy, 5/6/03)

REVISION HISTORY:

02 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers. Declare all REAL variables as REAL(fp).

3.2.4 Adjust_Press

Subroutine Adjust_Press initializes and calls the pressure fixer code.

INTERFACE:

```
SUBROUTINE Adjust_Press
```

- & (metdata_name_org, do_timinterp_winds, new_met_rec,
- & met_grid_type, advec_consrv_opt, pmet2_opt, press_fix_opt,
- & tdt, geofac_pc, geofac, cose, cosp, rel_area, dap, dbk,
- & pctm1, pctm2, pmet2, uu, vv, xmass, ymass)

INPUT PARAMETERS:

```
! First part of metdata_name, e.g., "NCAR"
CHARACTER(LEN=*) :: metdata_name_org
! Time interpolate wind fields?
LOGICAL :: do_timinterp_winds
! New met record?
LOGICAL :: new_met_rec
! Met grid type, A or C
INTEGER :: met_grid_type
! Advection_conserve option
INTEGER :: advec_consrv_opt
! pmet2 option
INTEGER :: pmet2_opt
! pressure fixer option
INTEGER :: press_fix_opt
! Model time step [s]
REAL(fp) :: tdt
! Special geometrical factor (geofac) for Polar cap
REAL(fp) :: geofac_pc
! Geometrical factor for meridional advection; geofac uses
! correct spherical geometry, and replaces acosp as the
! meridional geometrical factor in tpcore
REAL(fp) :: geofac (ju1_gl:j2_gl)
! Cosines of grid box edges and centers
REAL(fp) :: cose (ju1_gl:j2_gl)
REAL(fp) :: cosp (ju1_gl:j2_gl)
! Pressure difference across layer from (ai * pt) term [hPa]
REAL(fp) :: dap
                    (k1:k2)
! Difference in bi across layer - the dSigma term
REAL(fp) :: dbk
                    (k1:k2)
! Relative surface area of grid box (fraction)
REAL(fp) :: rel_area( i1_gl:i2_gl,
                                     ju1_gl:j2_gl)
! Metfield surface pressure at t1+tdt [hPa]
```

```
REAL(fp) :: pmet2(ilo_gl:ihi_gl, julo_gl:jhi_gl)
      ! CTM surface pressure at t1 [hPa]
      REAL(fp) :: pctm1(ilo_gl:ihi_gl, julo_gl:jhi_gl)
      ! CTM surface pressure at t1+tdt [hPa]
      REAL(fp) :: pctm2(ilo_gl:ihi_gl, julo_gl:jhi_gl)
      ! Wind velocity, x direction at t1+tdt/2 [m/s]
      REAL(fp) :: uu(ilo_gl:ihi_gl, julo_gl:jhi_gl, k1_gl:k2_gl)
      ! Wind velocity, y direction at t1+tdt/2 [m/s]
      REAL(fp) :: vv(ilo_gl:ihi_gl, julo_gl:jhi_gl, k1_gl:k2_gl)
INPUT/OUTPUT PARAMETERS:
      ! Horizontal mass flux in E-W direction [hPa]
      REAL(fp) :: xmass(ilo_gl:ihi_gl, julo_gl:jhi_gl, k1_gl:k2_gl)
      ! Horizontal mass flux in N-S direction [hPa]
      REAL(fp) :: ymass(ilo_gl:ihi_gl, julo_gl:jhi_gl, k1_gl:k2_gl)
AUTHOR:
```

Philip Cameron-Smith and John Tannahill, GMI project @ LLNL (2003)

REVISION HISTORY:

02 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers. Declare all REAL variables as REAL(fp).

3.2.5 Init_Press_Fix

Subroutine Init_Press_Fix initializes the pressure fixer.

! Model Time step [s]

INTERFACE:

```
SUBROUTINE Init_Press_Fix
     & (metdata_name_org, met_grid_type, tdt, geofac_pc, geofac,
         cose, cosp, dap, dbk, dps, dps_ctm, rel_area, pctm1, pmet2,
     & uu, vv, xmass, ymass)
INPUT PARAMETERS:
```

```
REAL(fp) :: tdt
! First part of metdata_name, e.g., "NCAR"
CHARACTER(LEN=*) :: metdata_name_org
```

```
! Met grid type, A or C
       TNTEGER.
                        :: met_grid_type
       ! Special geometrical factor (geofac) for Polar cap
      REAL(fp)
                          :: geofac_pc
       ! Cosine of grid box edges and centers
       REAL(fp)
                         :: cose(ju1_gl:j2_gl)
      REAL(fp)
                         :: cosp(ju1_gl:j2_gl)
       ! Geometrical factor for meridional advection; geofac uses
       ! correct spherical geometry, and replaces acosp as the
       ! meridional geometrical factor in tpcore
      REAL(fp)
                          :: geofac(ju1_gl:j2_gl)
       ! Pressure difference across layer from (ai * pt) term [hPa]
      REAL(fp)
                         :: dap(k1:k2)
       ! Difference in bi across layer - the dSigma term
      REAL(fp)
                         :: dbk(k1:k2)
       ! relative surface area of grid box (fraction)
      REAL(fp)
                         :: rel_area( i1_gl:i2_gl, ju1_gl:j2_gl)
       ! Metfield surface pressure at t1 [hPa]
      REAL(fp)
                         :: pmet2(ilo_gl:ihi_gl, julo_gl:jhi_gl)
       ! CTM surface pressure at t1 [hPa]
       REAL(fp)
                         :: pctm1(ilo_gl:ihi_gl, julo_gl:jhi_gl)
       ! CTM surface pressure at t1+tdt [hPa]
      REAL(fp)
                         :: pctm2(ilo_gl:ihi_gl, julo_gl:jhi_gl)
       ! Wind velocity, x direction at t1+tdt/2 [m/s]
      REAL(fp)
                        :: uu(ilo_gl:ihi_gl, julo_gl:jhi_gl, k1_gl:k2_gl)
       ! Wind velocity, y direction at t1+tdt/2 [m/s]
      REAL(fp)
                        :: vv(ilo_gl:ihi_gl, julo_gl:jhi_gl, k1_gl:k2_gl)
OUTPUT PARAMETERS:
       ! Horizontal mass flux in E-W direction [hPa]
      REAL(fp) :: xmass(ilo_gl:ihi_gl, julo_gl:jhi_gl, k1_gl:k2_gl)
       ! Horizontal mass flux in N-S direction [hPa]
      REAL(fp) :: ymass(ilo_gl:ihi_gl, julo_gl:jhi_gl, k1_gl:k2_gl)
       ! Change of surface pressure from met field pressure [hPa]
```

```
REAL(fp) :: dps(i1_gl:i2_gl, ju1_gl:j2_gl)
! CTM surface pressure tendency [hPa]
REAL(fp) :: dps_ctm(i1_gl:i2_gl, ju1_gl:j2_gl)
```

AUTHOR:

Philip Cameron-Smith and John Tannahill, GMI project @ LLNL (2003)

REVISION HISTORY:

```
02 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Declare all REAL variables as REAL(fp).
```

3.2.6 Do Press Fix Llnl

SUBROUTINE Do_Press_Fix_Llnl

Subroutine Do_Press_Fix_Llnl fixes the mass fluxes to match the met field pressure tendency.

& (geofac_pc, geofac, dbk, dps, dps_ctm, rel_area, & xmass, ymass, xmass_fixed, ymass_fixed)

INTERFACE:

```
INPUT PARAMETERS:
       ! Special geometrical factor (geofac) for Polar cap
      REAL(fp), INTENT(IN)
                            :: geofac_pc
      ! Geometrical factor for meridional advection; geofac uses
      ! correct spherical geometry, and replaces acosp as the
       ! meridional geometrical factor in tpcore
      REAL(fp), INTENT(IN)
                             :: geofac(ju1_gl:j2_gl)
      ! Difference in bi across layer - the dSigma term
      REAL(fp), INTENT(IN)
                             :: dbk(k1:k2)
      ! Change of surface pressure from met field pressure [hPa]
      REAL(fp), INTENT(IN)
                             :: dps(i1:i2, ju1:j2)
      ! Relative surface area of grid box (fraction)
      REAL(fp), INTENT(IN) :: rel_area(i1:i2, ju1:j2)
      ! Horizontal mass fluxes in E-W and N-S directions [hPa]
      REAL(fp), INTENT(IN) :: xmass(ilo:ihi, julo:jhi, k1:k2)
      REAL(fp), INTENT(IN) :: ymass(ilo:ihi, julo:jhi, k1:k2)
```

OUTPUT PARAMETERS:

```
! Sum over vertical of dpi calculated from original mass fluxes [hPa]
REAL(fp), INTENT(OUT) :: dps_ctm(i1:i2, ju1:j2)
! Horizontal mass flux in E-W and N-S directions after fixing [hPa]
REAL(fp), INTENT(OUT) :: xmass_fixed(ilo:ihi, julo:jhi, k1:k2)
REAL(fp), INTENT(OUT) :: ymass_fixed(ilo:ihi, julo:jhi, k1:k2)
```

AUTHOR:

Philip Cameron-Smith and John Tannahill, GMI project @ LLNL (2003)

REVISION HISTORY:

02 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Declare all REAL variables as REAL(fp).

3.2.7 Average_Press_Poles

Subroutine Average_Press_Poles averages pressure at the Poles when the Polar cap is enlarged. It makes the last two latitudes equal.

INTERFACE:

```
SUBROUTINE Average_Press_Poles
& (rel_area, press)
```

INPUT PARAMETERS:

```
! Relative surface area of grid box (fraction)
REAL(fp), INTENT(IN) :: rel_area(i1:i2, ju1:j2)
```

OUTPUT PARAMETERS:

```
! Surface pressure [hPa]
REAL(fp), INTENT(INOUT) :: press (ilo:ihi, julo:jhi)
```

AUTHOR:

Philip Cameron-Smith and John Tannahill, GMI project @ LLNL (2003)

REVISION HISTORY:

02 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Declare all REAL variables as REAL(fp).

3.2.8 Convert_Winds

Subroutine Convert_Winds converts winds on A or C grid to Courant # on C grid.

INTERFACE:

```
SUBROUTINE Convert_Winds
& (igd, tdt, cosp, crx, cry, uu, vv)
```

USES:

```
USE CMN_SIZE_MOD ! Size parameters
USE PhysConstants! Re, PI
```

INPUT PARAMETERS:

```
! A or C grid
INTEGER, INTENT(IN) :: igd

! Model time step [s]
REAL(fp), INTENT(IN) :: tdt

! Cosine of grid box centers
REAL(fp), INTENT(IN) :: cosp(ju1_gl:j2_gl)

! Wind velocity in E-W (UU) and N-S (VV) directions at t1+tdt/2 [m/s]
REAL(fp), INTENT(IN) :: uu (ilo:ihi, julo:jhi, k1:k2)
REAL(fp), INTENT(IN) :: vv (ilo:ihi, julo:jhi, k1:k2)
```

OUTPUT PARAMETERS:

```
! Courant number in E-W (CRX) and N-S (CRY) directions REAL(fp), INTENT(OUT) :: crx (ilo:ihi, julo:jhi, k1:k2) REAL(fp), INTENT(OUT) :: cry (ilo:ihi, julo:jhi, k1:k2)
```

AUTHOR:

Philip Cameron-Smith and John Tannahill, GMI project @ LLNL (2003)

REMARKS:

Use GEOS-CHEM physical constants Re, PI to be consistent with other usage everywhere (bmy, 5/5/03)

REVISION HISTORY:

```
02 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers. Declare all REAL variables as REAL(fp).
```

3.2.9 Calc_Horiz_Mass_Flux

Subroutine Calc_Horiz_Mass_Flux calculates the horizontal mass flux for non-GISS met data.

INTERFACE:

```
SUBROUTINE Calc_Horiz_Mass_Flux
& (cose, delpm, uu, vv, xmass, ymass, tdt, cosp)
```

USES:

```
USE CMN_SIZE_MOD ! Size parameters USE PhysConstants! Re, Pi
```

INPUT PARAMETERS:

```
! Timestep [s]
REAL(fp), INTENT(IN) :: tdt
! Cosine of grid box edges
REAL(fp), INTENT(IN) :: cose (ju1_g1:j2_g1)
! Cosine of grid box centers
REAL(fp), INTENT(IN) :: cosp (ju1_g1:j2_g1)
! Pressure thickness, the pseudo-density in a
! hdrostatic system at t1+tdt/2 (approximate) [hPa]
REAL(fp), INTENT(IN) :: delpm(ilo:ihi, julo:jhi, k1:k2)
! E-W (UU) and N-S (VV) winds [m/s]
REAL(fp), INTENT(IN) :: uu (ilo:ihi, julo:jhi, k1:k2)
REAL(fp), INTENT(IN) :: vv (ilo:ihi, julo:jhi, k1:k2)
```

OUTPUT PARAMETERS:

```
! Horizontal mass flux in E-W and N-S directions [hPa] REAL(fp), INTENT(OUT) :: xmass(ilo:ihi, julo:jhi, k1:k2) REAL(fp), INTENT(OUT) :: ymass(ilo:ihi, julo:jhi, k1:k2)
```

AUTHOR:

```
Original code from Shian-Jiann Lin, DAO John Tannahill, LLNL (jrt@llnl.gov)
```

REMARKS:

Use GEOS-CHEM physical constants Re, PI to be consistent with other usage everywhere (bmy, 5/5/03)

REVISION HISTORY:

02 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Declare all REAL variables as REAL(fp).

3.2.10 Calc_Divergence

Subroutine Calc_Divergence calculates the divergence.

INTERFACE:

```
SUBROUTINE Calc_Divergence
& (do_reduction, geofac_pc, geofac, dpi, xmass, ymass)
```

INPUT PARAMETERS:

INPUT/OUTPUT PARAMETERS:

```
! Divergence at a grid point; used to calculate vertical motion [hPa] REAL(fp), INTENT(INOUT) :: dpi (i1:i2, ju1:j2, k1:k2)
```

AUTHOR:

Philip Cameron-Smith and John Tannahill, GMI project @ LLNL (2003)

REVISION HISTORY:

```
02 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers. Declare all REAL variables as REAL(fp).
```

3.2.11 Set_Press_Terms

Subroutine Set_Press_Terms sets the pressure terms.

INTERFACE:

```
SUBROUTINE Set_Press_Terms
& (dap, dbk, pres1, pres2, delp1, delpm, pu)
```

INPUT PARAMETERS:

```
! Pressure difference across layer from (ai * pt) term [hPa]
REAL(fp), INTENT(IN) :: dap (k1:k2)
! Difference in bi across layer - the dSigma term
REAL(fp), INTENT(IN) :: dbk (k1:k2)
```

```
! Surface pressure at t1 [hPa] REAL(fp), INTENT(IN) :: pres1(ilo:ihi, julo:jhi)
```

```
! Surface pressure at t1+tdt [hPa]
REAL(fp), INTENT(IN) :: pres2(ilo:ihi, julo:jhi)
```

OUTPUT PARAMETERS:

```
! Pressure thickness, the psudo-density in a
! hydrostatic system at t1 [hPa]
REAL(fp), INTENT(OUT) :: delp1(ilo:ihi, julo:jhi, k1:k2)
! Pressure thickness, the psudo-density in a
! hydrostatic system at t1+tdt/2 (approximate) [hPa]
REAL(fp), INTENT(OUT) :: delpm(ilo:ihi, julo:jhi, k1:k2)
! Pressure at edges in "u" [hPa]
REAL(fp), INTENT(OUT) :: pu (ilo:ihi, julo:jhi, k1:k2)
```

AUTHOR:

Philip Cameron-Smith and John Tannahill, GMI project @ LLNL (2003)

REVISION HISTORY:

```
02 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Declare all REAL variables as REAL(fp).
```

3.2.12 Do_Divergence_Pole_Sum

Do_Divergence_Pole_Sum sets the divergence at the Poles.

INTERFACE:

```
SUBROUTINE Do_Divergence_Pole_Sum
& (do_reduction, geofac_pc, dpi, ymass)
```

INPUT PARAMETERS:

```
! Set to T if called on Master; set to F if called by Slaves
! (NOTE: This does not seem to be used!)
LOGICAL :: do_reduction
! Special geometrical factor (geofac) for Polar cap
REAL(fp) :: geofac_pc
! horizontal mass flux in N-S direction [hPa]
REAL(fp) :: ymass(ilo:ihi, julo:jhi, k1:k2)
```

OUTPUT PARAMETERS:

```
! Divergence at a grid point; used to calculate vertical motion [hPa] REAL(fp) :: dpi (i1:i2, ju1:j2, k1:k2)
```

AUTHOR:

Philip Cameron-Smith and John Tannahill, GMI project @ LLNL (2003)

REVISION HISTORY:

02 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Declare all REAL variables as REAL(fp).

3.2.13 Xpavg

!description: Subroutine Xpavg replaces each element of a vector with the average of the entire array. (bmy, 5/7/03)

INTERFACE:

```
SUBROUTINE Xpavg( P, IM )
```

USES:

```
! References to F90 modules USE ERROR_MOD, ONLY : ERROR_STOP
```

INPUT PARAMETERS:

```
! Dimension of P INTEGER, INTENT(IN) :: IM
```

INPUT/OUTPUT PARAMETERS:

```
! 1-D vector to be averaged REAL(fp), INTENT(INOUT) :: P(IM)
```

AUTHOR:

Philip Cameron-Smith and John Tannahill, GMI project @ LLNL (2003)

REVISION HISTORY:

02 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Now make all REAL variables REAL(fp).

3.2.14 Init_Pjc_Pfix

Subroutine Init_Pjc_Pfix allocates and initializes module arrays and variables. GMI dimension variables will be used for compatibility with the Phil Cameron-Smith P-fixer. (bdf, bmy, 5/8/03)

INTERFACE:

```
SUBROUTINE Init_Pjc_Pfix
```

USES:

```
! References to F90 modules

USE GC_GRID_MOD, ONLY : GET_AREA_M2, GET_YMID_R

USE ERROR_MOD, ONLY : ALLOC_ERR, ERROR_STOP

USE PRESSURE_MOD, ONLY : GET_AP, GET_BP

USE CMN_SIZE_MOD ! Size parameters

USE PhysConstants ! Re, PI, etc...
```

AUTHOR:

Brendan Field and Bob Yantosca (5/8/03)

REVISION HISTORY:

```
02 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.
01 Mar 2012 - R. Yantosca - Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
01 Mar 2012 - R. Yantosca - Now use GET_YMID_R(I,J,L) from grid_mod.F90
```

3.2.15 Cleanup_Pjc_Pfix

Subroutine Cleanup_Pjc_Pfix deallocates all module arrays (bmy, 5/8/03)

INTERFACE:

```
SUBROUTINE Cleanup_Pjc_Pfix
```

REVISION HISTORY:

02 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

3.3 Fortran: Module Interface tpcore_bc_mod.F

Module TPCORE_BC_MOD contains modules and variables which are needed to save and read TPCORE nested-grid boundary conditions to/from disk.

INTERFACE:

MODULE TPCORE_BC_MOD

USES:

```
USE PRECISION_MOD ! For GEOS-Chem Precision (fp)
IMPLICIT NONE
PRIVATE
```

PUBLIC DATA MEMBERS:

```
I-----
! IO_W : Lon offset of TPCORE REGION [# boxes]
! JO_W : Lat offset of TPCORE REGION [# boxes]
! IM_W : Lon extent of TPCORE REGION [# boxes]
! JM_W : Lat extent of TPCORE REGION [# boxes]
! I1_W : Lower left-hand (LL) lon index of NESTED WINDOW
! J1_W : Lower left-hand (LL) lat index of NESTED WINDOW
! I2_W : Upper right-hand (UR) lon index of NESTED WINDOW
! J2_W : Upper right-hand (UR) lat index of NESTED WINDOW
! IGZD : ???
! Please also see the diagram in the REMARKS section.
I-----
INTEGER, PUBLIC :: IO_W, JO_W
INTEGER, PUBLIC :: IO_E, JO_E
INTEGER, PUBLIC :: I1_W, J1_W
INTEGER, PUBLIC :: I2_W, J2_W
INTEGER, PUBLIC :: IM_W, JM_W
INTEGER, PUBLIC :: IGZD
```

PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: INIT_TPCORE_BC
PUBLIC :: DO_WINDOW_TPCORE_BC
```

PUBLIC :: SET_CLEAN_BC

PUBLIC :: SAVE_GLOBAL_TPCORE_BC

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: OPEN_BC_FILE

PRIVATE :: CLEAN_WINDOW_TPCORE_BC

PRIVATE :: READ_WINDOW_TPCORE_BC

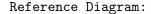
PRIVATE :: GET_4x5_BC

PRIVATE :: GET_4x5_BC_INIT

PRIVATE :: GET_2x25_BC

PRIVATE :: GET_2x25_BC_INIT
PRIVATE :: ITS_TIME_FOR_BC
PRIVATE :: CLEANUP_TPCORE_BC

REMARKS:



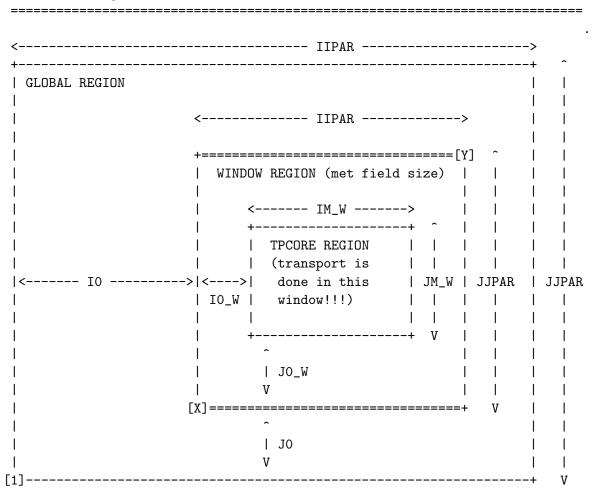


DIAGRAM NOTES:

- (a) The outermost box ("Global Region") is the global grid size. This region has IIPAR boxes in longitude and JJPAR boxes in latitude. The origin of the "Global Region" is at the south pole, at the lower left-hand corner (point [1]).
- (b) The next innermost box ("Window Region") is the nested-grid window. This region has IIPAR boxes in longitude and JJPAR boxes in latitude. This is the size of the trimmed met fields that will be used for a 1 x 1 "nested-grid" simulation.
- (c) The innermost region ("TPCORE Region") is the actual area in which TPCORE transport will be performed. Note that this region is smaller than the "Window Region". It is set up this way since a cushion of grid boxes is needed TPCORE Region for boundary conditions.
- (d) IO is the longitude offset (# of boxes) and JO is the latitude offset

(# of boxes) which translate between the "Global Region" and the "Window Region".

- (e) IO_W is the longitude offset (# of boxes), and JO_W is the latitude offset (# of boxes) which translate between the "Window Region" and the "TPCORE Region".
- (f) The lower left-hand corner of the "Window Region" (point [X]) has longitude and latitude indices (I1_W, J1_W). Similarly, the upper right-hand corner (point [Y]) has longitude and latitude indices (I2_W, J2_W).
- (g) Note that if IO=0, JO=0, IO_W=0, JO_W=0, IIPAR=IIPAR, JJPAR=JJPAR specifies a global simulation. In this case the "Window Region" totally coincides with the "Global Region".
- (h) In order for the nested-grid to work we must save out concentrations over the WINDOW REGION from a coarse model (e.g. 4x5) corresponding to the same WINDOW REGION at 1x1. These concentrations are copied along the edges of the 1x1 WINDOW REGION and are thus used as boundary conditions for TPCORE.

REVISION HISTORY:

- 04 Mar 2003 R. Yantosca Initial version
- (1) Bug fix for LINUX w/ TIMESTAMP_STRING (bmy, 9/29/03)
- (3) Now get HALFPOLAR for GEOS or GCAP grids (bmy, 6/28/05)
- (4) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (5) Rename arguments in GET_4x5_BC to avoid name conflict (bmy, 10/24/05)
- (6) Now use EXPAND_DATE instead of obsolete DATE_STRING (bmy, 3/15/06)
- (7) Added 2x2.5 boundary condition output (created GET_2x25_BC). Added multi-boundary condition output (NA, EU, CH and Custom region). Unternally defined boundary condition regions for NA, EU and CH. (amv, bmy, 12/18/09)
- 16 Feb 2011 R. Yantosca Add modifications for APM microphysics (G. Luo)
- 01 Mar 2012 R. Yantosca Now reference new grid_mod.F90
- 15 May 2012 R. Yantosca Added ProTeX headers
- 06 Aug 2012 R. Yantosca Now make IU_BC, IU_BC_NA, IU_BC_EU, IU_BC_CH local variables for findFreeLUN
- 07 Sep 2012 R. Yantosca Minor fixes for numerical stability
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 21 Nov 2014 M. Yannetti Added PRECISION_MOD
- 01 Apr 2015 R. Yantosca Now add IO_E and JO_E
- 03 Aug 2015 M. Sulprizio- Now make BC and BC_CU separate arrays to avoid confusion and error
- 23 Jun 2016 R. Yantosca Remove references to APM code; it is no longer compatible with the FlexChem implementation

```
29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90
```

3.3.1 set_clean_bc

Subroutine SET_CLEAN_BC initializes the CLEAN_BC logical flag. CLEAN_BC decides whether or not we will zero the nested-grid tpcore boundary conditions.

INTERFACE:

```
SUBROUTINE SET_CLEAN_BC( THIS_CLEAN_BC )
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: THIS_CLEAN_BC
```

REVISION HISTORY:

```
04 Mar 2003 - R. Yantosca - Initial versioni
15 May 2012 - R. Yantosca - Added ProTeX headers
```

3.3.2 open_bc_file

Subroutine OPEN_BC_FILE opens the file which contains boundary conditions saved from the coarse-grid WINDOW REGION for either reading or writing.

ONLY : OPEN_BPCH2_FOR_WRITE

INTERFACE:

```
SUBROUTINE OPEN_BC_FILE( am_I_Root, Input_Opt, RC, WINDOW, FOR_READ, FOR_WRITE )
```

USES:

```
USE BPCH2_MOD, ONLY : OPEN_BPCH2_FOR_READ
USE ErrCode_Mod
USE Input_Opt_Mod, ONLY : OptInput
USE inquireMod, ONLY : findFreeLUN
USE TIME_MOD, ONLY : EXPAND_DATE, GET_NYMD
USE TIME_MOD, ONLY : ITS_A_NEW_DAY
```

INPUT PARAMETERS:

USE BPCH2_MOD,

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

LOGICAL, INTENT(IN), OPTIONAL :: FOR_READ ! Open file for read?

LOGICAL, INTENT(IN), OPTIONAL :: FOR_WRITE ! Open file for write?

INTEGER, INTENT(IN) :: WINDOW ! Specifies nested region
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

```
Pass these values via the WINDOW argument to do the following actions;
WINDOW = 1 : Save BC's to file (Custom window, aka "CU")
WINDOW = 2 : Save BC's to file (North America window, aka "NA")
WINDOW = 3 : Save BC's to file (Europe window, aka "EU")
WINDOW = 4 : Save BC's to file (China/SE Asia window, aka "CH")
WINDOW = 5 : Read BC's from file
```

REVISION HISTORY:

3.3.3 save_global_tpcore_bc

Subroutine SAVE_GLOBAL_TPCORE_BC saves concentrations from the WINDOW RE-GION of a coarse-resolution model run to a bpch file. A new boundary conditions file is created for each day.

INTERFACE:

```
SUBROUTINE SAVE_GLOBAL_TPCORE_BC( am_I_Root, Input_Opt, & State_Chm, RC
```

USES:

```
USE BPCH2_MOD

USE CMN_SIZE_MOD

USE ErrCode_Mod

USE Input_Opt_Mod, ONLY : OptInput

USE State_Chm_Mod, ONLY : ChmState

USE TIME_MOD, ONLY : GET_NYMD, GET_NHMS

USE TIME_MOD, ONLY : GET_TAU, TIMESTAMP_STRING

USE UnitConv_Mod
```

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

- 04 Mar 2003 Y. Wang Initial version
- (1) Now references N_TRACERS and STT from "tracer_mod.f". Also now references TIMESTAMP_STRING from "time_mod.f". (bmy, 7/20/04)
- (2) Now call GET_HALFPOLAR from "bpch2_mod.f" to get the HALFPOLAR flag value for GEOS or GCAP grids (bmy, 6/28/05)
- (3) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (4) Can now save files to different directories (amv, bmy, 12/18/09)
- 16 Feb 2011 R. Yantosca Add modifications for APM microphysics (G. Luo)
- 15 May 2012 R. Yantosca Added ProTeX headers
- 06 Aug 2012 R. Yantosca Added comments & cosmetic changes
- 06 Aug 2012 R. Yantosca Now use file unit variables from this module instead of from GeosUtil/file_mod.F
- 25 Mar 2013 R. Yantosca Now accept am_I_Root, Input_Opt, State_Chm, RC
- 17 Dec 2014 R. Yantosca Leave time/date variables as 8-byte
- 17 Feb 2014 E. Lundgren Move temporary unit change to vol/vol to within this subroutine
- 13 Aug 2015 E. Lundgren Tracer units are now [kg/kg dry air]
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.
- 03 Aug 2016 R. Yantosca Remove temporary tracer removal code

3.3.4 do_window_tpcore_bc

Subroutine DO_WINDOW_TPCORE_BC is a driver routine for assigning TPCORE boundary conditions to the tracer array Spc.

INTERFACE:

USES:

USE CMN_SIZE_MOD

USE ErrCode_Mod

USE Input_Opt_Mod, ONLY : OptInput USE State_Chm_Mod, ONLY : ChmState

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INPUT/OUTPUT PARAMETERS:

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

- 07 Mar 2003 R. Yantosca Initial version
- (1) Now references N_TRACERS and STT from "tracer_mod.f" (bmy, 7/20/04)
- (2) Now can use 2×2.5 BC's (amv, bmy, 12/18/09)
- 16 Feb 2011 R. Yantosca Add modifications for APM microphysics (G. Luo)
- 08 Dec 2009 R. Yantosca Added ProTeX headers
- 25 Mar 2013 R. Yantosca Now accept am_I_Root, Input_Opt, State_Chm, RC
- 13 Aug 2014 E. Lundgren Tracer units are now [kg/kg dry air]
- 03 Aug 2016 R. Yantosca Remove temporary tracer removal code

3.3.5 clean_window_tpcore_bc

Subroutine CLEAN_WINDOW_TPCORE_BC zeroes the boundary conditions array BC at each timestep. (bmy, 3/7/03, 12/18/09)

INTERFACE:

SUBROUTINE CLEAN_WINDOW_TPCORE_BC(am_I_Root, Input_Opt, RC)

USES:

USE CMN_SIZE_MOD USE ErrCode_Mod

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

```
07 Mar 2003 - M. Prather - Initial version
(1 ) Now references N_TRACERS from "tracer_mod.f" (bmy, 7/20/04)
(2) Now zeroes the arrays for the different regions (amv, bmy, 12/18/09)
16 Feb 2011 - R. Yantosca - Add modifications for APM microphysics (G. Luo)
15 May 2012 - R. Yantosca - Added ProTeX headers
07 Sep 2012 - R. Yantosca - Simplify coding, remove parallel loops
07 Sep 2012 - R. Yantosca - Now use 0e+0_fp instead of 0e0 to zero BC arrays
25 Mar 2013 - R. Yantosca - Now accept am_I_Root, Input_Opt, RC
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
26 Sep 2013 - R. Yantosca - Removed SEAC4RS C-preprocessor switch
```

3.3.6 read_window_tpcore_bc

Subroutine READ_WINDOW_TPCORE_BC reads tracer concentrations saved on the WIN-DOW REGION of a coarse-grid simulation (e.g. 4x5, 2x2.5). These concentrations will be used as boundary conditions for TPCORE transport.

INTERFACE:

```
SUBROUTINE READ_WINDOW_TPCORE_BC( am_I_Root, Input_Opt,
                                   State_Chm, RC
&
```

USES:

```
USE CMN_SIZE_MOD
USE ErrCode_Mod
```

USE FILE_MOD, ONLY : IOERROR ONLY : Open ONLY : ChmState USE Input_Opt_Mod, USE State_Chm_Mod,

USE TIME_MOD, ONLY: GET_TAU, TIMESTAMP_STRING

INPUT PARAMETERS:

```
:: am_I_Root ! Are we on the root CPU?
               INTENT(IN)
LOGICAL,
TYPE(OptInput), INTENT(IN)
                              :: Input_Opt    ! Input Options object
```

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry state object

OUTPUT PARAMETERS:

INTENT(OUT) :: RC ! Success or failure? INTEGER,

REVISION HISTORY:

```
07 Mar 2003 - R. Yantosca - Initial version
```

(1) LINUX has a problem putting a function call w/in a WRITE statement. Now save output from TIMESTAMP_STRING to STAMP and print that. (bmy, 9/29/03)

- (2) Now references N_TRACERS from "tracer_mod.f" (bmy, 7/20/04)
- (3) Rewritten to be more generic (amv, bmy, 12/18/09)
- 15 May 2012 R. Yantosca Added ProTeX headers
- 25 Mar 2013 R. Yantosca Now accept am_I_Root, Input_Opt, State_Chm, RC

$3.3.7 \text{ get}_4x5_bc_init$

Function GET_4x5_BC_INIT initializes the MAP1x1 arrays.

INTERFACE:

SUBROUTINE GET_4x5_BC_INIT

USES:

```
USE CMN_SIZE_MOD
USE GC_GRID_MOD, ONLY : GET_XMID, GET_YMID
```

REMARKS:

NOTE: This routine was originally written for the 1 x 1 nested grid, but this now works for the GEOS-5 0.5 x 0.666 nested grid data. Keep variable names I_1x1 , J_1x1 , etc. unchanged for the present.

For now we will assume that we have saved tracer concentrations from a 4x5 window which overlays the corresponding 1x1 WINDOW REGION. These 4x5 tracer concentrations are used as boundary conditions for TPCORE.

REVISION HISTORY:

- 07 Mar 2003 Y. Wang, R. Yantosca Initial version
- (1) Rename arguments to avoid conflict w/ I1x1, J1x1 parameters in CMN_SIZE. (bmy, 10/24/05)
- 01 Mar 2012 R. Yantosca Now use GET_XMID(I,J,L) from grid_mod.F90
- 01 Mar 2012 R. Yantosca Now use GET_YMID(I,J,L) from grid_mod.F90
- 15 May 2012 R. Yantosca Added ProTeX headers
- 10 Nov 2014 C. Keller Split off from GET_4x5_BC

$3.3.8 \text{ get}_4x5_bc$

Function GET_4x5_BC returns a value from the 4x5 BC boundary conditions array at the location of a nested grid box.

INTERFACE:

```
FUNCTION GET_4x5_BC( I_1x1, J_1x1, L_1x1, N_1x1 ) RESULT( VALUE )
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I_1x1  ! Nested-grid lon index
INTEGER, INTENT(IN) :: J_1x1  ! Nested-grid lat index
INTEGER, INTENT(IN) :: L_1x1  ! Nested-grid level index
INTEGER, INTENT(IN) :: N_1x1  ! Nested-grid tracer index
```

RETURN VALUE:

REAL(fp) :: VALUE ! 4 x 5 BC @ location of nested grid box

REMARKS:

NOTE: This routine was originally written for the 1 x 1 nested grid, but this now works for the GEOS-5 0.5 x 0.666 nested grid data. Keep variable names I_1x1 , J_1x1 , etc. unchanged for the present.

For now we will assume that we have saved tracer concentrations from a 4x5 window which overlays the corresponding 1x1 WINDOW REGION. These 4x5 tracer concentrations are used as boundary conditions for TPCORE.

REVISION HISTORY:

- 07 Mar 2003 Y. Wang, R. Yantosca Initial version
- (1) Rename arguments to avoid conflict w/ I1x1, J1x1 parameters in CMN_SIZE. (bmy, 10/24/05)
- 01 Mar 2012 R. Yantosca Now use GET_XMID(I,J,L) from grid_mod.F90
- 01 Mar 2012 R. Yantosca Now use GET_YMID(I,J,L) from grid_mod.F90
- 15 May 2012 R. Yantosca Added ProTeX headers
- 10 Nov 2014 C. Keller Now initialize MAP1x1 array in separate routine

$3.3.9 \text{ get}_2x25\text{-bc}_i$ nit

Function GET_2x25_BC_INIT initializes the 2x25 mapping values.

INTERFACE:

SUBROUTINE GET_2x25_BC_INIT

USES:

```
USE CMN_SIZE_MOD
```

USE GC_GRID_MOD, ONLY : GET_XMID, GET_YMID

RETURN VALUE:

REMARKS:

NOTE: This routine was originally written for the 1 x 1 nested grid, but this now works for the GEOS-5 0.5 x 0.666 nested grid data. Keep variable names I_1x1 , J_1x1 , etc. unchanged for the present.

For now we will assume that we have saved tracer concentrations from a 2 x 2.5 window which overlays the corresponding NESTED WINDOW REGION. These 2 x 2.5 tracer concentrations are used as boundary conditions for TPCORE.

REVISION HISTORY:

```
18 Dec 2009 - A. van Donkeelar - Initial version
01 Mar 2012 - R. Yantosca - Now use GET_XMID(I,J,L) from grid_mod.F90
01 Mar 2012 - R. Yantosca - Now use GET_YMID(I,J,L) from grid_mod.F90
15 May 2012 - R. Yantosca - Added ProTeX headers
10 Nov 2014 - C. Keller - Split off from GET_2x25_BC. Now account for high-res midpoints on edges.
```

3.3.10 get_2x25_bc

Function GET_2x25_BC returns a value from the 2 x 2.5 BC boundary conditions array at the location of a nested grid box.

INTERFACE:

```
FUNCTION GET_2x25_BC( I_1x1, J_1x1, L_1x1, N_1x1 ) RESULT( VALUE ) USES:
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I_1x1 ! Nested-grid lon index
INTEGER, INTENT(IN) :: J_1x1 ! Nested-grid lat index
INTEGER, INTENT(IN) :: L_1x1 ! Nested-grid level index
INTEGER, INTENT(IN) :: N_1x1 ! Nested-grid tracer index
```

RETURN VALUE:

```
REAL(fp) :: VALUE ! 2 x 2.5 BC @ location of nested grid box
```

REMARKS:

NOTE: This routine was originally written for the 1 x 1 nested grid, but this now works for the GEOS-5 0.5 x 0.666 nested grid data. Keep variable names I_1x1 , J_1x1 , etc. unchanged for the present.

For now we will assume that we have saved tracer concentrations from a 2 x 2.5 window which overlays the corresponding NESTED WINDOW REGION. These 2×2.5 tracer concentrations are used as boundary conditions for TPCORE.

REVISION HISTORY:

```
18 Dec 2009 - A. van Donkeelar - Initial version
01 Mar 2012 - R. Yantosca - Now use GET_XMID(I,J,L) from grid_mod.F90
01 Mar 2012 - R. Yantosca - Now use GET_YMID(I,J,L) from grid_mod.F90
15 May 2012 - R. Yantosca - Added ProTeX headers
10 Nov 2014 - C. Keller - Now initialize MAP1x1 array in separate routine Also account for high-res midpoint on edges.
```

3.3.11 its_time_for_bc

Subroutine ITS_TIME_FOR_BC returns TRUE if it is time to read in the next set of boundary conditions for TPCORE, or FALSE otherwise.

INTERFACE:

```
FUNCTION ITS_TIME_FOR_BC() RESULT( FLAG )
```

USES:

```
USE TIME_MOD, ONLY : GET_ELAPSED_MIN
```

RETURN VALUE:

REVISION HISTORY:

```
05 Mar 2003 - R. Yantosca - Initial version
15 May 2012 - R. Yantosca - Added ProTeX headers
```

3.3.12 init_tpcore_bc

Subroutine INIT_TPCORE_BC initializes module variables and arrays.

INTERFACE:

```
SUBROUTINE INIT_TPCORE_BC( am_I_Root, Input_Opt, State_Chm, RC )
```

USES:

```
USE CMN_SIZE_MOD

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ALLOC_ERR

USE GC_GRID_MOD, ONLY : GET_XOFFSET, GET_YOFFSET

USE GC_GRID_MOD, ONLY : ITS_A_NESTED_GRID

USE Input_Opt_Mod, ONLY : OptInput

USE State_Chm_Mod, ONLY : ChmState
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REVISION HISTORY:

17 Oct 2012 - M. Payer - Bug fix: Define extent of coarse grid BC region even if LWINDO_CH = False to avoid out-of-bounds errors in array BC

```
of Jun 2013 - K. Yu - Define BC boundaries for GEOS_57 0.25 NA grid 20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete 26 Sep 2013 - R. Yantosca - Removed SEAC4RS C-preprocessor switch 26 Sep 2013 - R. Yantosca - Renamed GEOS_57 Cpp switch to GEOS_FP 01 Apr 2015 - L. Zhang - IM_W, JM_W are no longer symmetric, but are computed from IO_E and JO_E
```

3.3.13 cleanup_tpcore_bc

Subroutine CLEANUP_TPCORE_BC deallocates all module arrays.

INTERFACE:

SUBROUTINE CLEANUP_TPCORE_BC

REVISION HISTORY:

```
04 Mar 2003 - R. Yantosca - Initial version
15 May 2012 - R. Yantosca - Added ProTeX headers
```

3.4 Fortran: Module Interface tpcore_fvdas_mod.F90

Overview

Module Tpcore_Fvdas_Mod contains routines for the TPCORE transport scheme, as implemented in the GMI model (cf. John Tannahill), based on Lin Rood 1995. The Harvard Atmospheric Chemistry Modeling Group has added modifications to implement the Philip-Cameron Smith pressure fixer for mass conservation. Mass flux diagnostics have also been added.

References

- 1. Lin, S.-J., and R. B. Rood, 1996: Multidimensional flux form semi-Lagrangian transport schemes, Mon. Wea. Rev., 124, 2046-2070.
- 2. Lin, S.-J., W. C. Chao, Y. C. Sud, and G. K. Walker, 1994: A class of the van Leertype transport schemes and its applications to the moisture transport in a General Circulation Model, Mon. Wea. Rev., 122, 1575-1593.

Selecting E/W, N/S and vertical advection options

The flags IORD, JORD, KORD select which transport schemes are used in the E/W, N/S, and vertical directions, respectively. Here is a list of the possible values that IORD, JORD, KORD may be set to (original notes from S-J Lin):

- 1. 1st order upstream scheme (too diffusive, not a real option; it can be used for debugging purposes; this is THE only known "linear" monotonic advection scheme.).
- 2. 2nd order van Leer (full monotonicity constraint; see Lin et al 1994, MWR)
- 3. monotonic PPM* (Collela & Woodward 1984)
- 4. semi-monotonic PPM (same as 3, but overshoots are allowed)
- 5. positive-definite PPM (constraint on the subgrid distribution is only strong enough to prevent generation of negative values; both overshoots & undershoots are possible).
- 6. un-constrained PPM (nearly diffusion free; faster but positivity of the subgrid distribution is not quaranteed. Use this option only when the fields and winds are very smooth.
- 7. Huynh/Van Leer/Lin full monotonicity constraint. Only KORD can be set to 7 to enable the use of Huynh's 2nd monotonicity constraint for piece-wise parabolic distribution.

Recommended values:

- IORD=JORD=3 for high horizontal resolution.
- KORD=3 or 7

The implicit numerical diffusion decreases as _ORD increases. DO NOT use option 4 or 5 for non-positive definite scalars (such as Ertel Potential Vorticity).

In GEOS-Chem we have been using IORD=3, JORD=3, KORD=7. We have tested the OpenMP parallelization with these options. GEOS-Chem users who wish to use different (I,J,K)ORD options should consider doing single-processor vs. multi-processor tests to test the implementation of the parallelization.

GEOS-4 and GEOS-5 Hybrid Grid Definition

For GEOS-4 and GEOS-5 met fields, the pressure at the bottom edge of grid box (I,J,L) is defined as follows:

$$P_{edge}(I, J, L) = A_k(L) + [B_k(L) * P_{surface}(I, J)]$$

where

- $P_{surface}(I,J)$ is the "true" surface pressure at lon,lat (I,J)
- $A_k(L)$ has the same units as surface pressure [hPa]
- $B_k(L)$ is a unitless constant given at level edges

 $A_k(L)$ and $B_k(L)$ are supplied to us by GMAO.

REMARKS:

Note: surface pressure can be of any unit (e.g., pascal or mb) as long as it is consistent with the definition of (ak, bk) defined above. Winds (u,v), ps, and q are assumed to be defined at the same points.

The latitudes are given to the initialization routine: init_tpcore.

INTERFACE:

MODULE Tpcore_FvDas_Mod

USES:

USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

IMPLICIT NONE

PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: Init_Tpcore
PUBLIC :: Exit_Tpcore
PUBLIC :: Tpcore_FvDas

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: Average_Const_Poles
PRIVATE :: Set_Cross_Terms
PRIVATE :: Calc_Vert_Mass_Flux

PRIVATE :: Set_Jn_Js

PRIVATE :: Calc_Advec_Cross_Terms

PRIVATE :: Qckxyz PRIVATE :: Set_Lmts

PRIVATE :: Set_Press_Terms
PRIVATE :: Calc_Courant
PRIVATE :: Calc_Divergence

PRIVATE :: Do_Divergence_Pole_Sum
PRIVATE :: Do_Cross_Terms_Pole_I2d2

PRIVATE :: Xadv_Dao2
PRIVATE :: Yadv_Dao2

PRIVATE :: Do_Yadv_Pole_I2d2
PRIVATE :: Do_Yadv_Pole_Sum

PRIVATE :: Xtp
PRIVATE :: Xmist
PRIVATE :: Fxppm
PRIVATE :: Lmtppm
PRIVATE :: Ytp
PRIVATE :: Ymist

PRIVATE :: Do_Ymist_Pole1_I2d2
PRIVATE :: Do_Ymist_Pole2_I2d2

PRIVATE :: Fyppm

PRIVATE :: Do_Fyppm_Pole_I2d2
PRIVATE :: Do_Ytp_Pole_Sum

PRIVATE :: Fzppm

PRIVATE :: Average_Press_Poles

!PRIVATE DATA MEMBERS:

REAL(fp), ALLOCATABLE, SAVE :: dtdx5(:)
REAL(fp), ALLOCATABLE, SAVE :: dtdy5(:)
REAL(fp), ALLOCATABLE, SAVE :: cosp(:)
REAL(fp), ALLOCATABLE, SAVE :: cose(:)
REAL(fp), ALLOCATABLE, SAVE :: gw(:)
REAL(fp), ALLOCATABLE, SAVE :: DLAT(:)

AUTHOR:

Original code from Shian-Jiann Lin, GMAO Modified for GMI model by John Tannahill, LLNL (jrt@llnl.gov)

Implemented into GEOS-Chem by Claire Carouge (ccarouge@seas.harvard.edu)
ProTeX documentation added by Bob Yantosca (yantosca@seas.harvard.edu)
OpenMP parallelization added by Bob Yantosca (yantosca@seas.harvard.edu)

REVISION HISTORY:

```
O5 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin Yeh with the TPCORE routines from the GMI model. This eliminates the polar overshoot in the stratosphere.

O5 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers. Declare all REAL variables as REAL(fp). Added OpenMP parallel loops in various routines (and made some modifications to facilitate OpenMP).

O1 Apr 2009 - C. Carouge - Modified OpenMp parallelization and move the loops over vertical levels outside the horizontal transport routines for reducing processing time.

20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
21 Nov 2014 - M. Yannetti - Added PRECISION_MOD

19 Jan 2016 - E. Lundgren - Consolidated bpch and netcdf diagnostics code
```

3.4.1 Init_Tpcore

Subroutine Init_Tpcore allocates and initializes all module variables,

INTERFACE:

```
SUBROUTINE Init_Tpcore( IM, JM, KM, JFIRST, JLAST, NG, MG, dt, ae, clat )
USES:
```

USE PhysConstants

INPUT PARAMETERS:

```
! Global E-W dimension
INTEGER,
          INTENT(IN) :: IM
INTEGER,
          INTENT(IN) :: JM
                                   ! Global N-S dimension
INTEGER,
          INTENT(IN) :: KM
                                  ! Vertical dimension
                                  ! large ghost width
INTEGER,
          INTENT(IN) :: NG
INTEGER,
          INTENT(IN) :: MG
                                   ! small ghost width
REAL(fp),
          INTENT(IN) :: dt
                                  ! Time step in seconds
REAL(fp),
          INTENT(IN) :: ae
                                  ! Earth's radius (m)
REAL(fp),
          INTENT(IN) :: clat(JM) ! latitude in radian
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: JFIRST   ! Local first index for N-S direction
INTEGER, INTENT(OUT) :: JLAST   ! Local last index for N-S direction
```

REVISION HISTORY:

(05 Dec	2008 - C	. Carouge -	Replaced TPCORE routines by S-J Lin and Kevin
				Yeh with the TPCORE routines from GMI model.
				This eliminates the polar overshoot in the
				stratosphere.
(05 Dec	2008 - R	. Yantosca -	Updated documentation and added ProTeX headers.
				Declare all REAL variables as REAL(fp). Also
				make sure all numerical constants are declared

with the "D" double-precision exponent.

3.4.2 Exit_Tpcore

Subroutine Exit_Tpcore deallocates all module variables.

INTERFACE:

SUBROUTINE Exit_Tpcore

REVISION HISTORY:

05 Dec 2008 - C. Card	Yeh with the TPCORE routines from GMI model. This eliminates the polar overshoot in the
05 Dec 2008 - R. Yan	stratosphere. tosca - Updated documentation and added ProTeX headers. Declare all REAL variables as REAL(fp). Also make sure all numerical constants are declared
12 Feb 2015 - E. Lund	with the "D" double-precision exponent. dgren - Add new diagnostic arrays for writing diagnostics ND24, ND25, and ND26 to netcdf.

3.4.3 Tpcore_FvDas

Subroutine Tpcore_FvDas takes horizontal winds on sigma (or hybrid sigma-p) surfaces and calculates mass fluxes, and then updates the 3D mixing ratio fields one time step (tdt). The basic scheme is a Multi-Dimensional Flux Form Semi-Lagrangian (FFSL) based on the van Leer or PPM (see Lin and Rood, 1995).

INTERFACE:

SUBROUTINE Tpcore_FvDas(dt,	ae,	IM,	JM,	KM,	&
	JFIRST,	JLAST,	ng,	mg,	nq,	&
	ak,	bk,	u,	v,	ps1,	&
	ps2,	ps,	q,	iord,	jord,	&
	kord,	n_adj,	XMASS,	YMASS,	FILL,	&

#if defined(BPCH_DIAG) || defined(NC_DIAG)

- !%%% Adding DiagnArrays for writing diagnostics to netcdf (ewl, 2/12/15).
- !%%% MASSFLEW, MASSFLNS, and MASSFLUP are cumulative when BPCH=y.

&

```
! % They are instantaneous when using NETCDF
                           MASSFLEW, MASSFLNS, MASSFLUP,
 #endif
                           AREA_M2, ND24, ND25, ND26)
USES:
     ! Include files w/ physical constants and met values
    USE PhysConstants
INPUT PARAMETERS:
     ! Transport time step [s]
    REAL(fp), INTENT(IN) :: dt
     ! Earth's radius [m]
    REAL(fp), INTENT(IN) :: ae
     ! Global E-W, N-S, and vertical dimensions
    INTEGER, INTENT(IN) :: IM
                        :: JM
    INTEGER, INTENT(IN)
    INTEGER, INTENT(IN)
                          :: KM
     ! Latitude indices for local first box and local last box
     ! (NOTE: for global grids these are 1 and JM, respectively)
    INTEGER, INTENT(IN) :: JFIRST
    INTEGER, INTENT(IN)
                          :: JLAST
     ! Primary ghost region
     ! (NOTE: only required for MPI parallelization; use 0 otherwise)
    INTEGER, INTENT(IN)
                           :: ng
     ! Secondary ghost region
     ! (NOTE: only required for MPI parallelization; use 0 otherwise)
    INTEGER, INTENT(IN)
                         :: mg
     ! Ghosted latitudes (3 required by PPM)
     ! (NOTE: only required for MPI parallelization; use 0 otherwise)
    INTEGER, INTENT(IN)
                           :: nq
     ! Flags to denote E-W, N-S, and vertical transport schemes
    INTEGER, INTENT(IN) :: iord
    INTEGER, INTENT(IN) :: jord
    INTEGER, INTENT(IN) :: kord
     ! Number of adjustments to air_mass_flux (0 = no adjustment)
    INTEGER, INTENT(IN)
                          :: n_adj
     ! Ak and Bk coordinates to specify the hybrid grid
```

```
! (see the REMARKS section below)
    REAL(fp), INTENT(IN) :: ak(KM+1)
    REAL(fp), INTENT(IN) :: bk(KM+1)
    ! u-wind (m/s) at mid-time-level (t=t+dt/2)
    REAL(fp), INTENT(IN) :: u(:,:,:)
    ! E/W and N/S mass fluxes [kg/s]
    ! (These are computed by the pressure fixer, and passed into TPCORE)
    REAL(fp), INTENT(IN) :: XMASS(:,:,:)
    REAL(fp), INTENT(IN) :: YMASS(:,:,:)
    ! Grid box surface area for mass flux diag [m2]
    REAL(fp), INTENT(IN) :: AREA_M2(JM)
    ! Diagnostic flags
    INTEGER, INTENT(IN) :: ND25 ! Turns on N/S flux diagnostic
INTEGER, INTENT(IN) :: ND26 ! Turns on up/down flux diagnostic
    LOGICAL, INTENT(IN) :: FILL ! Fill negatives ?
INPUT/OUTPUT PARAMETERS:
     ! V-wind (m/s) at mid-time-level (t=t+dt/2)
    REAL(fp), INTENT(INOUT) :: v(:,:,:)
    ! surface pressure at current time
    REAL(fp), INTENT(INOUT) :: ps1(IM, JFIRST:JLAST)
    ! surface pressure at future time=t+dt
    REAL(fp), INTENT(INOUT) :: ps2(IM, JFIRST:JLAST)
    ! Tracer "mixing ratios" [kg tracer/moist air kg]
    REAL(fp), INTENT(INOUT), TARGET :: q(:,:,:,:)
 #if defined( BPCH_DIAG ) || defined( NC_DIAG )
    ! E/W, N/S, and up/down diagnostic mass fluxes
    REAL(fp), INTENT(INOUT) :: MASSFLEW(:,:,:) ! for ND24 diagnostic
    REAL(fp), INTENT(INOUT) :: MASSFLNS(:,:,:,:) ! for ND25 diagnostic
    REAL(fp), INTENT(INOUT) :: MASSFLUP(:,:,:) ! for ND26 diagnostic
 #endif
OUTPUT PARAMETERS:
    ! "Predicted" surface pressure [hPa]
    REAL(fp), INTENT(OUT) :: ps(IM, JFIRST: JLAST)
```

AUTHOR:

Original code from Shian-Jiann Lin, DAO)
John Tannahill, LLNL (jrt@llnl.gov)

REVISION HISTORY:

05	Dec	2008 -	- C.	Carouge	-	Replaced TPCORE routines by S-J Lin and Kevin Yeh with the TPCORE routines from GMI model. This eliminates the polar overshoot in the stratosphere.
05	Dec	2008 -	- R.	Yantosca	-	Updated documentation and added ProTeX headers. Declare all REAL variables as REAL(fp). Also make sure all numerical constants are declared
						with the "D" double-precision exponent. Added OpenMP parallel DO loops.
01	. Apr	2009 -	- C.	Carouge	-	Modified OpenMp parallelization and move the loops over vertical levels outside the horizontal transport routines for reducing processing time.
03	B Dec	2009 -	- C.	Carouge	-	Modify declarations of MASSFLEW, MASSFLNS and MASSFLUP to save memory space.
30) May	2013 -	- S.	Farina	-	For TOMAS, zero out UA and VA variables
04	Jun	2013 -	- R.	Yantosca	-	Use assumed-shape declarations for XMASS, YMASS, U, V, and $\mathbb Q$ arrays. These arrays are used to pass pointer references, so this may help to reduce the creation of array temporaries, which will reduce memory.
5	Jun	2013 -	- R.	Yantosca	_	Avoid array temporary in call to FZPPM
						Now use kg/kg total air as tracer units (previously v/v)
01	Jul	2015 -	- E.	Lundgren	-	Set tracer conc to small positive number if negative at end of advection (occurs at poles)

3.4.4 Average_Const_Poles

Subroutine Average_Const_Poles averages the species concentrations at the Poles when the Polar cap is enlarged. It makes the last two latitudes equal.

INTERFACE:

INPUT PARAMETERS:

! Global latitude indices of the South Pole and North Pole

```
INTEGER, INTENT(IN) :: JU1_GL, J2_GL
    ! Global max longitude index
    INTEGER, INTENT(IN)
                        :: I2_GL
     ! Local min & max longitude (I), latitude (J), altitude (K) indices
    INTEGER, INTENT(IN) :: I1, I2
    INTEGER, INTENT(IN)
                          :: JU1, J2
    ! Local min & max longitude (I) and latitude (J) indices
    INTEGER, INTENT(IN) :: ILO, IHI
    INTEGER, INTENT(IN) :: JULO, JHI
    ! Pressure difference across layer from (ai * pt) term [hPa]
    REAL(fp), INTENT(IN)
                          :: dap
    ! Difference in bi across layer - the dSigma term
    REAL(fp), INTENT(IN)
                          :: dbk
    ! Relative surface area of grid box [fraction]
    REAL(fp), INTENT(IN) :: rel_area(JU1:J2)
    ! CTM surface pressure at t1 [hPa]
    REAL(fp), INTENT(IN)
                          :: pctm1( ILO:IHI, JULO:JHI )
INPUT/OUTPUT PARAMETERS:
     ! Species concentration, known at zone center [mixing ratio]
    REAL(fp), INTENT(INOUT) :: const1( I1:I2, JU1:J2)
AUTHOR:
    Original code from Shian-Jiann Lin, DAO)
    John Tannahill, LLNL (jrt@llnl.gov)
```

REVISION HISTORY:

05 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin Yeh with the TPCORE routines from GMI model.

This eliminates the polar overshoot in the stratosphere.

05 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Declare all REAL variables as REAL(fp). Also

make sure all numerical constants are declared

with the "D" double-precision exponent.

3.4.5 Set_Cross_Terms

Subroutine Set_Cross_Terms sets the cross terms for E-W horizontal advection.

INTERFACE:

```
SUBROUTINE Set_Cross_Terms( crx, cry, ua, va, J1P, J2P, & I1_GL, I2_GL, JU1_GL, J2_GL, ILO, & IHI, JULO, JHI, I1, I2, & JU1, J2, CROSS)
```

INPUT PARAMETERS:

```
! Global latitude indices at the edges of the S/N polar caps
! J1P=JU1_GL+1; J2P=J2_GL-1 for a polar cap of 1 latitude band
! J1P=JU1_GL+2; J2P=J2_GL-2 for a polar cap of 2 latitude bands
INTEGER, INTENT(IN)
                      :: J1P,
                                 J2P
! Global min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN)
                      :: I1_GL, I2_GL
INTEGER, INTENT(IN)
                      :: JU1_GL, J2_GL
! Local min & max longitude (I), latitude (J), altitude (K) indices
INTEGER, INTENT(IN)
                      :: I1,
                                 12
INTEGER, INTENT(IN)
                      :: JU1,
                                 J2
! Local min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN)
                      :: ILO,
                                 IHI
INTEGER, INTENT(IN)
                      :: JULO,
                                 JHI
! Courant number in E-W direction
REAL(fp), INTENT(IN) :: crx(ILO:IHI, JULO:JHI)
! Courant number in N-S direction
REAL(fp), INTENT(IN) :: cry(ILO:IHI, JULO:JHI)
! Logical switch. If CROSS=T then cross-terms will be computed.
LOGICAL, INTENT(IN) :: CROSS
```

OUTPUT PARAMETERS:

```
! Average of Courant numbers from il and il+1
REAL(fp), INTENT(OUT) :: ua(ILO:IHI, JULO:JHI)
! Average of Courant numbers from ij and ij+1
REAL(fp), INTENT(OUT) :: va(ILO:IHI, JULO:JHI)
```

AUTHOR:

Original code from Shian-Jiann Lin, DAO)

John Tannahill, LLNL (jrt@llnl.gov)

REVISION HISTORY:

05 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin
Yeh with the TPCORE routines from GMI model.
This eliminates the polar overshoot in the
stratosphere.

05 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Declare all REAL variables as REAL(fp). Also
make sure all numerical constants are declared
with the "D" double-precision exponent. Added
OpenMP parallel DO loops.

01 Apr 2009 - C. Carouge - Moved the IK loop outside the subroutine.

3.4.6 Calc_Vert_Mass_Flux

Subroutine Calc_Vert_Mass_Flux calculates the vertical mass flux.

INTERFACE:

```
SUBROUTINE Calc_Vert_Mass_Flux( dbk, dps_ctm, dpi, wz, I1, & I2, JU1, J2, K1, K2)
```

INPUT PARAMETERS:

! Local min & max longitude (I), latitude (J), altitude (K) indices INTEGER, INTENT(IN) :: I1, I2
INTEGER, INTENT(IN) :: JU1, J2
INTEGER, INTENT(IN) :: K1, K2

! Difference in bi across layer - the dSigma term REAL(fp), INTENT(IN) :: dbk(K1:K2)

! CTM surface pressure tendency; sum over vertical of dpi

! calculated from original mass fluxes [hPa]
REAL(fp), INTENT(IN) :: dps_ctm(I1:I2, JU1:J2)

! Divergence at a grid point; used to calculate vertical motion [mb] REAL(fp), INTENT(IN) :: dpi(I1:I2, JU1:J2, K1:K2)

OUTPUT PARAMETERS:

! Large scale mass flux (per time step tdt) in the vertical ! direction as diagnosed from the hydrostatic relationship [hPa] REAL(fp), INTENT(OUT) :: wz(I1:I2, JU1:J2, K1:K2)

AUTHOR:

```
Original code from Shian-Jiann Lin, DAO)
John Tannahill, LLNL (jrt@llnl.gov)
```

REVISION HISTORY:

05 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin
Yeh with the TPCORE routines from GMI model.
This eliminates the polar overshoot in the
stratosphere.

05 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.
Declare all REAL variables as REAL(fp). Also
make sure all numerical constants are declared
with the "D" double-precision exponent. Added

OpenMP parallel DO loops

3.4.7 Set_Jn_Js

Subroutine Set_Jn_Js determines Jn and Js, by looking where Courant number is ¿ 1.

INTERFACE:

```
SUBROUTINE Set_Jn_Js( jn, js, crx, ILO, IHI, JULO, & JHI, JU1_GL, J2_GL, J1P, J2P, I1, & I2, JU1, J2, K1, K2)
```

INPUT PARAMETERS:

```
! Global latitude indices at the edges of the S/N polar caps
! J1P=JU1_GL+1; J2P=J2_GL-1 for a polar cap of 1 latitude band
! J1P=JU1_GL+2; J2P=J2_GL-2 for a polar cap of 2 latitude bands
INTEGER, INTENT(IN)
                      :: J1P,
! Global min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN)
                      :: JU1_GL, J2_GL
! Local min & max longitude (I), latitude (J), altitude (K) indices
INTEGER, INTENT(IN)
                      :: I1,
                                 12
INTEGER, INTENT(IN)
                      :: JU1,
                                 J2
INTEGER, INTENT(IN)
                      :: K1,
                                 K2
! Local min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN)
                      :: ILO,
                                 IHI
INTEGER, INTENT(IN)
                      :: JULO,
                                 JHI
! Courant number in E-W direction
REAL(fp), INTENT(IN) :: crx(ILO:IHI, JULO:JHI, K1:K2)
```

OUTPUT PARAMETERS:

```
! Northward of latitude index = jn; Courant numbers could be > 1,
! so use the flux-form semi-Lagrangian scheme
INTEGER, INTENT(OUT) :: jn(K1:K2)
! Southward of latitude index = js; Courant numbers could be > 1,
! so use the flux-form semi-Lagrangian scheme
INTEGER, INTENT(OUT) :: js(K1:K2)
```

AUTHOR:

```
Original code from Shian-Jiann Lin, DAO)
John Tannahill, LLNL (jrt@llnl.gov)
```

REMARKS:

We cannot parallelize this subroutine because there is a CYCLE statement within the outer loop.

REVISION HISTORY:

```
05 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin
Yeh with the TPCORE routines from GMI model.
This eliminates the polar overshoot in the
stratosphere.

05 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.
Declare all REAL variables as REAL(fp). Also
make sure all numerical constants are declared
with the "D" double-precision exponent.
```

3.4.8 Calc_Advec_Cross_Terms

Subroutine Calc_Advec_Cross_Terms calculates the advective cross terms.

INTERFACE:

```
SUBROUTINE Calc_Advec_Cross_Terms( jn,
                                           js,
                                                  qq1,
                                                        qqu,
                                                              qqv,
                                                  J1P,
                                                        J2P,
                                                              I2_GL, &
                                           va,
                                   JU1_GL, J2_GL, ILO,
                                                             JULO, &
                                                        IHI,
                                   JHI,
                                           I1,
                                                  I2,
                                                        JU1,
                                                              J2,
                                   CROSS )
```

INPUT PARAMETERS:

```
! Global latitude indices at the edges of the S/N polar caps ! J1P=JU1_GL+1; J2P=J2_GL-1 for a polar cap of 1 latitude band ! J1P=JU1_GL+2; J2P=J2_GL-2 for a polar cap of 2 latitude bands INTEGER, INTENT(IN) :: J1P, J2P
```

! Global min & max longitude (I) and latitude (J) indices

```
INTEGER, INTENT(IN) ::
                                    I2_GL
    INTEGER, INTENT(IN) :: JU1_GL, J2_GL
     ! Local min & max longitude (I), latitude (J), altitude (K) indices
    INTEGER, INTENT(IN) :: I1,
                                    12
    INTEGER, INTENT(IN) :: JU1,
     ! Local min & max longitude (I) and latitude (J) indices
    INTEGER, INTENT(IN) :: ILO,
                                    IHI
    INTEGER, INTENT(IN) :: JULO,
                                    JHI
     ! Northward of latitude index = jn, Courant numbers could be > 1,
     ! so use the flux-form semi-Lagrangian scheme
    INTEGER, INTENT(IN) :: Jn
     ! Southward of latitude index = js, Courant numbers could be > 1,
     ! so use the flux-form semi-Lagrangian scheme
    INTEGER, INTENT(IN) :: Js
     ! Species concentration (mixing ratio)
    REAL(fp), INTENT(IN) :: qq1(ILO:IHI, JULO:JHI)
     ! Average of Courant numbers from il and il+1
    REAL(fp), INTENT(IN) :: ua (ILO:IHI, JULO:JHI)
     ! Average of Courant numbers from ij and ij+1
    REAL(fp), INTENT(IN) :: va (ILO:IHI, JULO:JHI)
     ! Logical switch: If CROSS=T then cross-terms are being computed
    LOGICAL, INTENT(IN) :: CROSS
OUTPUT PARAMETERS:
     ! Concentration contribution from E-W advection [mixing ratio]
    REAL(fp), INTENT(OUT) :: qqu(ILO:IHI, JULO:JHI)
     ! concentration contribution from N-S advection [mixing ratio]
    REAL(fp), INTENT(OUT) :: qqv(ILO:IHI, JULO:JHI)
AUTHOR:
```

Original code from Shian-Jiann Lin, DAO) John Tannahill, LLNL (jrt@llnl.gov)

REVISION HISTORY:

05 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin Yeh with the TPCORE routines from GMI model. This eliminates the polar overshoot in the

```
stratosphere.
```

05 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Declare all REAL variables as REAL(fp). Also
make sure all numerical constants are declared
with the "D" double-precision exponent. Added
OpenMP parallel do loops.

01 Apr 2009 - C. Carouge - Moved the IK loop outside the subroutine.

3.4.9 Qckxyz

Subroutine Qckxyz routine checks for "filling".

INTERFACE:

```
SUBROUTINE Qckxyz( dq1, J1P, J2P, JU1_GL, J2_GL, & ILO, IHI, JULO, JHI, I1, & I2, JU1, J2, K1, K2)
```

INPUT PARAMETERS:

```
! Global latitude indices at the edges of the S/N polar caps
! J1P=JU1_GL+1; J2P=J2_GL-1 for a polar cap of 1 latitude band
! J1P=JU1_GL+2; J2P=J2_GL-2 for a polar cap of 2 latitude bands
INTEGER, INTENT(IN) :: J1P,
! Global min & max latitude (J) indices
INTEGER, INTENT(IN) :: JU1_GL, J2_GL
! Local min & max longitude (I), latitude (J), altitude (K) indices
INTEGER, INTENT(IN) :: I1,
                                T2
INTEGER, INTENT(IN) :: JU1,
                                J2
INTEGER, INTENT(IN) :: K1,
                                K2
! Local min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN)
                    :: ILO,
                                IHI
```

JHI

INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(IN) :: JULO,

```
! Species density [hPa]
REAL(fp), INTENT(INOUT) :: dq1(ILO:IHI, JULO:JHI, K1:K2)
```

AUTHOR:

```
Original code from Shian-Jiann Lin, DAO)
John Tannahill, LLNL (jrt@llnl.gov)
```

REVISION HISTORY:

05 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin
Yeh with the TPCORE routines from GMI model.
This eliminates the polar overshoot in the
stratosphere.

05 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Declare all REAL variables as REAL(fp). Also
make sure all numerical constants are declared
with the "D" double-precision exponent. Added
OpenMP parallel DO loops.

3.4.10 Set_Lmts

Subroutine Set_Lmts sets ILMT, JLMT, KLMT.

INTERFACE:

SUBROUTINE Set_Lmts(ilmt, jlmt, klmt, I2_GL, J2_GL, iord, jord, kord)

INPUT PARAMETERS:

- ! Global maximum longitude (I) and longitude (J) indices INTEGER, INTENT(IN) $:: I2_GL, J2_GL$
- ! Flags to denote E-W, N-S, and vertical transport schemes
- ! (See REMARKS section of routine Tpcore_FvDas for more info)

INTEGER, INTENT(IN) :: iord, jord, kord

OUTPUT PARAMETERS:

- ! Controls various options in E-W advection INTEGER, INTENT(OUT) :: ilmt
- ! Controls various options in N-S advection INTEGER, INTENT(OUT) :: jlmt
- ! Controls various options in vertical advection INTEGER, INTENT(OUT) :: klmt

AUTHOR:

Original code from Shian-Jiann Lin, DAO)
John Tannahill, LLNL (jrt@llnl.gov)

REVISION HISTORY:

05 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin Yeh with the TPCORE routines from GMI model.

This eliminates the polar overshoot in the stratosphere.

05 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Declare all REAL variables as REAL(fp). Also
make sure all numerical constants are declared
with the "D" double-precision exponent.

3.4.11 Set_Press_Terms

Subroutine Set_Press_Terms sets the pressure terms: DELP1, DELPM, PU.

INTERFACE:

```
SUBROUTINE Set_Press_Terms( dap, dbk, pres1, pres2, delp1, & delpm, pu, JU1_GL, J2_GL, ILO, & IHI, JULO, JHI, J1P, J2P, & I1, I2, JU1, J2)
```

INPUT PARAMETERS:

```
! Global latitude indices at the edges of the S/N polar caps
! J1P=JU1_GL+1; J2P=J2_GL-1 for a polar cap of 1 latitude band
! J1P=JU1_GL+2; J2P=J2_GL-2 for a polar cap of 2 latitude bands
INTEGER, INTENT(IN) :: J1P,
                                J2P
! Global min & max latitude (J) indices
INTEGER, INTENT(IN) :: JU1_GL, J2_GL
! Local min & max longitude (I), latitude (J), altitude (K) indices
INTEGER, INTENT(IN) :: I1,
INTEGER, INTENT(IN) :: JU1,
                                J2
! Local min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN) :: ILO,
                                IHI
INTEGER, INTENT(IN) :: JULO,
                                JHI
! Pressure difference across layer from (ai * pt) term [hPa]
REAL(fp), INTENT(IN) :: dap
! Difference in bi across layer - the dSigma term
REAL(fp), INTENT(IN) :: dbk
! Surface pressure at t1 [hPa]
REAL(fp), INTENT(IN) :: pres1(ILO:IHI, JULO:JHI)
! Surface pressure at t1+tdt [hPa]
REAL(fp), INTENT(IN) :: pres2(ILO:IHI, JULO:JHI)
```

OUTPUT PARAMETERS:

```
! Pressure thickness, the pseudo-density in a
! hydrostatic system at t1 [hPa]
REAL(fp), INTENT(OUT) :: delp1(ILO:IHI, JULO:JHI)

! Pressure thickness, the pseudo-density in a
! hydrostatic system at t1+tdt/2 (approximate) [hPa]
REAL(fp), INTENT(OUT) :: delpm(ILO:IHI, JULO:JHI)

! Pressure at edges in "u" [hPa]
REAL(fp), INTENT(OUT) :: pu(ILO:IHI, JULO:JHI)
```

AUTHOR:

Original code from Shian-Jiann Lin, DAO) John Tannahill, LLNL (jrt@llnl.gov)

REVISION HISTORY:

```
O5 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin Yeh with the TPCORE routines from GMI model.

This eliminates the polar overshoot in the stratosphere.

O5 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Declare all REAL variables as REAL(fp). Also make sure all numerical constants are declared with the "D" double-precision exponent. Added OpenMP parallel DO loops.

O1 Apr 2009 - C. Carouge - Moved the IK loop outside the subroutine.
```

3.4.12 Calc Courant

Subroutine Calc_Courant calculates courant numbers from the horizontal mass fluxes.

INTERFACE:

```
SUBROUTINE Calc_Courant( cose, delpm, pu, xmass, ymass, crx, cry, & J1P, J2P, JU1_GL, J2_GL, ILO, IHI, JULO, & JHI, I1, I2, JU1, J2)
```

```
! Global latitude indices at the edges of the S/N polar caps
! J1P=JU1_GL+1; J2P=J2_GL-1 for a polar cap of 1 latitude band
! J1P=JU1_GL+2; J2P=J2_GL-2 for a polar cap of 2 latitude bands
INTEGER, INTENT(IN) :: J1P, J2P

! Global min & max latitude (J) indices
INTEGER, INTENT(IN) :: JU1_GL, J2_GL
```

```
! Local min & max longitude (I), latitude (J), altitude (K) indices
    INTEGER, INTENT(IN) :: I1,
                                    T2
    INTEGER, INTENT(IN) :: JU1,
                                    .12
     ! Local min & max longitude (I) and latitude (J) indices
    INTEGER, INTENT(IN) :: ILO,
                                    IHI
    INTEGER, INTENT(IN) :: JULO,
                                    JHI
     ! Cosine of grid box edges
    REAL(fp), INTENT(IN) :: cose (JU1_GL:J2_GL)
     ! Pressure thickness, the pseudo-density in a hydrostatic system
     ! at t1+tdt/2 (approximate) (mb)
    REAL(fp), INTENT(IN) :: delpm(ILO:IHI, JULO:JHI)
     ! pressure at edges in "u" (mb)
    REAL(fp), INTENT(IN) :: pu (iLO:IHI, JULO:JHI)
     ! horizontal mass flux in E-W and N-S directions [hPa]
    REAL(fp), INTENT(IN) :: xmass(ILO:IHI, JULO:JHI)
    REAL(fp), INTENT(IN) :: ymass(ILO:IHI, JULO:JHI)
OUTPUT PARAMETERS:
     ! Courant numbers in E-W and N-S directions
    REAL(fp), INTENT(OUT) :: crx(ILO:IHI, JULO:JHI)
    REAL(fp), INTENT(OUT) :: cry(ILO:IHI, JULO:JHI)
```

AUTHOR:

Original code from Shian-Jiann Lin, DAO)
John Tannahill, LLNL (jrt@llnl.gov)

REVISION HISTORY:

```
05 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin
Yeh with the TPCORE routines from GMI model.
This eliminates the polar overshoot in the
stratosphere.

05 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.
Declare all REAL variables as REAL(fp). Also
make sure all numerical constants are declared
with the "D" double-precision exponent.

01 Apr 2009 - C. Carouge - Moved the IK loop outside the subroutine.
```

3.4.13 Calc_Divergence

Subroutine Calc_Divergence calculates the divergence.

INTERFACE:

```
SUBROUTINE Calc_Divergence( do_reduction, geofac_pc, geofac, dpi,
                           xmass,
                                         ymass,
                                                    J1P,
                                                            J2P,
                           I1_GL,
                                        I2_GL,
                                                    JU1_GL, J2_GL, &
                                         IHI,
                                                            JHI,
                           ILO,
                                                    JULO,
                           I1,
                                         I2,
                                                    JU1,
                                                            J2 )
```

```
INPUT PARAMETERS:
     ! Global latitude indices at the edges of the S/N polar caps
     ! J1P=JU1_GL+1; J2P=J2_GL-1 for a polar cap of 1 latitude band
     ! J1P=JU1_GL+2; J2P=J2_GL-2 for a polar cap of 2 latitude bands
    INTEGER, INTENT(IN) :: J1P,
                                    J2P
     ! Global min & max longitude (I) and latitude (J) indices
    INTEGER, INTENT(IN) :: I1_GL, I2_GL
    INTEGER, INTENT(IN) :: JU1_GL, J2_GL
     ! Local min & max longitude (I), latitude (J), altitude (K) indices
     INTEGER, INTENT(IN) :: I1,
                                    12
    INTEGER, INTENT(IN) :: JU1,
                                    J2
     ! Local min & max longitude (I) and latitude (J) indices
     INTEGER, INTENT(IN) :: ILO,
                                     IHI
    INTEGER, INTENT(IN) :: JULO,
                                     JHI
     ! Set to F if called on Master or T if called by Slaves
     ! (NOTE: This is only for MPI parallelization, for OPENMP it should be F)
    LOGICAL, INTENT(IN) :: do_reduction
     ! Special geometrical factor (geofac) for Polar cap
    REAL(fp) , INTENT(IN) :: geofac_pc
     ! Geometrical factor for meridional advection; geofac uses correct
     ! spherical geometry, and replaces acosp as the meridional geometrical
     ! factor in TPCORE
    REAL(fp) , INTENT(IN) :: geofac(JU1_GL:J2_GL)
     ! Horizontal mass flux in E/W and N/S directions [hPa]
    REAL(fp) , INTENT(IN) :: xmass(ILO:IHI, JULO:JHI)
    REAL(fp) , INTENT(IN) :: ymass(ILO:IHI, JULO:JHI)
```

OUTPUT PARAMETERS:

! Divergence at a grid point; used to calculate vertical motion [hPa]

```
REAL(fp), INTENT(OUT) :: dpi(I1:I2, JU1:J2)
```

AUTHOR:

Original code from Shian-Jiann Lin, DAO John Tannahill, LLNL (jrt@llnl.gov)

REVISION HISTORY:

O5 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin
Yeh with the TPCORE routines from GMI model.
This eliminates the polar overshoot in the
stratosphere.

O5 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.
Declare all REAL variables as REAL(fp). Also
make sure all numerical constants are declared
with the "D" double-precision exponent. Added
OpenMP parallel DO loops.

O1 Apr 2009 - C. Carouge - Moved the IK loop outside the subroutine.

3.4.14 Do_Divergence_Pole_Sum

Subroutine Do_Divergence_Pole_Sum sets the divergence at the Poles.

INTERFACE:

```
! Global latitude indices at the edges of the S/N polar caps
! J1P=JU1_GL+1; J2P=J2_GL-1 for a polar cap of 1 latitude band
! J1P=JU1_GL+2; J2P=J2_GL-2 for a polar cap of 2 latitude bands
INTEGER, INTENT(IN) :: J1P, J2P

! Global min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN) :: I1_GL, I2_GL
INTEGER, INTENT(IN) :: JU1_GL, J2_GL
! Local min & max longitude (I), latitude (J), altitude (K) indices
INTEGER, INTENT(IN) :: I1, I2
INTEGER, INTENT(IN) :: JU1, J2
```

```
! Local min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN) :: ILO, IHI
INTEGER, INTENT(IN) :: JULO, JHI

! Set to T if called on Master or F if called by slaves
! NOTE: This seems not to be used here....)
LOGICAL, INTENT(IN) :: do_reduction

! Special geometrical factor (geofac) for Polar cap
REAL(fp), INTENT(in) :: geofac_pc

! Horizontal mass flux in N-S direction [hPa]
REAL(fp), INTENT(IN) :: ymass(ILO:IHI, JULO:JHI)
```

! Divergence at a grid point; used to calculate vertical motion [hPa] REAL(fp), INTENT(OUT) :: dpi(I1:I2, JU1:J2)

AUTHOR:

Original code from Shian-Jiann Lin, DAO John Tannahill, LLNL (jrt@llnl.gov)

REVISION HISTORY:

```
O5 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin Yeh with the TPCORE routines from GMI model. This eliminates the polar overshoot in the stratosphere.

O5 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers. Declare all REAL variables as REAL(fp). Also make sure all numerical constants are declared with the "D" double-precision exponent. Added OpenMP parallel DO loops.

O1 Apr 2009 - C. Carouge - Moved the IK loop outside the subroutine.
```

3.4.15 Do_Cross_Terms_Pole_I2d2

Subroutine Do_Cross_Terms_Pole_I2d2 sets "va" at the Poles.

INTERFACE:

```
SUBROUTINE Do_Cross_Terms_Pole_I2d2( cry, va, I1_GL, I2_GL, JU1_GL, & J2_GL, J1P, ILO, IHI, JULO, & JHI, I1, I2, JU1, J2)
```

```
! Global latitude indices at the edge of the South polar cap
! J1P=JU1_GL+1 for a polar cap of 1 latitude band
! J1P=JU1_GL+2 for a polar cap of 2 latitude bands
INTEGER, INTENT(IN) :: J1P
! Global min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN) :: I1_GL, I2_GL
INTEGER, INTENT(IN) :: JU1_GL, J2_GL
! Local min & max longitude (I), latitude (J), altitude (K) indices
INTEGER, INTENT(IN) :: I1,
                                12
INTEGER, INTENT(IN) :: JU1,
                                J2
! Local min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN) :: ILO,
                                IHI
INTEGER, INTENT(IN) :: JULO,
                                JHI
! Courant number in N-S direction
REAL(fp), INTENT(IN) :: cry(ILO:IHI, JULO:JHI)
```

```
! Average of Courant numbers from ij and ij+1 REAL(fp), INTENT(OUT) :: va(ILO:IHI, JULO:JHI)
```

AUTHOR:

Original code from Shian-Jiann Lin, DAO John Tannahill, LLNL (jrt@llnl.gov)

REVISION HISTORY:

```
O5 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin
Yeh with the TPCORE routines from GMI model.
This eliminates the polar overshoot in the
stratosphere.

O5 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.
Declare all REAL variables as REAL(fp). Also
make sure all numerical constants are declared
with the "D" double-precision exponent.

O1 Apr 2009 - C. Carouge - Moved the IK loop outside the subroutine.
```

$3.4.16 \quad Xadv_Dao2$

Subroutine Xadv_Dao2 is the advective form E-W operator for computing the adx (E-W) cross term.

```
SUBROUTINE Xadv_Dao2( iad,
                            jn,
                                  js, adx, qqv, &
                           ILO, IHI, JULO, JHI, &
                    ua,
                    JU1_GL, J2_GL, J1P, J2P, I1, &
                    I2,
                           JU1,
                                  J2)
```

INPUT PARAMETERS:

```
! Global latitude indices at the edges of the S/N polar caps
     ! J1P=JU1_GL+1; J2P=J2_GL-1 for a polar cap of 1 latitude band
     ! J1P=JU1_GL+2; J2P=J2_GL-2 for a polar cap of 2 latitude bands
    INTEGER, INTENT(IN) :: J1P,
     ! Global min & max latitude (J) indices
    INTEGER, INTENT(IN) :: JU1_GL, J2_GL
     ! Local min & max longitude (I), latitude (J), altitude (K) indices
    INTEGER, INTENT(IN) :: I1,
    INTEGER, INTENT(IN) :: JU1,
     ! Local min & max longitude (I) and latitude (J) indices
    INTEGER, INTENT(IN) :: ILO,
                                    IHI
    INTEGER, INTENT(IN) :: JULO,
                                    JHI
     ! if iad = 1, use 1st order accurate scheme;
     ! if iad = 2, use 2nd order accurate scheme
    INTEGER, INTENT(IN) :: iad
     ! Northward of latitude index = jn, Courant numbers could be > 1,
     ! so use the flux-form semi-Lagrangian scheme
    INTEGER, INTENT(IN) :: jn
     ! southward of latitude index = js, Courant numbers could be > 1,
     ! so use the flux-form semi-Lagrangian scheme
    INTEGER, INTENT(IN) :: js
     ! Concentration contribution from N-S advection [mixing ratio]
    REAL(fp), INTENT(IN) :: qqv(ILO:IHI, JULO:JHI)
     ! Average of Courant numbers from il and il+1
    REAL(fp), INTENT(IN) :: ua(ILO:IHI, JULO:JHI)
OUTPUT PARAMETERS:
```

```
! Cross term due to E-W advection [mixing ratio]
REAL(fp), INTENT(OUT) :: adx(ILO:IHI, JULO:JHI)
```

AUTHOR:

```
Original code from Shian-Jiann Lin, DAO
John Tannahill, LLNL (jrt@llnl.gov)
```

REVISION HISTORY:

```
05 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin
Yeh with the TPCORE routines from GMI model.
This eliminates the polar overshoot in the
stratosphere.

05 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.
Declare all REAL variables as REAL(fp). Also
make sure all numerical constants are declared
with the "D" double-precision exponent. Added
```

OpenMP parallel DO loops.

01 Apr 2009 - C. Carouge $\,$ - Moved the IK loop outside the subroutine.

3.4.17 Yadv_Dao2

Subroutine Yadv_Dao2 is the advective form N-S operator for computing the ady (N-S) cross term.

INTERFACE:

```
SUBROUTINE Yadv_Dao2( iad, ady, qqu, va, I1_GL, & I2_GL, JU1_GL, J2_GL, J1P, J2P, & ILO, IHI, JULO, JHI, I1, & I2, JU1, J2)
```

```
! Global latitude indices at the edges of the S/N polar caps
! J1P=JU1_GL+1; J2P=J2_GL-1 for a polar cap of 1 latitude band
! J1P=JU1_GL+2; J2P=J2_GL-2 for a polar cap of 2 latitude bands
INTEGER, INTENT(IN) :: J1P,
                                J2P
! Global min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN) :: I1_GL, I2_GL
INTEGER, INTENT(IN) :: JU1_GL, J2_GL
! Local min & max longitude (I), latitude (J), altitude (K) indices
INTEGER, INTENT(IN) :: I1,
                                12
INTEGER, INTENT(IN) :: JU1,
                                J2
! Local min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN) :: ILO,
                                IHI
INTEGER, INTENT(IN) :: JULO,
                                JHI
! If iad = 1, use 1st order accurate scheme;
! If iad = 2, use 2nd order accurate scheme
INTEGER, INTENT(IN) :: iad
```

```
! Concentration contribution from E-W advection [mixing ratio]
REAL(fp), INTENT(IN) :: qqu(ILO:IHI, JULO:JHI)
! Average of Courant numbers from ij and ij+1
REAL(fp), INTENT(IN) :: va(ILO:IHI, JULO:JHI)
```

```
! Cross term due to N-S advection (mixing ratio) REAL(fp), INTENT(OUT) :: ady(ILO:IHI, JULO:JHI)
```

AUTHOR:

```
Original code from Shian-Jiann Lin, DAO John Tannahill, LLNL (jrt@llnl.gov)
```

REVISION HISTORY:

```
05 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin
Yeh with the TPCORE routines from GMI model.
This eliminates the polar overshoot in the
stratosphere.

05 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.
Declare all REAL variables as REAL(fp). Also
make sure all numerical constants are declared
with the "D" double-precision exponent.

01 Apr 2009 - C. Carouge - Moved the IK loop outside the subroutine.
```

3.4.18 Do_Yadv_Pole_I2d2

Subroutine Do_Yadv_Pole_I2d2 sets "qquwk" at the Poles.

INTERFACE:

```
SUBROUTINE Do_Yadv_Pole_I2d2 ( qqu, qquwk, I1_GL, I2_GL, JU1_GL, J2_GL, & J1P, ILO, IHI, JULO, JHI, I1, & I2, JU1, J2 )
```

```
! Global latitude indices at the edges of the South polar cap
! J1P=JU1_GL+1 for a polar cap of 1 latitude band
! J1P=JU1_GL+2 for a polar cap of 2 latitude bands
INTEGER, INTENT(IN) :: J1P
! Global min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN) :: I1_GL, I2_GL
INTEGER, INTENT(IN) :: JU1_GL, J2_GL
```

```
! qqu working array [mixing ratio]
REAL(fp), INTENT(OUT) :: qquwk(ILO:IHI, JULO-2:JHI+2)
```

AUTHOR:

Original code from Shian-Jiann Lin, DAO John Tannahill, LLNL (jrt@llnl.gov)

REVISION HISTORY:

```
O5 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin Yeh with the TPCORE routines from GMI model.

This eliminates the polar overshoot in the stratosphere.

O5 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Declare all REAL variables as REAL(fp). Also make sure all numerical constants are declared with the "D" double-precision exponent. Added OpenMP parallel DO loops.

O1 Apr 2009 - C. Carouge - Moved the IK loop outside the subroutine.
```

3.4.19 Do_Yadv_Pole_Sum

Subroutine Do_Yadv_Pole_Sum sets the cross term due to N-S advection at the Poles.

INTERFACE:

```
SUBROUTINE Do_Yadv_Pole_Sum( ady, I1_GL, I2_GL, JU1_GL, J2_GL, J1P, & ILO, IHI, JULO, JHI, I1, I2, & JU1, J2)
```

- ! Global latitude index at the edge of the South polar cap $% \left(1\right) =\left(1\right) +\left(1\right)$
- ! J1P=JU1_GL+1; for a polar cap of 1 latitude band

```
! J1P=JU1_GL+2; for a polar cap of 2 latitude bands
INTEGER, INTENT(IN)
                       :: J1P
! Global min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN) :: I1_GL, I2_GL
INTEGER, INTENT(IN)
                     :: JU1_GL, J2_GL
! Local min & max longitude (I), latitude (J), altitude (K) indices
INTEGER, INTENT(IN)
                       :: I1,
                                 12
INTEGER, INTENT(IN)
                       :: JU1,
                                  J2
! Local min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN)
                    :: ILO,
                                  IHI
INTEGER, INTENT(IN)
                     :: JULO,
                                  JHI
```

! Cross term due to N-S advection (mixing ratio) REAL(fp), INTENT(INOUT) :: ady(ILO:IHI, JULO:JHI)

AUTHOR:

Original code from Shian-Jiann Lin, DAO John Tannahill, LLNL (jrt@llnl.gov)

REVISION HISTORY:

```
O5 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin Yeh with the TPCORE routines from GMI model.

This eliminates the polar overshoot in the stratosphere.

O5 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Declare all REAL variables as REAL(fp). Also make sure all numerical constants are declared with the "D" double-precision exponent. Added OpenMP parallel DO loops. Also make a logical to test if we are using an extended polar cap.

O1 Apr 2009 - C. Carouge - Moved the IK loop outside the subroutine.
```

3.4.20 Xtp

Subroutine Xtp does horizontal advection in the E-W direction.

```
SUBROUTINE Xtp( ilmt, jn, js, pu, crx, dq1, qqv, xmass, fx, & J1P, J2P, I2_GL, JU1_GL, J2_GL, ILO, IHI, JULO, JHI, & I1, I2, JU1, J2, iord )
```

```
! Global latitude indices at the edges of the S/N polar caps
     ! J1P=JU1_GL+1; J2P=J2_GL-1 for a polar cap of 1 latitude band
     ! J1P=JU1_GL+2; J2P=J2_GL-2 for a polar cap of 2 latitude bands
     INTEGER, INTENT(IN) :: J1P,
                                      J<sub>2</sub>P
     ! Global min & max longitude (I) and latitude (J) indices
    INTEGER, INTENT(IN) ::
                                     I2_GL
    INTEGER, INTENT(IN) :: JU1_GL, J2_GL
     ! Local min & max longitude (I), latitude (J), altitude (K) indices
     INTEGER, INTENT(IN) :: I1,
                                      12
    INTEGER, INTENT(IN)
                          :: JU1,
                                      J2
     ! Local min & max longitude (I) and latitude (J) indices
    INTEGER, INTENT(IN)
                         :: ILO,
                                      IHI
    INTEGER, INTENT(IN)
                          :: JULO,
                                      JHI
     ! Controls various options in E-W advection
    INTEGER, INTENT(IN)
                          :: ilmt
     ! Northward of latitude index = jn, Courant numbers could be > 1,
     ! so use the flux-form semi-Lagrangian scheme
    INTEGER, INTENT(IN)
                         :: jn
     ! Southward of latitude index = js, Courant numbers could be > 1,
     ! so use the flux-form semi-Lagrangian scheme
    INTEGER, INTENT(IN)
                           :: js
     ! Option for E-W transport scheme. See module header for more info.
    INTEGER, INTENT(IN)
                          :: iord
     ! pressure at edges in "u" [hPa]
    REAL(fp), INTENT(IN) :: pu(ILO:IHI, JULO:JHI)
     ! Courant number in E-W direction
    REAL(fp), INTENT(IN) :: crx(ILO:IHI, JULO:JHI)
     ! Horizontal mass flux in E-W direction [hPa]
    REAL(fp), INTENT(IN) :: xmass(ILO:IHI, JULO:JHI)
INPUT/OUTPUT PARAMETERS:
     ! Species density [hPa]
    REAL(fp), INTENT(INOUT) :: dq1(ILO:IHI, JULO:JHI)
     ! Concentration contribution from N-S advection [mixing ratio]
    REAL(fp), INTENT(INOUT) :: qqv(ILO:IHI, JULO:JHI)
```

```
! E-W flux [mixing ratio]
REAL(fp), INTENT(OUT) :: fx(ILO:IHI, JULO:JHI)
```

AUTHOR:

Original code from Shian-Jiann Lin, DAO John Tannahill, LLNL (jrt@llnl.gov)

REVISION HISTORY:

05 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin
Yeh with the TPCORE routines from GMI model.
This eliminates the polar overshoot in the
stratosphere.

05 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.
Declare all REAL variables as REAL(fp). Also
make sure all numerical constants are declared
with the "D" double-precision exponent. Added

OpenMP parallel DO loops.

01 Apr 2009 - C. Carouge - Moved the IK loop outside the subroutine.

3.4.21 Xmist

Subroutine Xmist computes the linear tracer slope in the E-W direction. It uses the Lin et. al. 1994 algorithm.

INTERFACE:

```
SUBROUTINE Xmist( dcx, qqv, J1P, J2P, I2_GL, JU1_GL, J2_GL, ILO, IHI, & JULO, JHI, I1, I2, JU1, J2)
```

```
! Global latitude indices at the edges of the S/N polar caps
! J1P=JU1_GL+1; J2P=J2_GL-1 for a polar cap of 1 latitude band
! J1P=JU1_GL+2; J2P=J2_GL-2 for a polar cap of 2 latitude bands
INTEGER, INTENT(IN) :: J1P, J2P

! Global min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN) :: I2_GL
INTEGER, INTENT(IN) :: JU1_GL, J2_GL

! Local min & max longitude (I), latitude (J), altitude (K) indices
INTEGER, INTENT(IN) :: J1, I2
INTEGER, INTENT(IN) :: JU1, J2

! Local min & max longitude (I) and latitude (J) indices
```

```
INTEGER, INTENT(IN) :: ILO, IHI
INTEGER, INTENT(IN) :: JULO, JHI
```

! Concentration contribution from N-S advection [mixing ratio] REAL(fp), INTENT(IN) :: qqv(-I2/3:I2+I2/3, JULO:JHI)

OUTPUT PARAMETERS:

! Slope of concentration distribution in E-W direction [mixing ratio] REAL(fp), INTENT(OUT) :: dcx(-I2/3:I2+I2/3, JULO:JHI)

AUTHOR:

Original code from Shian-Jiann Lin, DAO John Tannahill, LLNL (jrt@llnl.gov)

REVISION HISTORY:

```
05 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin
Yeh with the TPCORE routines from GMI model.
This eliminates the polar overshoot in the
stratosphere.

05 Dec 2008 - B. Yantosca - Updated documentation and added ProTeX headers
```

05 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Declare all REAL variables as REAL(fp). Also

make sure all numerical constants are declared

with the "D" double-precision exponent. Added

OpenMP parallel DO loops.

01 Apr 2009 - C. Carouge - Moved the IK loop outside the subroutine.

3.4.22 Fxppm

Subroutine Fxppm is the 1D "outer" flux form operator based on the Piecewise Parabolic Method (PPM; see also Lin and Rood 1996) for computing the fluxes in the E-W direction.

INTERFACE:

INPUT PARAMETERS:

```
! Local min & max longitude (I) and altitude (K) indices INTEGER, INTENT(IN) \ :: \ \mbox{I1}, \ \ \mbox{I2}
```

```
! Local min & max longitude (I) and latitude (J) indices INTEGER, INTENT(IN) :: ILO, IHI INTEGER, INTENT(IN) :: JULO, JHI
```

! Latitude (IJ) and altitude (IK) indices

```
INTEGER, INTENT(IN)
                     :: ij
! Controls various options in E-W advection
INTEGER, INTENT(IN)
                     :: ilmt
! Courant number in E-W direction
REAL(fp), INTENT(IN)
                       :: crx(I1:I2, JULO:JHI)
```

INPUT/OUTPUT PARAMETERS:

! Concentration contribution from N-S advection [mixing ratio] REAL(fp), INTENT(INOUT) :: qqv(ILO:IHI, JULO:JHI)

OUTPUT PARAMETERS:

```
! Slope of concentration distribution in E-W direction (mixing ratio)
REAL(fp), INTENT(OUT) :: dcx(ILO:IHI, JULO:JHI)
! E-W flux [mixing ratio]
REAL(fp), INTENT(OUT)
                      :: fx(I1:I2, JULO:JHI)
```

AUTHOR:

Original code from Shian-Jiann Lin, DAO John Tannahill, LLNL (jrt@llnl.gov)

REMARKS:

This routine is called from w/in a OpenMP parallel loop fro

REVISION HISTORY:

```
05 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin
                            Yeh with the TPCORE routines from GMI model.
                            This eliminates the polar overshoot in the
                            stratosphere.
05 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.
                            Declare all REAL variables as REAL(fp). Also
                            make sure all numerical constants are declared
                            with the "D" double-precision exponent.
                            Also remove the allocatable arrays, which
                            interfere w/ OpenMP parallelization.
01 Apr 2009 - C. Carouge - The input arrays are now 2D only.
```

3.4.23 Lmtppm

Subroutine Lmtppm enforces the full monotonic, semi-monotonic, or the positive-definite constraint to the sub-grid parabolic distribution of the Piecewise Parabolic Method (PPM).

```
SUBROUTINE Lmtppm(lenx, lmt, a6, a1, ar, dc, qa)
```

INPUT PARAMETERS:

```
! If 0 => full monotonicity;
! If 1 => semi-monotonic constraint (no undershoots);
! If 2 => positive-definite constraint
INTEGER, INTENT(IN) :: lmt
```

! Vector length

INTEGER, INTENT(IN) :: lenx

INPUT/OUTPUT PARAMETERS:

```
! Curvature of the test parabola REAL(fp), INTENT(INOUT) :: a6(lenx)
```

```
! Left edge value of the test parabola REAL(fp), INTENT(INOUT) :: al(lenx)
```

```
! Right edge value of the test parabola REAL(fp), INTENT(INOUT) :: ar(lenx)
```

```
! 0.5 * mismatch
```

REAL(fp), INTENT(INOUT) :: dc(lenx)

! Cell-averaged value

REAL(fp), INTENT(INOUT) :: qa(lenx)

AUTHOR:

Original code from Shian-Jiann Lin, DAO John Tannahill, LLNL (jrt@llnl.gov)

REVISION HISTORY:

```
05 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin Yeh with the TPCORE routines from GMI model.

This eliminates the polar overshoot in the stratosphere.
```

05 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Declare all REAL variables as REAL(fp). Also
make sure all numerical constants are declared
with the "D" double-precision exponent.

3.4.24 Ytp

Subroutine Ytp does horizontal advection in the N-S direction.

```
SUBROUTINE Ytp( jlmt, geofac_pc, geofac, cry, dq1, qqu, qqv, & ymass, fy, J1P, J2P, I1_GL, I2_GL, JU1_GL, & J2_GL, ilong, ILO, IHI, JULO, JHI, I1, & I2, JU1, J2, jord)

INPUT PARAMETERS:

! Global latitude indices at the edges of the S/N polar caps
```

```
! J1P=JU1_GL+1; J2P=J2_GL-1 for a polar cap of 1 latitude band
! J1P=JU1_GL+2; J2P=J2_GL-2 for a polar cap of 2 latitude bands
INTEGER, INTENT(IN)
                     :: J1P,
! Global min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN) :: I1_GL, I2_GL
INTEGER, INTENT(IN) :: JU1_GL, J2_GL
! Local min & max longitude (I), latitude (J), altitude (K) indices
INTEGER, INTENT(IN)
                   :: I1,
                                 12
INTEGER, INTENT(IN)
                   :: JU1,
                                 .J2
! Local min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN) :: ILO,
                                 IHI
INTEGER, INTENT(IN)
                     :: JULO,
                                 JHI
! ???
INTEGER, INTENT(IN) :: ilong
! Controls various options in N-S advection
INTEGER, INTENT(IN) :: jlmt
! N-S transport scheme (see module header for more info)
INTEGER, INTENT(IN)
                      :: jord
! special geometrical factor (geofac) for Polar cap
REAL(fp), INTENT(IN)
                      :: geofac_pc
! geometrical factor for meridional advection; geofac uses correct
! spherical geometry, and replaces acosp as the meridional geometrical
! factor in tpcore
REAL(fp), INTENT(IN) :: geofac(JU1_GL:J2_GL)
! Courant number in N-S direction
REAL(fp), INTENT(IN) :: cry(ILO:IHI, JULO:JHI)
! Concentration contribution from E-W advection [mixing ratio]
                      :: qqu(ILO:IHI, JULO:JHI)
REAL(fp), INTENT(IN)
! Horizontal mass flux in N-S direction [hPa]
REAL(fp), INTENT(IN) :: ymass(ILO:IHI, JULO:JHI)
```

INPUT/OUTPUT PARAMETERS:

```
! Species density [hPa]
REAL(fp), INTENT(INOUT) :: dq1(ILO:IHI, JULO:JHI)
! Concentration contribution from N-S advection [mixing ratio]
REAL(fp), INTENT(INOUT) :: qqv(ILO:IHI, JULO:JHI)
```

OUTPUT PARAMETERS:

```
! N-S flux [mixing ratio]
REAL(fp), INTENT(OUT) :: fy(ILO:IHI, JULO:JHI+1)
```

AUTHOR:

```
Original code from Shian-Jiann Lin, DAO John Tannahill, LLNL (jrt@llnl.gov)
```

REVISION HISTORY:

```
O5 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin
Yeh with the TPCORE routines from GMI model.
This eliminates the polar overshoot in the
stratosphere.

O5 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.
Declare all REAL variables as REAL(fp). Also
make sure all numerical constants are declared
with the "D" double-precision exponent. Added
OpenMP parallel DO loops.

O1 Apr 2009 - C. Carouge - Moved the IK loop outside the subroutine.
```

3.4.25 Ymist

Subroutine Ymist computes the linear tracer slope in the N-S direction. It uses the Lin et. al. 1994 algorithm.

INTERFACE:

```
SUBROUTINE Ymist( id, dcy, qqu, I1_GL, I2_GL, JU1_GL, & J2_GL, J1P, ILO, IHI, JULO, JHI, & I1, I2, JU1, J2)
```

```
! Global latitude index at the edge of the South polar cap
! J1P=JU1_GL+1 for a polar cap of 1 latitude band
! J1P=JU1_GL+2 for a polar cap of 2 latitude bands
INTEGER, INTENT(IN) :: J1P
```

```
! Global min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN) :: I1_GL, I2_GL
INTEGER, INTENT(IN) :: JU1_GL, J2_GL
! Local min & max longitude (I), latitude (J), altitude (K) indices
INTEGER, INTENT(IN) :: I1,
                                T2
INTEGER, INTENT(IN) :: JU1,
                                J2
! Local min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN) :: ILO,
                                IHI
INTEGER, INTENT(IN) :: JULO,
                                JHI
! The "order" of the accuracy in the computed linear "slope"
! (or mismatch, Lin et al. 1994); it is either 2 or 4.
INTEGER, INTENT(IN) :: id
! Concentration contribution from E-W advection (mixing ratio)
REAL(fp), INTENT(IN) :: qqu(ILO:IHI, JULO:JHI)
```

! Slope of concentration distribution in N-S direction [mixing ratio] REAL(fp), INTENT(OUT) :: dcy(ILO:IHI, JULO:JHI)

AUTHOR:

Original code from Shian-Jiann Lin, DAO John Tannahill, LLNL (jrt@llnl.gov)

REVISION HISTORY:

```
O5 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin
Yeh with the TPCORE routines from GMI model.
This eliminates the polar overshoot in the
stratosphere.

O5 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.
Declare all REAL variables as REAL(fp). Also
make sure all numerical constants are declared
with the "D" double-precision exponent. Added
OpenMP parallel DO loops.

O1 Apr 2009 - C. Carouge - Moved the IK loop outside the subroutine.
```

3.4.26 Do_Ymist_Pole1_I2d2

Subroutine Do_Ymist_Pole1_I2d2 sets "dcy" at the Poles.

```
SUBROUTINE Do_Ymist_Pole1_I2d2( dcy,
                                    qqu, I1_GL, I2_GL, JU1_GL,
                              J2_GL, ILO, IHI, JULO, JHI,
                                    I2, JU1,
                              I1,
                                                J2 )
```

INPUT PARAMETERS:

```
! Global min & max longitude (I) and latitude (J) indices
```

! J1P=JU1_GL+1; J2P=J2_GL-1 for a polar cap of 1 latitude band

! J1P=JU1_GL+2; J2P=J2_GL-2 for a polar cap of 2 latitude bands

INTEGER, INTENT(IN) :: I1_GL, I2_GL INTEGER, INTENT(IN) :: JU1_GL, J2_GL

! Local min & max longitude (I), latitude (J), altitude (K) indices

INTEGER, INTENT(IN) :: I1, T2 INTEGER, INTENT(IN) :: JU1, J2

! Local min & max longitude (I) and latitude (J) indices

INTEGER, INTENT(IN) :: ILO, IHI INTEGER, INTENT(IN) :: JULO, JHI

! Concentration contribution from E-W advection [mixing ratio] REAL(fp), INTENT(IN) :: qqu(ILO:IHI, JULO-2:JHI+2)

OUTPUT PARAMETERS:

! Slope of concentration distribution in N-S direction [mixing ratio] REAL(fp), INTENT(OUT) :: dcy(ILO:IHI, JULO:JHI)

AUTHOR:

Original code from Shian-Jiann Lin, DAO John Tannahill, LLNL (jrt@llnl.gov)

REVISION HISTORY:

05 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin Yeh with the TPCORE routines from GMI model. This eliminates the polar overshoot in the

stratosphere.

05 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Declare all REAL variables as REAL(fp). Also make sure all numerical constants are declared with the "D" double-precision exponent. Added OpenMP parallel DO loops.

01 Apr 2009 - C. Carouge - Moved the IK loop outside the subroutine.

3.4.27 Do_Ymist_Pole2_I2d2

Subroutine Do_Ymist_Pole2_I2d2 sets "dcy" at the Poles.

```
SUBROUTINE Do_Ymist_Pole2_I2d2( dcy, qqu, I1_GL, I2_GL, JU1_GL, & J2_GL, J1P, ILO, IHI, JULO, & JHI, I1, I2, JU1, J2)
```

INPUT PARAMETERS:

```
! Global latitude index at the edge of the South polar cap
! J1P=JU1_GL+1 for a polar cap of 1 latitude band
! J1P=JU1_GL+2 for a polar cap of 2 latitude bands
INTEGER, INTENT(IN) :: J1P
! Global min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN) :: I1_GL, I2_GL
INTEGER, INTENT(IN) :: JU1_GL, J2_GL
! Local min & max longitude (I), latitude (J), altitude (K) indices
INTEGER, INTENT(IN) :: I1,
                                12
INTEGER, INTENT(IN) :: JU1,
                                J2
! Local min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN) :: ILO,
                                IHI
INTEGER, INTENT(IN) :: JULO,
                                JHT
! Concentration contribution from E-W advection [mixing ratio]
```

OUTPUT PARAMETERS:

! Slope of concentration distribution in N-S direction [mixing ratio] REAL(fp), INTENT(OUT) :: dcy(ILO:IHI, JULO:JHI)

REAL(fp), INTENT(IN) :: qqu(ILO:IHI, JULO-2:JHI+2)

AUTHOR:

Original code from Shian-Jiann Lin, DAO John Tannahill, LLNL (jrt@llnl.gov)

REVISION HISTORY:

```
O5 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin
Yeh with the TPCORE routines from GMI model.
This eliminates the polar overshoot in the
stratosphere.

O5 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.
Declare all REAL variables as REAL(fp). Also
make sure all numerical constants are declared
with the "D" double-precision exponent. Added
OpenMP parallel DO loops.

O1 Apr 2009 - C. Carouge - Moved the IK loop outside the subroutine.
```

3.4.28 Fyppm

Subroutine Fyppm is the 1D "outer" flux form operator based on the Piecewise Parabolic Method (PPM; see also Lin and Rood 1996) for computing the fluxes in the N-S direction.

INTERFACE:

```
SUBROUTINE Fyppm(jlmt, cry, dcy, qqu,
                                               j1p, j2p,
                                         qqv,
                                                           &
                i1_gl, i2_gl, ju1_gl, j2_gl, ilong, ilo, ihi,
                julo, jhi, i1,
                                  i2,
                                         ju1,
                                               j2 )
```

INPUT PARAMETERS:

```
! Global latitude indices at the edges of the S/N polar caps
! J1P=JU1_GL+1; J2P=J2_GL-1 for a polar cap of 1 latitude band
! J1P=JU1_GL+2; J2P=J2_GL-2 for a polar cap of 2 latitude bands
INTEGER, INTENT(IN) :: J1P,
                               J2P
! Global min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN) :: I1_GL, I2_GL
INTEGER, INTENT(IN) :: JU1_GL, J2_GL
! Local min & max longitude (I), latitude (J), altitude (K) indices
INTEGER, INTENT(IN) :: I1,
INTEGER, INTENT(IN) :: JU1,
                                J2
! Local min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN) :: ILO,
                               IHI
INTEGER, INTENT(IN) :: JULO,
                               JHI
! ILONG ??
INTEGER, INTENT(IN) :: ilong
! Controls various options in N-S advection
INTEGER, INTENT(IN) :: jlmt
! Courant number in N-S direction
REAL(fp), INTENT(IN) :: cry(ILO:IHI, JULO:JHI)
! Slope of concentration distribution in N-S direction [mixing ratio]
REAL(fp), INTENT(IN) :: dcy(ILO:IHI, JULO:JHI)
! Concentration contribution from E-W advection [mixing ratio]
REAL(fp), INTENT(IN) :: qqu(ILO:IHI, JULO:JHI)
```

OUTPUT PARAMETERS:

! Concentration contribution from N-S advection [mixing ratio] REAL(fp), INTENT(OUT) :: qqv(ILO:IHI, JULO:JHI)

AUTHOR:

Original code from Shian-Jiann Lin, DAO John Tannahill, LLNL (jrt@llnl.gov)

REVISION HISTORY:

05 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin
Yeh with the TPCORE routines from GMI model.
This eliminates the polar overshoot in the
stratosphere.

05 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.
Declare all REAL variables as REAL(fp). Also

Declare all REAL variables as REAL(fp). Also make sure all numerical constants are declared with the "D" double-precision exponent. Added OpenMP parallel DO loops

01 Apr 2009 - C. Carouge - Moved the IK loop outside the subroutine.

3.4.29 Do_Fyppm_Pole_I2d2

Subroutine Do_Fyppm_Pole_I2d2 sets "al" & "ar" at the Poles.

INTERFACE:

```
SUBROUTINE Do_Fyppm_Pole_I2d2( al, ar, I1_GL, I2_GL, JU1_GL, J2_GL, & ILO, IHI, JULO, JHI, I1, I2, & JU1, J2 )
```

INPUT PARAMETERS:

```
! Global min & max longitude (I) and latitude (J) indices INTEGER, INTENT(IN) :: I1_GL, I2_GL INTEGER, INTENT(IN) :: JU1_GL, J2_GL
```

! Local min & max longitude (I), latitude (J), altitude (K) indices INTEGER, INTENT(IN) :: I1, I2
INTEGER, INTENT(IN) :: JU1, J2

! Local min & max longitude (I) and latitude (J) indices INTEGER, INTENT(IN) :: ILO, IHI INTEGER, INTENT(IN) :: JULO, JHI

OUTPUT PARAMETERS:

```
! Left (al) and right (ar) edge values of the test parabola REAL(fp), INTENT(INOUT) :: al(ILO:IHI, JULO:JHI)
REAL(fp), INTENT(INOUT) :: ar(ILO:IHI, JULO:JHI)
```

AUTHOR:

Original code from Shian-Jiann Lin, DAO John Tannahill, LLNL (jrt@llnl.gov)

REVISION HISTORY:

05 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin
Yeh with the TPCORE routines from GMI model.
This eliminates the polar overshoot in the
stratosphere.

05 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.
Declare all REAL variables as REAL(fp). Also

make sure all numerical constants are declared with the "D" double-precision exponent. Added OpenMP parallel DO loops.

01 Apr 2009 - C. Carouge - Moved the IK loop outside the subroutine.

3.4.30 Do_Ytp_Pole_Sum

Subroutine Do_Ytp_Pole_Sum sets "dq1" at the Poles.

INTERFACE:

```
SUBROUTINE Do_Ytp_Pole_Sum( geofac_pc, dq1,
                                              qqv,
                                                     fy, I1_GL,
                            I2_GL,
                                       JU1_GL, J2_GL, J1P, J2P,
                                                                   &
                            ILO,
                                       IHI,
                                              JULO, JHI, I1,
                                               J2 )
                            I2,
                                       JU1,
!input PARAMETERS:
  ! Global latitude indices at the edges of the S/N polar caps
  ! J1P=JU1_GL+1; J2P=J2_GL-1 for a polar cap of 1 latitude band
  ! J1P=JU1_GL+2; J2P=J2_GL-2 for a polar cap of 2 latitude bands
  INTEGER, INTENT(IN)
                       :: J1P,
  ! Global min & max longitude (I) and latitude (J) indices
  INTEGER, INTENT(IN) :: I1_GL, I2_GL
  INTEGER, INTENT(IN)
                        :: JU1_GL, J2_GL
  ! Local min & max longitude (I), latitude (J), altitude (K) indices
  INTEGER, INTENT(IN)
                         :: I1,
                                   12
  INTEGER, INTENT(IN)
                        :: JU1,
                                   J2
```

! Local min & max longitude (I) and latitude (J) indices

INTEGER, INTENT(IN) :: ILO, IHI
INTEGER, INTENT(IN) :: JULO, JHI

! Special geometrical factor (geofac) for Polar cap
REAL(fp), INTENT(IN) :: geofac_pc

```
! Concentration contribution from N-S advection [mixing ratio] REAL(fp), INTENT(IN) :: qqv(ILO:IHI, JULO:JHI)
```

INPUT/OUTPUT PARAMETERS:

```
! Species density [hPa]
REAL(fp), INTENT(INOUT) :: dq1(ILO:IHI, JULO:JHI)
! N-S mass flux [mixing ratio]
REAL(fp), INTENT(INOUT) :: fy (ILO:IHI, JULO:JHI+1)
```

AUTHOR:

```
Original code from Shian-Jiann Lin, DAO John Tannahill, LLNL (jrt@llnl.gov)
```

REVISION HISTORY:

```
O5 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin
Yeh with the TPCORE routines from GMI model.
This eliminates the polar overshoot in the
stratosphere.

O5 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.
Declare all REAL variables as REAL(fp). Also
make sure all numerical constants are declared
with the "D" double-precision exponent. Added
OpenMP parallel DO loops.

O1 Apr 2009 - C. Carouge - Moved the IK loop outside the subroutine.
```

3.4.31 Fzppm

Subroutine Fzppm is the 1D "outer" flux form operator based on the Piecewise Parabolic Method (PPM; see also Lin and Rood 1996) for computing the fluxes in the vertical direction.

Fzppm was modified by S.-J. Lin, 12/14/98, to allow the use of the KORD=7 (klmt=4) option. KORD=7 enforces the 2nd monotonicity constraint of Huynh (1996). Note that in Huynh's original scheme, two constraints are necessary for the preservation of monotonicity. To use Huynh's algorithm, it was modified as follows. The original PPM is still used to obtain the first guesses for the cell edges, and as such Huynh's 1st constraint is no longer needed. Huynh's median function is also replaced by a simpler yet functionally equivalent in-line algorithm.

```
SUBROUTINE Fzppm( klmt, delp1, wz, dq1, qq1, fz, & J1P, JU1_GL, J2_GL, ILO, IHI, JULO, JHI, & ILONG, IVERT, I1, I2, JU1, J2, K1, K2)
```

INPUT PARAMETERS:

```
! Global latitude index at the edges of the South polar cap
    ! J1P=JU1_GL+1 for a polar cap of 1 latitude band
    ! J1P=JU1_GL+2 for a polar cap of 2 latitude bands
    INTEGER, INTENT(IN) :: J1P
     ! Global min & max longitude (I) and latitude (J) indices
    INTEGER, INTENT(IN) :: JU1_GL, J2_GL
    ! Local min & max longitude (I), latitude (J), altitude (K) indices
    INTEGER, INTENT(IN) :: I1,
                                     T2
    INTEGER, INTENT(IN) :: JU1,
                                     .12
    INTEGER, INTENT(IN) :: K1,
                                     K2
    ! Local min & max longitude (I) and latitude (J) indices
    INTEGER, INTENT(IN)
                        :: ILO,
                                      IHI
    INTEGER, INTENT(IN)
                          :: JULO,
                                     JHI
    ! Dimensions in longitude & altitude ???
    INTEGER, INTENT(IN)
                        :: ilong, ivert
    ! Controls various options in vertical advection
    INTEGER, INTENT(IN)
                          :: klmt
    ! Pressure thickness, the pseudo-density in a
    ! hydrostatic system at t1 [hPa]
                          :: delp1(ILO:IHI, JULO:JHI, K1:K2)
    REAL(fp), INTENT(IN)
    ! Large scale mass flux (per time step tdt) in the vertical
    ! direction as diagnosed from the hydrostatic relationship [hPa]
    REAL(fp), INTENT(IN)
                            :: wz(I1:I2, JU1:J2, K1:K2)
    ! Species concentration [mixing ratio]
    REAL(fp), INTENT(IN)
                             :: qq1(:,:,:)
INPUT/OUTPUT PARAMETERS:
    ! Species density [hPa]
    REAL(fp), INTENT(INOUT) :: dq1(ILO:IHI, JULO:JHI, K1:K2)
OUTPUT PARAMETERS:
     ! Vertical flux [mixing ratio]
    REAL(fp), INTENT(OUT) :: fz(ILO:IHI, JULO:JHI, K1:K2)
AUTHOR:
    Original code from Shian-Jiann Lin, DAO
    John Tannahill, LLNL (jrt@llnl.gov)
```

REVISION HISTORY:

```
O5 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin
Yeh with the TPCORE routines from GMI model.
This eliminates the polar overshoot in the
stratosphere.

O5 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.
Declare all REAL variables as REAL(fp). Also
make sure all numerical constants are declared
with the "D" double-precision exponent.
```

3.4.32 Average_Press_Poles

Subroutine Average_Press_Poles averages pressure at the Poles when the Polar cap is enlarged. It makes the last two latitudes equal.

INTERFACE:

```
SUBROUTINE Average_Press_Poles( area_1D, press, I1, I2, JU1, & J2, ILO, IHI, JULO, JHI)
```

INPUT PARAMETERS:

```
! Local min & max longitude (I), latitude (J)
INTEGER, INTENT(IN)
                      :: I1,
                                 12
INTEGER, INTENT(IN)
                      :: JU1,
                                 J2
! Local min & max longitude (I) and latitude (J) indices
INTEGER, INTENT(IN)
                      :: ILO,
                                 IHI
INTEGER, INTENT(IN)
                      :: JULO,
                                 JHI
! Surface area of grid box
REAL(fp), INTENT(IN)
                       :: AREA_1D(JU1:J2)
```

INPUT/OUTPUT PARAMETERS:

```
! Surface pressure [hPa]
REAL(fp), INTENT(INOUT) :: press(ILO:IHI, JULO:JHI)
```

AUTHOR:

```
Philip Cameron-Smith and John Tannahill, GMI project @ LLNL (2003) Implemented into GEOS-Chem by Claire Carouge (ccarouge@seas.harvard.edu)
```

REMARKS:

Subroutine from pjc_pfix. Call this one once everything is working fine.

05 Dec 2008 - C. Carouge - Replaced TPCORE routines by S-J Lin and Kevin Yeh with the TPCORE routines from GMI model.

This eliminates the polar overshoot in the stratosphere.

05 Dec 2008 - R. Yantosca - Updated documentation and added ProTeX headers.

Declare all REAL variables as REAL(fp). Also

make sure all numerical constants are declared

with the "D" double-precision exponent.

4 Convection and scavenging modules

These modules contain routines to perform the convective transport and to scavenge soluble species out of the atmosphere.

4.1 Fortran: Module Interface convection_mod.F90

Module CONVECTION_MOD contains routines which select the proper convection code for GEOS-3, GEOS-4, GEOS-5, MERRA, or GCAP met field data sets.

INTERFACE:

MODULE CONVECTION_MOD

USES:

USE ErrCode_Mod

USE PhysConstants ! Physical constants

USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

IMPLICIT NONE PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: DO_CONVECTION

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: DO_GEOS4_CONVECT PRIVATE :: DO_GCAP_CONVECT

PRIVATE :: NFCLDMX

PRIVATE :: DO_MERRA_CONVECTION

REVISION HISTORY:

27 Jan 2004 - R. Yantosca - Initial version

(1) Contains new updates for GEOS-4/fvDAS convection. Also now references "error_mod.f". Now make F in routine NFCLDMX a 4-D array to avoid

```
memory problems on the Altix. (bmy, 1/27/04)
(2) Bug fix: Now pass NTRACE elements of TCVV to FVDAS_CONVECT in routine
      DO_CONVECTION (bmy, 2/23/04)
(3) Now references "logical_mod.f" and "tracer_mod.f" (bmy, 7/20/04)
(4) Now also references "ocean_mercury_mod.f" and "tracerid_mod.f"
      (sas, bmy, 1/19/05)
(5) Now added routines DO_GEOS4_CONVECT and DO_GCAP_CONVECT by breaking
      off code from DO_CONVECTION, in order to implement GCAP convection
      in a much cleaner way. (swu, bmy, 5/25/05)
(6) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
(7) Shut off scavenging in shallow convection for GCAP (swu, bmy, 11/1/05)
(8) Modified for tagged Hg simulation (cdh, bmy, 1/6/06)
(9) Bug fix: now only call ADD_Hg2_WD if LDYNOCEAN=T (phs, 2/8/07)
(10) Fix for GEOS-5 met fields in routine NFCLDMX (swu, 8/15/07)
(11) Resize DTCSUM array in NFCLDMX to save memory (bmy, 1/31/08)
13 Aug 2010 - R. Yantosca - Added ProTeX headers
13 Aug 2010 - R. Yantosca - Treat MERRA in the same way as for GEOS-5
29 Sep 2010 - R. Yantosca - Added modifications for MERRA
05 Oct 2010 - R. Yantosca - Added ND14 and ND38 diagnostics to
                            DO_MERRA_CONVECTION routine
16 Aug 2011 - J. Fisher - Minor bug fixes in DO_MERRA_CONVECTION
15 Feb 2011 - R. Yantosca - Add modifications for APM from G. Luo
28 Feb 2012 - R. Yantosca - Removed support for GEOS-3
02 Mar 2012 - R. Yantosca - Now reference the new grid_mod.F90
22 Oct 2012 - R. Yantosca - Now reference Headers/gigc_errcode_mod.F90
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
07 Nov 2014 - M. Yannetti - Added PRECISION_MOD
23 Jun 2015 - E. Lundgren - Convert tracer units from v/v dry air to
```

kg/kg total air for convection

compatible with the FlexChem implementation

23 Jun 2016 - R. Yantosca - Remove references to APM code; it is no longer

06 Jul 2016 - E. Lundgren - Spc units are now kg/kg dry air in convection

4.1.1 do_convection

Subroutine DO_CONVECTION calls the appropriate convection driver program for different met field data sets.

29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90

INTERFACE:

```
SUBROUTINE DO_CONVECTION( am_I_Root, Input_Opt, & State_Met, State_Chm, RC )

USES:

USE CMN_DIAG_MOD
```

USE CMN_DIAG_MOD

USE DIAG_MOD, ONLY : CONVFLUP USE ERROR_MOD, ONLY : GC_Error USE UnitConv_Mod #if defined(BPCH_DIAG) USE DIAG_MOD, ONLY: AD38 #endif USE ErrCode_Mod USE ERROR_MOD, ONLY : GEOS_CHEM_STOP USE GC_GRID_MOD, ONLY : GET_AREA_M2 USE Input_Opt_Mod, ONLY : OptInput USE Species_Mod, ONLY : Species USE State_Chm_Mod, ONLY : ChmState USE State_Met_Mod, ONLY : MetState USE TIME_MOD, ONLY : GET_TS_DYN USE TIME_MOD, ONLY : GET_TS_CONV ONLY : COMPUTE_F USE WETSCAV_MOD, USE WETSCAV_MOD, ONLY: H2O2s USE WETSCAV_MOD, ONLY : SO2s #if defined(NC_DIAG) USE HCO_ERROR_MOD USE HCO_INTERFACE_MOD USE ERROR_MOD, ONLY : ERROR_STOP USE HCO_DIAGN_MOD, ONLY : Diagn_Update #endif #if defined(USE_TEND) USE TENDENCIES_MOD USE State_Chm_Mod, ONLY : Ind_ #endif

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

25 May 2005 - S. Wu - Initial version
08 Feb 2007 - R. Yantosca - Now reference "CMN_SIZE". Now references
CLDMAS, CMFMC, DTRAIN from "dao_mod.f" so that
we can pass either GEOS-5 or GEOS-3 meteorology

to NFCLDMX.

```
13 Aug 2010 - R. Yantosca - Added ProTeX headers
```

- 13 Aug 2010 R. Yantosca Treat MERRA in the same way as for GEOS-5
- 29 Sep 2010 R. Yantosca Now call DO_MERRA_CONVECTION for MERRA met
- 05 Oct 2010 R. Yantosca Now attach diagnostics to MERRA conv routine
- 06 Oct 2010 R. Yantosca Parallelized call to DO_MERRA_CONVECTION
- 15 Oct 2010 H. Amos Now get BXHEIGHT, T from dao_mod.f
- 15 Oct 2010 R. Yantosca Now get LDYNOCEAN from logical_mod.f
- 15 Oct 2010 R. Yantosca Now get ITS_A_MERCURY_SIM from tracer_mod.f
- 15 Oct 2010 R. Yantosca Now get IDTHg2, IDTHgP from tracerid_mod.f
- 15 Oct 2010 R. Yantosca Now get H2O2s, SO2s from wetscav_mod.f
- 15 Oct 2010 H. Amos Now pass BXHEIGHT, T, to DO_MERRA_CONVECTION
- 15 Oct 2010 R. Yantosca Now pass H2O2s, SO2s to DO_MERRA_CONVECTION
- 15 Feb 2011 R. Yantosca Add modifications for APM from G. Luo
- 29 Aug 2011 R. Yantosca Bug fix: reposition #if defined(APM) statement
- 09 Feb 2012 R. Yantosca For GEOS-5.7, PFICU and PFLCU fields are defined on level edges. Pass the top edge of each level to DO_MERRA_CONVECTION
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 01 Mar 2012 R. Yantosca Now use GET_AREA_M2(I,J,L) from grid_mod.F90
- 21 Jun 2012 R. Yantosca Now use poiners to pass array slices to routines
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 04 Feb 2013 S. Kim Bug fix: H202s, S02s, STT are not in State_Met
- 25 Mar 2013 R. Yantosca Now accept am_I_Root, Input_Opt, State_Chm, RC
- 31 May 2013 R. Yantosca Now pass objects to NFCLDMX
- 03 Jun 2013 R. Yantosca Bug fix: pass State_Chm to DO_MERRA_CONVECTION
- 26 Sep 2013 R. Yantosca Renamed GEOS_57 Cpp switch to GEOS_FP
- 17 Apr 2014 R. Yantosca Speed up MERRA and GEOS-FP convection by adding !\$OMP+SCHEDULE(DYNAMIC)
- 17 Apr 2014 R. Yantosca Test if (ND14>0) and (ND38>0) outside OMP loop
- 18 Apr 2014 R. Yantosca Now use a pointer to pass a slice of the F array to subroutine COMPUTE_F
- 18 Apr 2014 R. Yantosca Clean up call to DO_MERRA_CONVECTION, remove stuff that was leftover from the column code
- 18 Apr 2014 R. Yantosca Now use proper # of tracers for APM in the call to DO_MERRA_CONVECTION (MERRA & GEOS-FP)
- 25 Jun 2014 R. Yantosca Now pass Input_Opt to COMPUTE_F
- 26 Feb 2015 E. Lundgren Replace GET_PEDGE with State_Met%PEDGE.
 Remove dependency on pressure_mod
- 28 Apr 2015 E. Lundgren Consolidate NFCLDMX arguments to remove passing State_Met array slice
- 15 Jun 2015 E. Lundgren Now use kg/kg total air as tracer units (previously v/v)
- 10 Aug 2015 E. Lundgren Incoming tracer units are now kg/kg dry air
- 11 Aug 2015 R. Yantosca Added support for MERRA2 data
- 29 Apr 2016 R. Yantosca Don't initialize pointers in declaration stmts
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected

```
species ID from State_Chm%Map_Advect.

06 Jul 2016 - R. Yantosca - Use State_Chm%Map_WetDep to get species ID's

07 Jul 2016 - R. Yantosca - Now dimension DIAG14 and DIAG38 for the #

of soluble species (State_Chm%nWetDep)

07 Jul 2016 - E. Lundgren - Now use spc kg/kg dry instead of kg/kg total

8 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code
```

4.1.2 do_geos4_convect

Subroutine DO_GEOS4_CONVECT is a wrapper for the GEOS-4/fvDAS convection code. This was broken off from the old DO_CONVECTION routine above.

INTERFACE:

```
SUBROUTINE DO_GEOS4_CONVECT( am_I_Root, Input_Opt,
& State_Met, State_Chm, RC )
```

USES:

```
USE CMN_DIAG_MOD
USE CMN_SIZE_MOD
```

USE DIAG_MOD, ONLY : AD37

USE ErrCode_Mod

USE ERROR_MOD, ONLY : DEBUG_MSG

USE FVDAS_CONVECT_MOD, ONLY : INIT_FVDAS_CONVECT, FVDAS_CONVECT

USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState
USE TIME_MOD, ONLY : GET_TS_CONV
USE WETSCAV_MOD, ONLY : COMPUTE_F

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

As of July 2016, we assume that all of the advected species are listed first in the species database. This is the easiest way to pass a slab to the TPCORE routine. This may change in the future. (bmy, 7/13/16)

%%% GEOS-4 IS DEPRECATED AND MAY BE REMOVED SOON %%%%

REVISION HISTORY:

```
25 May 2005 - S. Wu
                         - Initial version
(1 ) Now use array masks to flip arrays vertically in call to FVDAS_CONVECT
      (bmy, 5/25/05)
(2) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
(3) Add a check to set negative values in STT to TINY (ccc, 4/15/09)
13 Aug 2010 - R. Yantosca - Added ProTeX headers
15 Feb 2011 - R. Yantosca - Add modifications for APM from G. Luo
09 Nov 2012 - M. Payer
                          - Replaced all met field arrays with State_Met
                            derived type object
25 Mar 2013 - R. Yantosca - Now accept am_I_Root, Input_Opt, State_Chm, RC
14 Apr 2014 - R. Yantosca - Remove array temporary in call to FVDAS_CONVECT
18 Apr 2014 - R. Yantosca - Now use a pointer to pass a slice of the
                            F array to subroutine COMPUTE_F
23 Jun 2014 - R. Yantosca - Now pass Input_Opt to CONVTRAN
25 Jun 2014 - R. Yantosca - Now pass Input_Opt to COMPUTE_F
26 Feb 2015 - E. Lundgren - Replace GET_PEDGE differences with
                            State_Met%DELP. Remove dependency on
                            pressure_mod
23 Jun 2015 - E. Lundgren - Now use kg/kg total air as tracer units
                            (previously v/v)
22 Apr 2016 - R. Yantosca - Now pass State_Chm to FVDAS_CONVECT_MOD
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected
                            species ID from State_Chm%Map_Advect.
06 Jul 2016 - E. Lundgren - Now use kg/kg dry air as spc units, requiring
                            use of DELP_DRY instead of DELP
```

4.1.3 do_gcap_convect

Subroutine DO_GCAP_CONVECT is a wrapper for the GCAP convection code. This was broken off from the old DO_CONVECTION routine above.

INTERFACE:

```
SUBROUTINE DO_GCAP_CONVECT( am_I_Root, Input_Opt, & State_Met, State_Chm, RC )
```

USES:

```
USE CMN_DIAG_MOD

USE CMN_SIZE_MOD

USE DIAG_MOD, ONLY : AD37

USE ErrCode_Mod

USE ERROR_MOD, ONLY : DEBUG_MSG

USE GCAP_CONVECT_MOD, ONLY : GCAP_CONVECT

USE Input_Opt_Mod, ONLY : OptInput

USE State_Chm_Mod, ONLY : ChmState
```

USE State_Met_Mod, ONLY : MetState
USE TIME_MOD, ONLY : GET_TS_CONV
USE WETSCAV_MOD, ONLY : COMPUTE_F

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

- 25 May 2005 S. Wu Initial version
- (1) Now use array masks to flip arrays vertically in call to GCAP_CONVECT (bmy, 5/25/05)
- (2) Shut off scavenging in shallow convection for GCAP below 700 hPa (swu, bmy, 11/1/05)
- (3) Add a check to set negative values in STT to TINY (ccc, 4/15/09)
- 13 Aug 2010 R. Yantosca Added ProTeX headers
- 15 Feb 2011 R. Yantosca Add modifications for APM from G. Luo
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 25 Mar 2013 R. Yantosca Now accept am_I_Root, Input_Opt, State_Chm, RC
- 04 Nov 2013 M. Sulprizio- Now use pointer variables to flip met fields in the vertical
- 15 Apr 2014 R. Yantosca Remove array temporaries in call to GCAP_CONVECT
- 18 Apr 2014 R. Yantosca Now use a pointer to pass a slice of the F array to subroutine COMPUTE_F
- 25 Jun 2014 R. Yantosca Now pass Input_Opt to COMPUTE_F
- 26 Feb 2015 E. Lundgren Replace GET_PCENTER with State_Met%PMID.

Replace PEDGE difference with State_Met%DELP.

Remove dependency on pressure_mod.

- 23 Jun 2015 E. Lundgren Now use kg/kg total air as tracer units
- (previously v/v) 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected
- species ID from State_Chm%Map_Advect.
- 06 Jul 2016 E. Lundgren Now use kg/kg dry air as spc units, requiring use of DELP_DRY instead of DELP

4.1.4 nfcldmx

Subroutine NFCLDMX is S-J Lin's cumulus transport module for 3D GSFC-CTM, modified for the GEOS-Chem model. The "NF" stands for "no flipping", and denotes that you

don't have to flip the species array Q in the main program before passing it to NFCLDMX.

NOTE: NFCLDMX can be used with GEOS-1, GEOS-STRAT, and GEOS-3 met fields. For GEOS-4/fVDAS, you must use the routines in "fvdas_convect_mod.f"

INTERFACE:

```
SUBROUTINE NFCLDMX( am_I_Root, Input_Opt, State_Met,
& State_Chm, RC )
```

USES:

USE CMN_DIAG_MOD USE CMN_SIZE_MOD

USE DEPO_MERCURY_MOD, ONLY : ADD_Hg2_WD USE DEPO_MERCURY_MOD, ONLY : ADD_HgP_WD

USE DEPO_MERCURY_MOD, ONLY : ADD_Hg2_SNOWPACK

USE DIAG_MOD, ONLY : AD37

#if defined(BPCH_DIAG)

USE DIAG_MOD, ONLY : AD38

#endif

USE DIAG_MOD, ONLY : CONVFLUP

USE ErrCode_Mod

USE GC_GRID_MOD, ONLY : GET_AREA_M2 USE Input_Opt_Mod, ONLY : OptInput USE PRESSURE_MOD, ONLY : GET_BP USE Species_Mod, ONLY : Species USE State_Chm_Mod, ONLY : ChmState USE State_Met_Mod, ONLY : MetState USE TIME_MOD, ONLY : GET_TS_CONV USE WETSCAV_MOD, ONLY : COMPUTE_F USE ERROR_MOD, ONLY : ALLOC_ERR

IMPLICIT NONE

INPUT PARAMETERS:

! Are we on the root CPU

LOGICAL, INTENT(IN) :: am_I_Root

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REMARKS:

k+1

CMFMC(k+1)

- (1) The "NF" stands for "no flipping", and denotes that you don't have to flip the species array $\mathbb Q$ in the main program before passing it to NFCLDMX. (bmy, 2/12/97, 1/31/08)
- (2) This version has been customized to work with ${\tt GEOS-5}$ met fields. Reference:

Lin, SJ. "Description of the parameterization of cumulus transport in the 3D Goddard Chemistry Transport Model, NASA/GSFC, 1996. Vertical indexing:

The indexing of the vertical sigma levels has been changed from SJ-Lin's original code:

Lin's origi	Old Method	New Method	-
_	(SJ Lin)		Top of Atm.
	k = 1	k = NLAY	
=		k = NLAY-1	
-		k = 4	
-	k = NLAY-2	k = 3	Cloud hage
_	k = NLAY-1	k = 2	Cloud base
=	k = NLAY	k = 1	Ground
which mean	ns that:		
	Old Method (SJ Lin)	New	Method
	(55 LIII) 	k+1	^ -
	CMFMC(k)		MC(k)
		becomes	
k	DTRAIN(k), QC(k), Q(k)	k DT: QC(RAIN(k), k), Q(k)
	^		•
			-

k-1 CMFMC(k-1)

i.e., the lowest level used to be NLAY but is now 1 the level below k used to be k+1 but is now k-1. the level above k used to be k-1 but is now k+1 the top of the atm. used to be 1 but is now NLAY.

The old method required that the vertical dimensions of the CMFMC, DTRAIN, and Q arrays had to be flipped before and after calling CLDMX. Also, diagnostic arrays generated within CLDMX also had to be flipped. The new indexing eliminates this requirement (and also saves on array operations). Major Modifications:

Original Author: Shian-Jiann Lin, Code 910.3, NASA/GSFC

Original Release: 12 February 1997

Version 3, Detrainment and Entrainment are considered. The algorithm reduces to that of version 2 if Dtrn = 0.

Modified By: Bob Yantosca, for Harvard Atmospheric Sciences

Modified Release: 27 January 1998

Version 3.11, contains features of V.3 but also scavenges soluble tracer in wet convective updrafts.

28 April 1998

Version 3.12, now includes mass flux diagnostic

11 November 1999

Added mass-flux diagnostics

04 January 2000

Updated scavenging constant AS2

14 March 2000

Added new wet scavenging code and diagnostics

based on the GMI algorithm

02 May 2000

Added parallel loop over species!

- 12 Feb 1997 M. Prather Initial version
- (1) NFCLDMX is written in Fixed-Form Fortran 90.
- (2) Added TCVV to the argument list. Also cleaned up argument and local variable declarations. (bey, bmy, 11/10/99)
- (3) AD38 and CONVFLUP are now declared allocatable in "diag_mod.f". (bmy, 11/29/99)
- (4) Bug fix for tagged CO tracer run (bey, bmy, 1/4/00)
- (5) Add new routines for computing scavenging coefficients, as well as adding the AD37 diagnostic array. (bmy, 3/14/00)
- (6) Updated comments (bmy, 10/2/01)

- (7) Now print a header to stdout on the first call, to confirm that NFCLDMX has been called (bmy, 4/15/02)
- (8) Remove PZ from the arg list -- it isn't used! (bmy, 8/22/02)
- (9) Fixed ND38 diagnostic so that it now reports correctly (must divide by DNS). Updatec comments, cosmetic changes. (bmy, 1/27/03)
- (10) Bug fix: remove duplicate K from PRIVATE declaration (bmy, 3/23/03)
- (11) Now removed all arguments except NC, TCVV, Q from the arg list -- the other arguments can be supplied via F90 modules. Now references "dao_mod.f", "grid_mod.f", "pressure_mod.f", and "time_mod.f". (bmy, 3/27/03)
- (12) Bundled into "convection_mod.f" (bmy, 6/26/03)
- (13) Make sure K does not go out of bounds in ND38 diagnostic. Now make F a 4-D array in order to avoid memory problems on the Altix. (bmy, 1/27/04)
- (14) Now references both "ocean_mercury_mod.f" and "tracerid_mod.f".

 Now call ADD_Hg2_WD from "ocean_mercury_mod.f" to pass the amt of Hg2 lost by wet scavenging (sas, bmy, 1/19/05)
- (15) Now references IS_Hg2 from "tracerid_mod.f". Now pass tracer # IC to ADD_Hg2_WD. (cdh, bmy, 1/6/06)
- (16) Bug fix: now only call ADD_Hg2_WD if LDYNOCEAN=T (phs, 2/8/07)
- (17) Now make CLDMAS, DTRN as arguments, so that we can pass either GEOS-3 or GEOS-3 met data. Redimension DTCSUM with NC instead of NNPAR. In many cases, NC is less than NNPAR and this will help to save memory especially when running at 2x25 or greater resolution (bmy, 1/31/08)
- (18) Add a check to set negative values in Q to TINY (ccc, 4/15/09)
- (19) Updates for mercury simulation (ccc, 5/17/10)
- 13 Aug 2010 R. Yantosca Added ProTeX headers
- 01 Mar 2012 R. Yantosca Now use GET_AREA_M2(I,J,L) from grid_mod.F90
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 29 May 2013 R. Yantosca Now set TINY = 1d-60 only for TOMAS code
- 31 May 2013 R. Yantosca Now pass State_Chm and then have Q point to State_Chm%Tracers. This is for TOMAS.
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 26 Sep 2013 R. Yantosca Renamed GEOS_57 Cpp switch to GEOS_FP
- 04 Feb 2014 R. Yantosca Bug fix for TOMAS: call COMPUTE_F In its own separate parallel loop. Also save the values of ISOL in the ISOL_SAVE array so that we can pass them to the parallel tracer loop.
- 18 Apr 2014 R. Yantosca Now use a pointer to pass a slice of the F array to subroutine COMPUTE_F
- 25 Jun 2014 R. Yantosca Now pass Input_Opt to COMPUTE_F
- 26 Feb 2015 E. Lundgren Replace GET_PEDGE dinnerences with DELP and remove dependency on pressure_mod
- 20 Apr 2015 E. Lundgren Use DELP*100/g instead of AD/area for BMASS to keep definition as grid box moist mass/area
- 28 Apr 2015 E. Lundgren Remove CLDMAS and DTRM as arguments since

```
now included in State_Met

09 Jun 2015 - R. Yantosca - Now deposit Hg2, HgP to snowpack regardless of whether the dynamic ocean is used

15 Jun 2015 - E. Lundgren - Now use kg/kg total air as tracer units (previously v/v)

22 Apr 2016 - R. Yantosca - Now get Is_Hg2 and Is_HgP from species database

22 Apr 2016 - R. Yantosca - Now pass ThisSpc to ADD_HG2_SNOWPACK

29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts

30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

01 Jul 2016 - R. Yantosca - Now rename species DB object ThisSpc to SpcInfo

06 Jul 2016 - E. Lundgren - Now use kg/kg dry air as spc units, requiring use of DELP_DRY instead of DELP
```

4.1.5 do_merra_convection

Subroutine DO_MERRA_CONVECTION (formerly called NFCLDMX) is S-J Lin's cumulus transport module for 3D GSFC-CTM, modified for the GEOS-Chem model.

INTERFACE:

8		DO_MERRA_CONVECTION(<pre>am_I_Root, Input_Opt,</pre>	
8	;		State_Met,	
8	;		State_Chm,	
8	;		I,	
8	;		J,	
8	;		AREA_M2,	
8	;		F,	
8	:		TS_DYN,	
8	:		USE_DIAG14,	
8	:		DIAG14,	
8	;		USE_DIAG38,	
8	;		DIAG38,	
8	:		RC)

USES:

```
USE CMN_SIZE_MOD
USE DEPO_MERCURY_MOD,
                        ONLY : ADD_Hg2_SNOWPACK
USE DEPO_MERCURY_MOD,
                        ONLY: ADD_Hg2_WD
USE DEPO_MERCURY_MOD,
                        ONLY : ADD_HgP_WD
                        ONLY : IT_IS_NAN
USE ERROR_MOD,
USE ERROR_MOD,
                        ONLY : IT_IS_FINITE
USE ERROR_MOD,
                        ONLY: GEOS_CHEM_STOP ! hma Nov 3, debug
USE Input_Opt_Mod,
                        ONLY : OptInput
USE State_Chm_Mod,
                        ONLY : ChmState
USE State_Met_Mod,
                        ONLY : MetState
```

```
USE Species_Mod, ONLY : Species

USE WETSCAV_MOD, ONLY : H202s_3D => H202s ! [v/v]

USE WETSCAV_MOD, ONLY : S02s_3D => S02s ! [v/v]

USE WETSCAV_MOD, ONLY : WASHOUT

USE WETSCAV_MOD, ONLY : LS_K_RAIN

USE WETSCAV_MOD, ONLY : LS_F_PRIME
```

INPUT PARAMETERS:

```
:: am_I_Root ! Are we on the root CPU?
LOGICAL,
            INTENT(IN)
TYPE(OptInput), INTENT(IN)
                       :: Input_Opt ! Input Options object
TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
! for updraft scavenging
                                  ! [unitless]. Computed by
                                   ! routine COMPUTE_F.
REAL(fp), INTENT(IN) :: TS_DYN
                                  ! Dynamic timestep [min]
           INTENT(IN) :: USE_DIAG14 ! Archive DIAG14?
LOGICAL,
           INTENT(IN) :: USE_DIAG38 ! Archive DIAG38?
LOGICAL,
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT) :: DIAG14(:,:) ! Array for ND14 diagnostic REAL(fp), INTENT(OUT) :: DIAG38(:,:) ! Array for ND38 diagnostic INTEGER, INTENT(OUT) :: RC ! Return code
```

REMARKS:

Reference:

Lin, SJ. "Description of the parameterization of cumulus transport in the 3D Goddard Chemistry Transport Model, NASA/GSFC, 1996.

Unit conversion for BMASS:

NOTE: We are passing I & J down to this routine so that it can call the proper code from "mercury_mod.f". Normally, we wouldn't pass I & J as arguments to columnized code. This prevents rewriting the mercury_mod.f routines ADD_Hg2_

```
15 Jul 2009 - R. Yantosca - Columnized and cleaned up.
                          - CLDMAS renamed to CMFMC and DTRN renamed
                            to DTRAIN for consistency w/ GEOS-5.
17 Jul 2009 - R. Yantosca - Now do unit conversion of Q array from
                            [kg] --> [v/v] and vice versa internally
14 Dec 2009 - R. Yantosca - Now remove internal unit conversion, since
                            Q now comes in as [mol/mol] (=[v/v]) from the
                            calling routine.
14 Dec 2009 - R. Yantosca - Remove COEF from the argument list
06 May 2010 - R. Yantosca - Now add IDENT via the argument list
29 Sep 2010 - R. Yantosca - Modified for MERRA met fields
05 Oct 2010 - R. Yantosca - Now pass COEF via the argument list
05 Oct 2010 - R. Yantosca - Attach ND14 and ND38 diagnostics
15 Oct 2010 - H. Amos
                          - Added BXHEIGHT and T as arguments
15 Oct 2010 - R. Yantosca - Added I, J, H2O2s and SO2s as arguments
15 Oct 2010 - H. Amos
                          - Added scavenging below cloud base
06 Apr 2011 - M.Fu, H.Amos- Bug fix: make sure washout adheres to the same
                            algorithm as in the wet deposition code.
27 Jul 2011 - R. Yantosca - Declare CLDBASE as INTEGER to avoid PGI errors
16 Aug 2011 - J. Fisher - Bug fix: use IS_Hg2() and IS_HgP to test if
                            a tracer is Hg2 or HgP (for tagged species)
16 Aug 2011 - J. Fisher - Now use WETLOSS instead of TO_SUM in the ND38
                            diagnostic below the cloud. Using TO_SUM leads
                            us to over-count the tracer scavenged out of
                            the column.
22 Oct 2012 - R. Yantosca - Now reference Headers/gigc_errcode_mod.F90
09 Nov 2012 - M. Payer
                          - Replaced all met field arrays with State_Met
                            derived type object
31 May 2013 - R. Yantosca - Now pass State_Chm to WASHOUT
05 Sep 2013 - R. Yantosca - Bug fix: DT is apparently undefined, but still
                            passed to WASHOUT. Use SDT instead. This
                            avoids a floating-point error.
18 Apr 2014 - R. Yantosca - Now point to 3-D arrays internally
18 Apr 2014 - R. Yantosca - Now also pass N_TRACERS (to facilitate APM)
18 Apr 2014 - R. Yantosca - Remove code that we don't need anymore
04 Feb 2015 - M. Sulprizio- Fix calculation of WETLOSS for non-aerosol
                            tracers below the cloud base (C. Friedman)
20 Apr 2015 - E. Lundgren - Use DELP*100/g instead of AD/area as grid box
                            moist mass per area and remove AD from routine
20 May 2015 - M. Sulprizio- Apply bug fixes provided by Viral Shah:
                            -- Remove F(K,IC) > 0 condition that prevents
                               archiving of deposited mass in DIAG38
                            -- Add statement that subtracts the wet deposited
                               amount from the atmospheric mass
                            -- Fix inconsistency in units when TO_SUM is used
04 Jun 2015 - E. Lundgren - Adapt Viral Shah bug fixes to moist mixing ratio
09 Jun 2015 - R. Yantosca - Now deposit Hg2, HgP to snowpack regardless of
                            whether the dynamic ocean is used
```

```
15 Jun 2015 - E. Lundgren - Now use kg/kg total air as tracer units not v/v
22 Jun 2015 - E. Lundgren - Move QB_NUM calculation to within timestep loop
12 Aug 2015 - R. Yantosca - Treat MERRA2 in same way as we do for GEOS-FP
14 Sep 2015 - E. Lundgren - Apply bug fixes provided by Viral Shah:
                            -- Prevent ALPHA > 1 in washout of aerosols
                            -- Add tracer GAINED to Q before WETLOSS
                               calculation in aerosol washout
22 Apr 2016 - R. Yantosca - Now get Is_Hg2 & Is_HgP from species database
25 Apr 2016 - R. Yantosca - Now pass Hg category # to ADD_Hg2_* functions
28 Apr 2016 - R. Yantosca - Rewrite Is_Hg block to avoid unassociated
                            pointer seg faults
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected
                            species ID from State_Chm%Map_Advect.
01 Jul 2016 - R. Yantosca - Now rename species DB object ThisSpc to SpcInfo
05 Jul 2016 - R. Yantosca - Now replace N_TRACERS argument with the
                            State_Chm%nAdvect field
06 Jul 2016 - E. Lundgren - Now use kg/kg dry air as spc units, requiring
                            use of DELP_DRY instead of DELP and PEDGE_DRY
                            for avg mixing ratio
07 Jul 2016 - R. Yantosca - Bug fix: F and ISOL need to be indexed with
                            the advected species index NA
07 Jul 2016 - R. Yantosca - DIAG14 and DIAG38 now are dimensioned with
                            of size State_Chm%nWetDep instead of N_TRACERS
20 Sep 2016 - R. Yantosca - Rewrote IF test to avoid Gfortran compiler error
```

4.2 Fortran: Module Interface wetscav_mod.F

Module WETSCAV_MOD contains routines and variables used in the wet scavenging of species in cloud updrafts, rainout, and washout.

INTERFACE:

MODULE WETSCAV_MOD

USES:

```
USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

IMPLICIT NONE

PRIVATE
```

PUBLIC DATA MEMBERS:

```
! Save H202 and S02 [v/v] for sulfate chemistry REAL(fp), PUBLIC, ALLOCATABLE, TARGET :: H202s(:,:,:) REAL(fp), PUBLIC, ALLOCATABLE, TARGET :: S02s(:,:,:)
```

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: CLEANUP_WETSCAV

PUBLIC :: COMPUTE_F
PUBLIC :: DO_WETDEP
PUBLIC :: INIT_WETSCAV
PUBLIC :: SETUP_WETSCAV

PUBLIC :: WASHOUT
PUBLIC :: LS_K_RAIN
PUBLIC :: LS_F_PRIME

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: COMPUTE_L2G
PRIVATE :: CONV_F_PRIME

PRIVATE :: E_ICE
PRIVATE :: RAINOUT

PRIVATE :: GET_RAINFRAC

PRIVATE :: SAFETY

PRIVATE :: WASHFRAC_FINE_AEROSOL
PRIVATE :: WASHFRAC_COARSE_AEROSOL

PRIVATE :: WASHFRAC_LIQ_GAS
PRIVATE :: WASHFRAC_HNO3

PRIVATE :: GET_VUD

REMARKS:

References:

- (1) Liu, H., D.J. Jacob, I. Bey and R.M. Yantosca, "Constraints from 210Pb and 7Be on wet deposition and transport in a global three-dimensional chemical tracer model driven by assimilated meteorological fields", JGR, Vol 106, pp 12109-12128, 2001.
- (2) D.J. Jacob, H. Liu, C. Mari, and R. M. Yantosca, "Harvard wet deposition scheme for GMI", Harvard Atmospheric Chemistry Modeling Group, March 2000.
- (3) Chin, M., D.J. Jacob, G.M. Gardner, M.S. Foreman-Fowler, and P.A. Spiro, "A global three-dimensional model of tropospheric sulfate", J. Geophys. Res., 101, 18667-18690, 1996.
- (4) Balkanski, Y D.J. Jacob, G.M. Gardner, W.C. Graustein, and K.K. Turekian, "Transport and Residence Times of Tropospheric Aerosols from a Global Three-Dimensional Simulation of 210Pb", JGR, Vol 98, (D11) pp 20573-20586, 1993.
- (5) Giorgi, F, & W.L. Chaimedes, "Rainout Lifetimes of Highly Soluble Aerosols and Gases as Inferred from Simulations With a General Circulation Model", JGR, Vol 86 (D13) pp 14367-14376, 1986.

- (1) Now trap allocation errors with routine ALLOC_ERR. (bmy, 7/11/00)
- (2) Moved routine MAKE_QQ here from "dao_mod.f" (bmy, 10/12/00)
- (3) Reordered arguments in INIT_PRECIP (bmy, 10/12/00)

- (4) Updated comments (bmy, 9/4/01)
- (5) Bug fix in MAKE_QQ: BXHEIGHT is sized IIPAR, JJPAR, LLPAR (bmy, 10/4/01)
- (6) Removed obsolete, commented-out code from 10/01 (bmy, 11/26/01)
- (7) Now divide module header into MODULE PRIVATE, MODULE VARIABLES, and MODULE ROUTINES sections. Updated comments (bmy, 5/28/02)
- (8) Now zero allocatable arrays (bmy, 8/5/02)
- (9) Bug fix: ND39 diagnostic now closes the budget. Also bundled several standalone routines into this module. Now references F90 module "tracerid_mod.f". Also set NSOLMAX=10 since we now have sulfate tracers for wetdep. Now prevent out-of-bounds errors in routine WETDEP. Added GET_WETDEP_NMAX function to return max # of soluble tracers for allocating diagnostic arrays. Added functions GET_WETDEP_NSOL and GET_WETDEP_IDWETD. Now init H2O2s and SO2s to the initial H2O2 and SO2 from STT. Updated comments. (qli, bmy, 1/14/03)
- (10) Improvements for SO2/SO4 scavenging (rjp, bmy, 3/23/03)
- (11) Now references "time_mod.f". Added driver routine DO_WETDEP to remove cumbersome calling sequence from MAIN program. Also declared WETDEP and MAKE_QQ PRIVATE to this module. (bmy, 3/27/03)
- (11) Add parallelization to routine WETDEP (bmy, 3/17/04)
- (12) Added carbon and dust aerosol tracers (rjp, tdf, bmy, 4/5/04)
- (13) Added seasalt aerosol tracers (rjp, bec, bmy, 4/20/04)
- (14) Added secondary organic aerosol tracers (rjp, bmy, 7/13/04)
- (15) Now references "logical_mod.f" and "tracer_mod.f". Now move all internal routines to the module and pass arguments explicitly in order to facilitate parallelization on the Altix. (bmy, 7/20/04)
- (16) Updated for mercury aerosol tracers (eck, bmy, 12/9/04)
- (17) Updated for AS, AHS, LET, NH4aq, SO4aq. Also now pass Hg2 wetdep loss to "ocean_mercury_mod.f". (cas, sas, bmy, 1/20/05)
- (18) Bug fix to avoid numerical blowup in WETDEP. Now use analytical function for E_ICE(T). (bmy, 3/7/05)
- (19) Added SO4s, NITs. Increased NSOLMAX to 31. Also block out parallel loop in WETDEP for SGI MIPS compiler. (bec, bmy, 5/5/05)
- (20) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (21) Bug fixes: do not over-deplete H2O2s. Also include updates for tagged Hg simulation. (dkh, rjp, eck, cdh, bmy, 1/6/06)
- (22) Now wet deposit SOG4, SOA4. Remove unnecessary variables in WETDEP. (dkh, bmy, 5/18/06)
- (23) Bug fixes in COMPUTE_F (bmy, 7/26/06)
- (24) Resize DSTT array in WETDEP to save memory. Added fixes for GEOS-5 wet deposition per Hongyu Liu's suggestions. (bmy, 3/5/08)
- (25) Add wet scavenging of GLYX, MGLY, GLYC, SOAG, SOAM (tmf, 1/7/09)
- (26) Effective Henry's law constant and coefficient from Sander, R, 1999, Compilation of Henry's Law Constants for Inorganic and Organic Species of Potential Importance in Environmental Chemistry.
 - http://www.mpch-mainz.mpg.de/~sander/res/henry.html (tmf, 1/7/09)

- (27) Remove support for SGI compiler. Bug fix in RAINOUT. (bmy, 7/20/09) (28) Update mercury simulation. (ccc, 5/17/10)
- (29) Add LGTMM as condition to output AD39. (ccc, 11/18/09)
- (30) Add snow scavenging, different washout/rainout ratio (wqq, ccc, 7/13/10)
- 13 Aug 2010 R. Yantosca Add modifications for MERRA (treat like GEOS-5)
- 16 Sep 2010 R. Yantosca Added ProteX headers
- 20 Sep 2010 H. Amos, R. Yantosca Implement new algorithms for MERRA
- 08 Oct 2010 H. Amos - WASHFRAC_LIQ_GAS is now a subroutine
- 08 Oct 2010 H. Amos - Various other modifications in WETDEP_MERRA
- 01 Aug 2011 H. Amos - Bug fix for function WASHFRAC_LIQ_GAS
- 01 Aug 2011 H. Amos - Updated comments
- 09 Feb 2012 R. Yantosca Add modifications for GEOS-5.7.x
- 21 Jun 2012 R. Yantosca Declare H2O2s, SO2s as TARGETs for pointers
- 23 Apr 2013 R. Yantosca Bug fix, eliminate white space from #if block
- 23 Apr 2013 R. Yantosca Remove LTOMAS logical, since we now invoke TOMAS with either TOMAS=yes or TOMAS40=yes
- 13 Aug 2013 M. Sulprizio- Add modifications for updated SOA and SOA + semivolatile POA simulations (H. Pye)
- 12 Sep 2013 M. Sulprizio- Add modifications for acid uptake on dust aerosols (T.D. Fairlie)
- 24 Nov 2014 M. Yannetti Added PRECISION_MOD
- 12 Feb 2015 C. Keller - Added GET_F and GET_VUD. VUD is now stored in State_Met. In an ESMF environment, it's values are directly taken from the GEOS-5 model. In the traditional GEOS-Chem, the updraft velocity is still calculated in the old manner (5 m/s over water, 10 m/s over land/ice).
- 23 Jun 2015 M. Sulprizio- Add impaction scavenging for hydrophobic BC and homogeneous IN removal from Qiaoqiao Wang
- 08 Jul 2015 E. Lundgren Add marine organic aerosols (B.Gantt, M.Johnson)
- 03 Sep 2015 R. Yantosca Remove NSOLMAX, we now get the # of wetdep species from State_Chm%nWetDep
- 03 Sep 2015 R. Yantosca INIT_WETSCAV now just allocates arrays; SETUP_WETSCAV now just sets up quantities
- 03 Sep 2015 R. Yantosca Remove WETDEPID routine, it's not needed
- 22 Sep 2015 R. Yantosca Re-introduce GET_WETDEP_NSOL routine
- 25 Sep 2015 R. Yantosca Use species database to collapse down routines COMPUTE_F, RAINOUT, WASHOUT
- 16 Jun 2016 L. Hu - Replaced IDTXXX with Ind_('XXX')
- 20 Jun 2016 R. Yantosca Now define species ID's only in the INIT phase
- 20 Jun 2016 R. Yantosca Renamed species ID's IDTxxxx to id_XXXX
- 06 Jul 2016 R. Yantosca Removed GET_WETDEP_NSOL and GET_WETDEP_IDWETD, these are now replaced by State_Chm fields

4.2.1 do_wetdep

Subroutine DO₋WETDEP is a driver for the wet deposition code, called from the MAIN program.

INTERFACE:

```
SUBROUTINE DO_WETDEP( am_I_Root, Input_Opt,
& State_Met, State_Chm, RC )
```

USES:

USE CMN_SIZE_MOD
USE ErrCode_Mod
USE ERROR_MOD

USE PhysConstants

USE State_Chm_Mod, ONLY : ChmState USE State_Met_Mod, ONLY : MetState

#if defined(USE_TEND)

USE TENDENCIES_MOD

#endif

USE TIME_MOD, ONLY : GET_TS_DYN

USE UnitConv_Mod

#if defined(NC_DIAG)

USE SPECIES_MOD

USE HCO_ERROR_MOD

USE HCO_INTERFACE_MOD, ONLY : HcoState
USE HCO_DIAGN_MOD, ONLY : Diagn_Update

#endif

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REMARKS:

```
NOTE FROM HONGYU LIU (hyl@nianet.org) -- 3/5/08
```

Rainout and washout from convective precipitation for previous GEOS archives were intended to represent precipitation from cloud anvils

[Liu et al., 2001]. For GEOS-5 (as archived at Harvard), the cloud anvil precipitation was already included in the large-scale precipitation.

Therefore, we insert a #if block to ensure that call MAKE_QQ and WETDEP are not called for convective precip in GEOS-5. (hyl, bmy, 3/5/08)

REVISION HISTORY:

4.2.2 make_qq

Subroutine MAKE_QQ computes the large-scale or convective precipitation fields for use with WETDEP

INTERFACE:

```
SUBROUTINE MAKE_QQ( State_Met, LS )
```

USES:

```
USE CMN_SIZE_MOD
```

USE ERROR_MOD, ONLY : ALLOC_ERR
USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: LS ! =T, denotes large scale precip ! =F, denotes convective precip TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

REMARKS:

```
%%%%%% FOR MERRA, MERRA2, and GEOS-FP MET FIELDS ONLY %%%%%
```


Construct QQ and PDOWN directly from GEOS-FP, MERRA, MERRA2 met fields.

This only applies to large-scale precip, as the #if defined block in routine DO_WETDEP prevents the wet deposition routines from being called if it is convective precip.

MERRA met fields:

```
DQRLSAN = 3-D precip production rate (LS+anvil) [kg/kg/s]
PFILSAN = Dwnwd flux of ice precip (LS+anvil) [kg/m2/s]
PFLLSAN = Dwnwd flux of liquid precip (LS+anvil) [kg/m2/s]
REEVAPLS = Evap of precip'ing LS+anvil condensate [kg/kg/s]
```

Unit conversion for QQ:

and $[m^3 H20/m3 air] = [cm^3 H20/cm3 air]$ because the same conversion factor from $m^3 -> cm^3$ is in both the numerator and the denominator.

Unit conversion for PDOWN:

= [(PFILSAN/1000) * 100] + [(PFILSAN/1000) * 100]

If there is total precipitation in the (I,J) column, then:

(1) Compute FRAC, the large scale fraction (if LS = .TRUE.) or convective fraction (if LS = .FALSE.) total precipitation. FRAC is computed from PREACC and PRECON. (2) Compute QQ, the rate of formation of precipitation [cm3 H2O/cm3 air/s]. From MOISTQ [kg H2O/kg air/s], defined as the tendency in specific humidity, the unit conversion is:

and

since the same conversion factor $(10^6 \text{ cm}^3/\text{m}^3)$ is in both the numerator and the denominator.

Therefore, the equation for QQ is:

$$QQ(L,I,J) = FRAC * MOISTQ(I,J,L) * MAIRDEN(I,J,L) / 1000.0$$

- (3) Compute PDOWN, the column precipitation [cm3 H2O/cm2 air/s], by multiplying QQ(L,I,J) by BXHEIGHT(I,J,L) * 100 cm.
- (4) The reason why we do not force PTEMP to be positive is that PREACC is the integral of the MOISTQ field. MOISTQ contains both negative (evap) and positive (precip) values. If we forced PTEMP to be positive, then we would be adding extra precipitation to PDOWN (hyl, bmy, 3/6/99).

- 29 Feb 2000 H. Liu, R. Yantosca Initial version
- (1) Now we partition MOISTQ into large-scale and convective parts, using total precipitation PREACC and convective precipitation PRECON (both are vertical integral amounts). The precipitation field at altitudes (PDOWN) is also made (hyl, djj, 10/17/98).
- (2) MAKE_QQ is written in Fixed-Form Fortran 90. (bmy, 4/2/99)!
- (3) AIRDEN, MOISTQ, QQ, and PDOWN are dimensioned (LLPAR, IIPAR, JJPAR) in order to maximize loop efficiency when processing an (I, J) column layer by layer. (bmy, 3/14/00)
- (4) MOISTQ is originally [g H2O/kg air/day], and is converted in READ_A6 to [kg H2O/kg air/s]. (bmy, 3/14/00)
- (5) Now reference PREACC, PRECON from "dao_mod.f" instead of from common block header file "CMN_PRECIP" (bmy, 6/26/00)
- (6) Now pass BXHEIGHT as an argument. Also added to "dao_mod.f". (bmy, 6/26/00)

```
(7) Moved from "dao_mod.f" to "wetscav_mod.f". Also made PREACC
      and PRECON into arguments. (bmy, 10/12/00)
(8) Updated comments (bmy, 9/4/01)
(9) BXHEIGHT is now sized (IIPAR, JJPAR, LLPAR) (bmy, 10/4/01)
(10) Removed obsolete, commented-out code from 10/01 (bmy, 11/26/01)
(11) Now reference met field arrays directly from "dao_mod.f" (bmy, 11/8/02)
16 Sep 2010 - R. Yantosca - Added ProTeX headers
16 Sep 2010 - R. Yantosca - Compute QQ and PDOWN from MERRA met fields
09 Feb 2012 - R. Yantosca - Added modifications for GEOS-5.7.x met fields
09 Nov 2012 - M. Payer
                          - Replaced all met field arrays with State_Met
                            derived type object
26 Sep 2013 - R. Yantosca - Renamed GEOS_57 Cpp switch to GEOS_FP
06 Nov 2014 - R. Yantosca - Now use State_Met%AIRDEN(I,J,L)
06 Nov 2014 - R. Yantosca - Now use State_Met%MOISTQ(I,J,L)
29 Apr 2015 - E. Lundgren - Now use State_Met%MAIRDEN instead of AIRDEN
                            since AIRDEN is now dry air density and MAIRDEN
                            is moist air density, needed for use with MOISTQ
```

12 Aug 2015 - R. Yantosca - Add support for MERRA2 meteorology

4.2.3 e_ice

Subroutine E_ICE computes Eice(T), the saturation vapor pressure of ice at a given Celsius temperature.

INTERFACE:

```
FUNCTION E_ICE( TK ) RESULT( VALUE )
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: TK    ! Temperature [K]
```

RETURN VALUE:

```
REAL(fp) :: VALUE ! Saturation vapor pressure [hPa]
```

REMARKS:

```
Marti & Mauersberber (GRL '93) formulation of saturation vapor pressure of ice [Pa] is: log P = A/TK + B
```

```
08 Feb 2005 - R. Yantosca - Initial version
(1 ) Now use the same analytic function as the Goddard CTM (bmy, 2/8/05)
16 Sep 2010 - R. Yantosca - Added ProTeX headers
```

4.2.4 compute_l2g

Subroutine COMPUTE_L2G computes the ratio L2G = Cliq / Cgas, which is the mixing ratio of species in the liquid phase, divided by the mixing ratio of species in the gas phase.

INTERFACE:

```
SUBROUTINE COMPUTE_L2G( KO, CR, pKa, TK, H2OLIQ, L2G )
```

USES:

```
USE Henry_Mod, ONLY : Calc_KH
USE Henry_Mod, ONLY : Calc_Heff
```

INPUT PARAMETERS:

```
REAL(f8), INTENT(IN) :: KO ! Henry's solubility constant [M/atm]
REAL(f8), INTENT(IN) :: CR ! Henry's volatility constant [K]
REAL(f8), INTENT(IN) :: pKa ! Henry's pH correction factor [1]
REAL(fp), INTENT(IN) :: TK ! Temperature [K]
REAL(fp), INTENT(IN) :: H2OLIQ ! Liquid water content [cm3 H2O/cm3 air]
```

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT) :: L2G  ! Cliq/Cgas ratio [1]
```

REMARKS:

```
The ratio Cliq / Cgas is obtained via Henry's law. The appropriate values of Kstar298 and H298_R must be supplied for each species. (cf Jacob et al 2000, p. 3)
```

REVISION HISTORY:

```
23 Feb 2000 - R. Yantosca - Initial version
(1 ) Bundled into "wetscav_mod.f" (bmy, 11/8/02)
16 Sep 2010 - R. Yantosca - Added ProTeX headers
10-Jan-2011 - H. Amos - Corrected the units on KStar298 from moles/atm to M/atm
15-May-2013 - F. Paulot - Fix R constant
08 Dec 2015 - R. Yantosca - Now use functions from henry_mod.F
```

4.2.5 compute_f

Subroutine COMPUTE_F computes F, the fraction of soluble species lost by scavenging in convective cloud updrafts.

INTERFACE:

```
SUBROUTINE COMPUTE_F( am_I_Root, N,
                                                  F,
                            Input_Opt, State_Met, State_Chm, RC
USES:
      USE CMN_Size_Mod
```

USE ErrCode_Mod USE Error_Mod USE Input_Opt_Mod, ONLY : OptInput USE Species_Mod, ONLY : Species USE State_Chm_Mod, ONLY : ChmState USE State_Met_Mod, UNLY : ChmState
USE State_Met_Mod, ONLY : MetState #if defined(TOMAS)

USE Tomas_Mod, ONLY : GetFraction

#endif

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? INTENT(IN) INTEGER, :: N ! Species ID TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object TYPE(MetState), INTENT(IN) :: State_Met ! Met State object

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State

OUTPUT PARAMETERS:

INTENT(OUT) :: ISOL ! Index for ND38 diag INTEGER, REAL(fp), INTENT(OUT) :: F(:,:,:) ! Soluble fraction of species INTEGER, :: RC ! Success or failure? INTENT(OUT)

- 23 Feb 2000 H. Liu, R. Yantosca Initial version
- (1) Currently works computes scavenging fractions for either full chemistry simulation (NSRCX == 3) or Rn-Pb-Be chemistry simulation (NSRCX == 1). Set the scavenging fraction to zero for other simulations which do not carry soluble tracers. (bmy, 3/2/00)
- (2) Need to call INIT_SCAV to initialize the Vud, C_H2O, CLDLIQ, and CLDICE fields once per timestep. (bmy, 2/23/00)
- (3) For aerosols only: now apply Eq. 2 for all temperatures. Also use the distance between the grid box centers in Eq. 2. Updated comments and made some cosmetic changes (hyl, bmy, 6/18/01)
- (4) Remove IREF, JREF -- these are obsolete. T is now dimensioned (IIPAR, JJPAR, LLPAR). T(IREF, JREF, L) is now T(I, J, L). (bmy, 9/27/01)
- (5) Removed obsolete code from 9/01 (bmy, 10/23/01)
- (6) Fix 2 bugs for aerosol scavenging in Rn-Pb-Be simulation: (a) set F(:,:,1) = 0 since we don't do any scavenging there. (b) DO L = 2, LLPAR to avoid any subscript range out of bounds errors (rjp, hyl, bmy, 1/10/02)

- (7) Now set F=0 in the first level for all tracers. Also now compute the distance between grid box centers and use that in in Eq. 10 from Jacob et al, 2000 to compute F. (hyl, bmy, 1/24/02)
- (8) Eliminated obsolete code from 1/02 (bmy, 2/27/02)
- (9) Now reference T from "dao_mod.f" instead of from "CMN". Also reference BXHEIGHT from "dao_mod.f" instead of from "CMN_NOX". Now bundled into "wetscav_mod.f". Now references IDTHNO3, IDTH202, etc, from F90 module "tracerid_mod.f". Added internal routines F_AEROSOL and GET_ISOL. Rewritten so that we don't duplicate code for different chemistry simulations. (bmy, 1/17/03)
- (10) Now compute F for SO2 in the same way for both fullchem and offline simulations (rjp, bmy, 3/23/03)
- (11) Added slots for carbon aerosol & dust tracers. Now modified internal routine GET_ISOL so it's not hardwired anymore. (rjp, bmy, 4/5/04)
- (12) Added slots for sea salt aerosol tracers (rjp, bec, bmy, 4/20/04)
- (13) Added slots for secondary organic aerosol tracers (rjp, bmy, 7/13/04)
- (14) Remove reference to CMN, it's not needed. Made internal routine F_AEROSOL a module procedure rather than an internal routine to COMPUTE_F in order to facilitate parallelization on the Altix. Also now pass all arguments explicitly to F_AEROSOL. (bmy, 7/20/04)
- (15) Now wet scavenge mercury aerosol tracers (eck, bmy, 12/9/04)
- (16) Updated for AS, AHS, LET, NH4aq, SO4aq. Also condensed the IF statement by combining branches for aerosols. (cas, bmy, 12/20/04)
- (17) Updated for SO4s, NITs (bec, bmy, 4/25/05)
- (18) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (19) Bug fix: Now do not over-deplete H2O2s. Also change Henry's law constant for Hg2 to 1.0d+14. Now use functions IS_Hg2 and IS_HgP to determine if a tracer is an Hg2 or HgP tagged tracer.

 (dkh, rjp, eck, cdh, bmy, 1/6/06)
- (20) Updated for SOG4 and SOA4 (dkh, bmy, 5/18/06)
- (21) Bug fix: now use separate conversion factors for H2O2 and NH3. (havala, bmy, 7/26/06)
- 16 Sep 2010 R. Yantosca Added ProTeX headers
- 10-Jan-2011 H.Amos Changed Hg2 Henry's law constant from 1.0d14 (no citation) to 1.4d6 M/atm (HgCl2, Lindqvist & Rhode, 1985). Henry's law constant in wetscav_mod.f is now consistent with what's used in mercury_mod.f
- 27 Sep 2011 H. Amos remove LHg_WETDasHNO3 logical, it's obsolete
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 06 Mar 2013 H. Amos merge C. Friedman's POP code
- 31 May 2013 R. Yantosca Now accept State_Chm, and pass it to TOMAS code
- 13 Aug 2013 M. Sulprizio- Add modifications for updated SOA and SOA + semivolatile POA simulations (H. Pye)
- 12 Sep 2013 M. Sulprizio- Add modifications for acid uptake on dust aerosols (T.D. Fairlie)
- 18 Apr 2014 R. Yantosca Now make the F argument an assumed-shape array

```
so that we can pass a pointer array slice to it
25 Jun 2014 - R. Yantosca - Now accept Input_Opt via the arg list
19 Dec 2014 - M. Sulprizio- Add bug fixes for CONV_H2O2 and CONV_NH3 from
                            Duncan Fairlie. The square root term should be
                            inverted to be consistent with Mari et al (2000).
04 Jun 2015 - E. Lundgren - Now accept am_I_Root and RC as arguments
23 Jun 2015 - M. Sulprizio- Add impaction scavenging for hydrophobic BC and
                            homogeneous IN removal from Qiaoqiao Wang
04 Sep 2015 - R. Yantosca - Use species database to radically simplify
                            the structure of this routine.
24 Sep 2015 - E. Lundgren - Convert kg/kg total air <-> kg for TOMAS
25 Sep 2015 - R. Yantosca - Move the computation of the Ki rate (Eq. 1 from
                            Jacob et al 2000) into routine COMPUTE_Ki
25 Sep 2015 - R. Yantosca - Remove T pointer, it's not needed here
30 Sep 2015 - R. Yantosca - Now use ThisSpc%WD_Is_HN03 and ThisSpc%WD_Is_S02
                            to flag the special cases of HNO3 & SO2 wetdep
05 Oct 2015 - R. Yantosca - Need to make ThisSpc !$OMP THREADPRIVATE
06 Oct 2015 - R. Yantosca - Add missing variables for TOMAS
16 Oct 2015 - E. Lundgren - Consolidate remaining embedded ifelse blocks
01 Jul 2016 - R. Yantosca - Now rename species DB object ThisSpc to SpcInfo
07 Jul 2016 - R. Yantosca - Now set ISOL = -1 if not a wetdep species
07 Jul 2016 - R. Yantosca - Remove pointer nullification from declarations
```

4.2.6 compute_ki

Subroutine COMPUTE_Ki computes the loss of species by scavenging according to Jacob et al 2000, eq. 1.

INTERFACE:

SUBROUTINE COMPUTE_Ki(SpcInfo, C_H2O, CLDICE, CLDLIQ, Kc, T, Ki)

USES:

USE Species_Mod, ONLY : Species

INPUT PARAMETERS:

```
TYPE(Species), INTENT(IN) :: SpcInfo ! Species database object
REAL(fp),
              INTENT(IN) :: C_H20
                                    ! Mixing ratio of H2O [v/v]
              INTENT(IN) :: CLDICE ! Cloud ice mixing ratio
REAL(fp),
                                     ! [cm3 ice/cm3 air]
REAL(fp),
              INTENT(IN) :: CLDLIQ
                                     ! Cloud liquid water mix ratio
                                     ! [cm3 H2O/cm3 air]
                                     ! Rate for conversion of cloud
REAL(fp),
              INTENT(IN) :: Kc
                                     ! condensate -> precip [1/s]
                                     ! Temperature [K]
REAL(fp),
              INTENT(IN) :: T
```

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT) :: Ki ! Loss of species from updraft ! (cf Eq. 1, Jacob et al, 2000)
```

REMARKS:

This routine centralizes computations that are used in routines ${\tt COMPUTE_F}$ and ${\tt RAINOUT}$.

REVISION HISTORY:

```
25 Sep 2015 - R. Yantosca - Initial version
08 Dec 2015 - R. Yantosca - Make KO, CR, pKa 8-byte variables for compatibility w/ CALC_KH, CALC_HEFF routines
01 Jul 2016 - R. Yantosca - Now rename species DB object ThisSpc to SpcInfo
```

4.2.7 f_aerosol

Subroutine F_AEROSOL returns the fraction of aerosol scavenged in updrafts

INTERFACE:

```
SUBROUTINE F_AEROSOL( KC, KcScale, State_Met, F)
```

USES:

```
USE CMN_SIZE_MOD
USE State_Met_Mod, ONLY: MetState
```

INPUT PARAMETERS:

REAL(fp),	INTENT(IN)	:: KC	! Cloud condensate to
			! precipitation rate
			! [1/s]
REAL(fp),	INTENT(IN)	:: KcScale(3)	! Scale factors for Kc
			! for 3 temperature
			! regimes
TYPE(MetState),	INTENT(IN)	:: State_Met	! Meteorology State

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT) :: F(IIPAR, JJPAR, LLPAR) ! Fraction of aerosol ! scavenged in ! convective updrafts
```

```
07 Nov 2002 - R. Yantosca - Initial version
16 Sep 2010 - R. Yantosca - Added ProTeX headers
09 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met derived type object
29 May 2013 - R. Yantosca - Segregate TOMAS-specific code with #ifdefs
```

```
10 Nov 2014 - C. Keller - Now also apply TINY check in ESMF environment.

23 Jun 2015 - M. Sulprizio- Add impaction scavenging for hydrophobic BC and homogeneous IN removal from Qiaoqiao Wang

25 Sep 2015 - R. Yantosca - Rewrite this routine to avoid testing on the tracer number. Remove the N argument.
```

4.2.8 rainout

Subroutine RAINOUT computes RAINFRAC, the fraction of soluble species lost to rainout events in precipitation.

INTERFACE:

```
SUBROUTINE RAINOUT( I, J, L, N, & K_RAIN, DT, F, RAINFRAC, & Input_Opt, State_Met, State_Chm
```

USES:

```
USE CMN_Size_Mod

USE Error_Mod, ONLY : Error_Stop

USE Input_Opt_Mod, ONLY : OptInput

USE Species_Mod, ONLY : Species

USE State_Chm_Mod, ONLY : ChmState

USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

```
INTEGER,
               INTENT(IN) :: I
                                         ! Longitude index
               INTENT(IN) :: J
                                         ! Latitude index
INTEGER,
                                         ! Level index
INTEGER.
               INTENT(IN) :: L
INTEGER,
               INTENT(IN) :: N
                                         ! Species number
REAL(fp),
                                         ! Rainout rate constant [1/s]
               INTENT(IN) :: K_RAIN
REAL(fp),
               INTENT(IN) :: DT
                                         ! Timestep for rainout event [s]
                                         ! Fraction of grid box that is
REAL(fp),
               INTENT(IN) :: F
                                         ! precipitating [unitless]
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input options
TYPE(MetState), INTENT(IN) :: State_Met
                                         ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT) :: RAINFRAC ! Fraction of species lost ! to rainout [unitless]
```

- 28 Feb 2000 R. Yantosca Initial version
- (1) Currently works for either full chemistry simulation (NSRCX == 3) or Rn-Pb-Be chemistry simulation (NSRCX == 1). Other simulations do not carry soluble tracer, so set RAINFRAC = 0. (bmy, 2/28/00)
- (2) Need to call INIT_SCAV to initialize the Vud, C_H2O, CLDLIQ, and CLDICE fields once per dynamic timestep. (bmy, 2/28/00)
- (3) K_RAIN, the rainout rate constant, and F, the areal fraction of the grid box undergoing precipitiation, are computed according to Giorgi & Chaimedes, as described in Jacob et al, 2000.
- (4) Now no longer suppress scavenging of HNO3 and aerosol below 258K. Updated comments, cosmetic changes. Now set TK = T(I,J,L) since T is now sized (IIPAR,JJPAR,LLPAR) in "CMN". (djj, hyl, bmy, 1/24/02)
- (5) Eliminated obsolete code (bmy, 2/27/02)
- (6) Now reference T from "dao_mod.f". Updated comments. Now bundled into "wetscav_mod.f". Now references "tracerid_mod.f". Also removed reference to CMN since we don't need NSRCX. (bmy, 11/8/02)
- (7) Now updated for carbon & dust aerosol tracers (rjp, bmy, 4/5/04)
- (8) Now updated for seasalt aerosol tracers (rjp, bec, bmy, 4/20/04)
- (9) Now updated for secondary aerosol tracers (rjp, bmy, 7/13/04)
- (10) Now treat rainout of mercury aerosol tracers (eck, bmy, 12/9/04)
- (11) Updated for AS, AHS, LET, NH4aq, SO4aq. Also condensed the IF statement by grouping blocks together. (cas, bmy, 12/20/04)
- (12) Updated for SO4s, NITs (bec, bmy, 4/25/05)
- (13) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (14) Change Henry's law constant for Hg2 to 1.0d+14. Now use functions IS_Hg2 and IS_HgP to determine if the tracer is a tagged Hg0 or HgP tracer. (eck, cdh, bmy, 1/6/06)
- (15) Updated for SOG4 and SOA4 (dkh, bmy, 5/18/06)
- (16) For GEOS-5, suppress rainout when T < 258K (hyl, bmy, 3/5/08)
- (17) Bug fix: need to use separate conversion parameters for H2O2 and NH3. This was the same fix as in COMPUTE_F but until now we had overlooked this. (havala, bmy, 7/20/09)
- 25 Aug 2010 R. Yantosca Treat MERRA in the same way as GEOS-5
- 16 Sep 2010 R. Yantosca Added ProTeX headers
- 27 Sep 2011 H. Amos remove LHg_WETDasHNO3 logical, it's obsolete
- 09 Feb 2012 R. Yantosca Treat GEOS-5.7.x in the same way as MERRA
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 13 Aug 2013 M. Sulprizio- Add modifications for updated SOA and SOA + semivolatile POA simulations (H. Pye)
- 12 Sep 2013 M. Sulprizio- Add modifications for acid uptake on dust aerosols (T.D. Fairlie)
- 26 Sep 2013 R. Yantosca Renamed GEOS_57 Cpp switch to GEOS_FP
- 25 Aug 2014 M. Sulprizio- Now accept Input_Opt as an argument
- 19 Dec 2014 M. Sulprizio- Add bug fixes for CONV_H2O2 and CONV_NH3 from Duncan Fairlie. The square root term should be inverted to be consistent with Mari et al (2000).
- 23 Jun 2015 M. Sulprizio- Add impaction scavenging for hydrophobic BC and

4.2.9 apply_rainout_eff

Subroutine APPLY_RAINOUT_EFF multiplies the rainout fraction computed by RAINOUT with the rainout efficiency for one of 3 temperature ranges: (1) T ; 237 K; (2) 237 K $_{\rm i}$ = T ; 258 K; (3) T $_{\rm i}$ 258 K. The rainout efficiencies for each aerosol species are defined in the species database object (i.e. State_Chm

This allows us to apply the impaction scavenging of certain aerosol species (BC, dust, HNO3) as implemented by Qiaoqiao Wang, while also suppressing rainout for other aerosol species. The prior code achieved this by using a large and confusing IF statement, whose logic was hard to understand.

INTERFACE:

```
SUBROUTINE APPLY_RAINOUT_EFF( TK, SpcInfo, RainFrac )
```

USES:

```
USE Species_Mod, ONLY : Species
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: TK ! Temperature [K]
TYPE(Species), INTENT(IN) :: SpcInfo ! Species Database object
```

INPUT/OUTPUT PARAMETERS:

```
REAL(fp), INTENT(INOUT) :: RainFrac ! Rainout fraction
```

```
06 Jan 2015 - R. Yantosca - Initial version
```

4.2.10 get_rainfrac

Function GET_RAINFRAC computes the fraction of species lost to rainout according to Jacob et al 2000.

INTERFACE:

```
FUNCTION GET_RAINFRAC( K, F, DT ) RESULT( RAINFRAC )
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: K ! Rainout rate constant [1/s]
REAL(fp), INTENT(IN) :: F ! Timestep for rainout event [s]
REAL(fp), INTENT(IN) :: DT ! Fraction of grid box that is
! undergoing precipitation [unitless]
```

RETURN VALUE:

```
REAL(fp) :: RAINFRAC ! Fraction of species lost to rainout
```

REVISION HISTORY:

```
08 Nov 2002 - R. Yantosca - Initial version
(1 ) Now move internal routines GET_RAINFRAC to the module and pass all
arguments explicitly. This facilitates parallelization on the
Altix platform (bmy, 7/20/04)
16 Sep 2010 - R. Yantosca - Added ProTeX headers
```

4.2.11 washout

Subroutine WASHOUT computes WASHFRAC, the fraction of soluble species lost to washout events in precipitation.

INTERFACE:

```
SUBROUTINE WASHOUT( am_I_Root, I, J, L, N, BXHEIGHT, TK, PP, & DT, F, H2O2s, SO2s, WASHFRAC, KIN, & Input_Opt, State_Met, State_Chm, RC)
```

USES:

```
USE CMN_SIZE_MOD
     USE ErrCode_Mod
     USE ERROR_MOD,
                              ONLY : ERROR_STOP
     USE Input_Opt_Mod,
                              ONLY : OptInput
     USE Species_Mod,
                              ONLY : Species
     USE State_Chm_Mod,
                              ONLY : ChmState
                              ONLY : MetState
     USE State_Met_Mod,
#if defined( TOMAS )
     USE ERROR_MOD
     USE TOMAS_MOD,
                             ONLY : IBINS,
                                               ICOMP
     USE UnitConv_Mod
#endif
```

INPUT PARAMETERS:

:: am_I_Root ! Are we on the root CPU? LOGICAL. INTENT(IN) INTEGER, INTENT(IN) :: I ! Longitude index :: J ! Latitude index INTEGER, INTENT(IN) INTEGER, INTENT(IN) :: L ! Level index INTENT(IN) ! Species number INTEGER, :: N REAL(fp), INTENT(IN) :: BXHEIGHT ! Grid box height [m] REAL(fp), ! Temperature [K] INTENT(IN) :: TK ! Precip rate thru bottom REAL(fp), :: PP INTENT(IN) ! of grid (I,J,L) ! [cm3 H2O/cm2 air/s] REAL(fp), :: DT ! Timestep [s] INTENT(IN) :: F REAL(fp), INTENT(IN) ! Fraction of grid box that ! is precipitating [1] TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options :: State_Met ! Meteorology State TYPE(MetState), INTENT(IN)

INPUT/OUTPUT PARAMETERS:

OUTPUT PARAMETERS:

REAL(fp), ! Fraction of species lost INTENT(OUT) :: WASHFRAC ! to washout [1] INTENT(OUT) :: KIN ! =T washout is a LOGICAL, kinetic process ! =F washout is an equilibrium process INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

28 Feb 2000 - R. Yantosca - Initial version

- (1) Currently works for either full chemistry simulation (NSRCX == 3) or Rn-Pb-Be chemistry simulation (NSRCX == 1). Other simulations do not carry soluble tracers, so set WASHFRAC = 0.
- (2) K_WASH, the rainout rate constant, and F, the areal fraction of the grid box undergoing precipitiation, are computed according to Giorgi & Chaimedes, as described in Jacob et al, 2000.
- (3) Washout is only done for $T \ge 268 \text{ K}$, when the cloud condensate is in the liquid phase.

- (4) T(I+I0,J+J0,L) is now T(I,J,L). Removed IREF, JREF -- these are obsolete. Updated comments. (bmy, 9/27/01)
- (5) Removed obsolete commented out code from 9/01 (bmy, 10/24/01)
- (6) Now reference BXHEIGHT, T from "dao_mod.f". Also remove reference to "CMN_NOX". Updated comments. Now bundled into "wetscav_mod.f". Now also references "tracerid_mod.f". Added internal routines WASHFRAC_AEROSOL and WASHFRAC_LIQ_GAS. Also removed reference to CMN since we don't need to use NSRCX here. (bmy, 11/6/02)
- (7) Updated for carbon aerosol and dust tracers (rjp, bmy, 4/5/04)
- (8) Updated for seasalt aerosol tracers (rjp, bec, bmy, 4/20/04)
- (9) Updated for secondary organic aerosol tracers (rjp, bmy, 7/13/04)
- (10) Now move internal routines WASHFRAC_AEROSOL and WASHFRAC_LIQ_GAS to the module and pass all arguments explicitly. This facilitates parallelization on the Altix platform (bmy, 7/20/04)
- (11) Now handle washout of mercury aerosol tracers (eck, bmy, 12/9/04)
- (13) Updated for AS, AHS, LET, NH4aq, SO4aq. Also condensed the IF statement by grouping blocks together (cas, bmy, 12/20/04)
- (14) Updated for SO4s, NITs (bec, bmy, 4/25/05)
- (15) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (16) Bug fix: Deplete H2O2s the same as SO2s. Also change Henry's law constant for Hg2 to 1.0d+14. Now use functions IS_Hg2 and IS_HgP to determine if a tracer is a tagged HgO or HgP tracer.

 (dkh, rjp, eck, cdh, bmy, 1/6/06)
- (17) Updated for SOG4 and SOA4 (bmy, 5/18/06)
- 16 Sep 2010 R. Yantosca Added ProTeX headers
- 30 Sep 2010 H. Amos WASHFRAC_LIQ_GAS now a subroutine (was an external function)
- 14 Oct 2010 H. Amos Remove dependence on I, J. That means removing I, J as input arguments and adding T, BXHEIGHT, H202s, and S04s and input arguments.
- 16 Aug 2011 H. Amos move K_WASH to WASHFRAC_AEROSOL, WASHFRAC_HNO3, and WASHFRAC_LIQ_GAS
- Replace logical AER with KIN. Serves the same purpose in the code, but emphasizes to the user that the difference in washout isn't whether or not the tracer is an aerosol, it's whether or not washout is modeled as a kinetic vs equilibrium process.
- 27 Sep 2011 H. Amos remove LHg2_WETDasHNO3 logical, it's obsolete
- 20 Jan 2012 H. Amos WASHFRAC for aerosol is now either computed by WASHFRAC_FINE_AEROSOL or WASHFRAC_COARSE_AEROSOL
- 31 May 2013 R. Yantosca Now accept State_Chm, and pass it to TOMAS code
- 13 Aug 2013 M. Sulprizio- Add modifications for updated SOA and SOA + semivolatile POA simulations (H. Pye)
- 12 Sep 2013 M. Sulprizio- Add modifications for acid uptake on dust aerosols (T.D. Fairlie)
- 27 Sep 2013 M. Sulprizio- DST2-DST4 are now considered coarse mode aerosol following the recommendation of T.D. Fairlie.

```
NITd, SO4d, and DALK are similarly updated.

25 Aug 2014 - M. Sulprizio- Now accept Input_Opt as an argument

12 May 2015 - E. Lundgren - Change tracer units from v/v -> kg for TOMAS if not already in kg (ie. called from convection)

04 Jun 2015 - E. Lundgren - Now accept am_I_Root and RC as arguments

23 Jun 2015 - E. Lundgren - Adjust 5/12/15 TOMAS bug fix to convert kg/kg total air <-> kg for new convection units

08 Jul 2015 - E. Lundgren - Add marine organic aerosols (B.Gantt, M.Johnson)

22 Sep 2015 - E. Lundgren - Add kg/m2 <-> kg conversion for TOMAS

30 Sep 2015 - R. Yantosca - Now use ThisSpc%WD_Is_HNO3 and ThisSpc%WD_Is_SO2 to flag the special cases of HNO3 & SO2 wetdep

16 Oct 2015 - E. Lundgren - Use ThisSpc%WD_Is_H2SO4 to treat H2SO4 as aerosol for wetdep, and consolidate ifelse blocks

27 Jul 2016 - E. Lundgren - Now expect dry mixing ratio not total
```

4.2.12 washfrac_fine_aerosol

Function WASHFRAC_FINE_AEROSOL returns the fraction of soluble aerosol species lost to washout.

INTERFACE:

```
FUNCTION WASHFRAC_FINE_AEROSOL( DT, F, PP, TK )
& RESULT( WASHFRAC )
```

USES:

INPUT PARAMETERS:

RETURN VALUE:

```
REAL(fp) :: WASHFRAC ! Fraction of soluble species ! lost to washout [1]
```

REVISION HISTORY:

```
08 Nov 2002 - R. Yantosca - Initial version
```

(1) WASHFRAC_AEROSOL used to be an internal function to subroutine WASHOUT. This caused NaN's in the parallel loop on Altix, so we moved it to the module and now pass Iall arguments explicitly (bmy, 7/20/04)

4.2.13 washfrac_coarse_aerosol

Function WASHFRAC_COARSE_AEROSOL returns the fraction of soluble aerosol species lost to washout.

INTERFACE:

```
FUNCTION WASHFRAC_COARSE_AEROSOL( DT, F, PP, TK ) & RESULT( WASHFRAC )
```

USES:

INPUT PARAMETERS:

RETURN VALUE:

```
REAL(fp) :: WASHFRAC ! Fraction of soluble species ! lost to washout
```

REVISION HISTORY:

```
08 Nov 2002 - R. Yantosca - Initial version
(1 ) WASHFRAC_AEROSOL used to be an internal function to subroutine WASHOUT.
    This caused NaN's in the parallel loop on Altix, so we moved it to
    the module and now pass Iall arguments explicitly (bmy, 7/20/04)
16 Sep 2010 - R. Yantosca - Added ProTeX headers
```

16 Aug 2011 - H Amos - Remove K_WASH from input list, make a defined parameter.

```
20 Jan 2012 - H Amos - WASHFRAC_COARSE_AEROSOL created to handle
SALC and DST4

04 Sep 2013 - R. Yantosca - Bug fix: Prevent div-by-zero if F=0. Because F
multiplies the whole expression for WASHFRAC,
WASHFRAC=0 whenever F=0 anyway.
```

4.2.14 washfrac_size_aerosol

Subroutine WASHFRAC_SIZE_AEROSOL retrieves fraction of soluble aerosol species lost to washout. Size resolved version for TOMAS.

INTERFACE:

```
SUBROUTINE WASHFRAC_SIZE_AEROSOL( DT, F, PP, TK, N, I, J, L, & State_Met, State_Chm, WASHFRAC, & RC )
```

USES:

```
USE ErrCode_Mod
USE ERROR_MOD
```

USE State_Chm_Mod, ONLY : ChmState USE State_Met_Mod, ONLY : MetState

USE TOMAS_MOD, ONLY : IBINS, GETDP, STRATSCAV

INPUT PARAMETERS:

REAL(fp),	INTENT(IN)	:: DT	! Dynamic timestep [s]
REAL(fp),	<pre>INTENT(IN)</pre>	:: F	! Fraction of grid box
			! that is precipitating
REAL(fp),	<pre>INTENT(IN)</pre>	:: PP	! Precip rate thru bottom
			! of grid box (I,J,L)
			! [cm3 H2O/cm2 air/s]
REAL(fp),	<pre>INTENT(IN)</pre>	:: TK	! Temperature [K]
INTEGER,	<pre>INTENT(IN)</pre>	:: I	! Longitude index
INTEGER,	<pre>INTENT(IN)</pre>	:: J	! Latitude index
INTEGER,	<pre>INTENT(IN)</pre>	:: L	! Level index
INTEGER,	<pre>INTENT(IN)</pre>	:: N	! Species index

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

OUTPUT PARAMETERS:

REAL(fp),	INTENT(OUT)	:: WASHFRAC	! Fraction of species
			! lost to washout [1]
INTEGER,	INTENT(OUT)	:: RC	! Success or failure?

REVISION HISTORY:

```
31 May 2013 - R. Yantosca - Now accept State_Met, State_Chm as arguments
04 Sep 2013 - R. Yantosca - Bug fix: Prevent div-by-zero if F=0. Because F
multiplies the whole expression for WASHFRAC,
WASHFRAC=0 whenever F=0 anyway.

24 Sep 2015 - E. Lundgren - Function is now a subroutine and outputs RC
```

4.2.15 washfrac_hno3

Function WASHFRAC_HNO3 returns the fraction of HNO3 species lost to washout.

INTERFACE:

```
FUNCTION WASHFRAC_HNO3( DT, F, PP, TK ) RESULT( WASHFRAC )
```

USES:

INPUT PARAMETERS:

RETURN VALUE:

```
REAL(fp) :: WASHFRAC ! Fraction of soluble species
```

```
13 Aug 2011, H Amos: Initial version, modeled after WASHFRAC_AEROSOL.

Seperate function created to emphasize that the new, updated washout coefficients from Feng et al (2007; 2009) should only be applied to aerosol species. It was a coincidence before that the original washout coefficients for aerosols and HNO3 were the same.

16 Aug 2011, H Amos: Remove K_WASH from input list, now a defined parameter 04 Sep 2013 - R. Yantosca - Bug fix: Prevent div-by-zero if F=0. Because F multiplies the whole expression for WASHFRAC, WASHFRAC=0 whenever F=0 anyway.
```

4.2.16 washfrac_liq_gas

!Subroutine WASHFRAC_LIQ_GAS returns the fraction of soluble liquid/gas phase species lost to washout.

INTERFACE:

```
SUBROUTINE WASHFRAC_LIQ_GAS( KO, CR, pKa, PP, DT, & F, DZ, TK, WASHFRAC, KIN )
```

INPUT PARAMETERS:

```
REAL(f8), INTENT(IN) :: KO
                                   ! Henry's solubility constant [M/atm]
REAL(f8), INTENT(IN) :: CR
                                   ! Henry's volatility constant [K]
                                   ! Henry's pH correction [1]
REAL(f8), INTENT(IN) :: pKa
REAL(fp), INTENT(IN) :: PP
                                   ! Precip rate thru bottom of the
                                   ! grid box [cm3 H2O/cm2 air/s]
REAL(fp), INTENT(IN) :: DT
                                   ! Timestep for washout event [s]
REAL(fp), INTENT(IN) :: F
                                   ! Fraction of grid box that is
                                   ! precipitating [unitless]
REAL(fp), INTENT(IN) :: DZ
                                   ! Height of grid box [cm]
                                   ! Temperature in grid box [K]
REAL(fp), INTENT(IN)
                     :: TK
```

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT) :: WASHFRAC ! Fraction of species lost to washout
LOGICAL, INTENT(OUT) :: KIN ! T = washout is a kinetic process
! F = washout is an equilibrium process
```

REVISION HISTORY:

```
20 Jul 2004 - R. Yantosca - Initial version
```

(1) WASHFRAC_LIQ_GAS used to be an internal function to subroutine WASHOUT. This caused NaN's in the parallel loop on Altix, so we moved it to the module and now pass all arguments explicitly (bmy, 7/20/04)

```
16 Sep 2010 - R. Yantosca - Added ProTeX headers
```

```
10 Jan 2011 - H. Amos - Remove AER from the argument list
```

03 Jun 2011 - H. Amos - convert from a function to a subroutine and add AER to the argument list

16 Aug 2011 - H. Amos - remove K_WASH from input list, now a defined parameter

16 Aug 2911 - H. Amos - rename AER logical KIN to emphasize that washout is either a kinetic or equilibrium process

4.2.17 wetdep

Subroutine WETDEP computes the downward mass flux of species due to washout and rainout of aerosols and soluble species in a column. The timestep is the dynamic timestep.

INTERFACE:

SUBROUTINE WETDEP(am_I_Root, Input_Opt, State_Met, State_Chm, & RC, LS)

USES:

USE CMN_DIAG_MOD USE CMN_SIZE_MOD

USE DEPO_MERCURY_MOD, ONLY : ADD_Hg2_WD USE DEPO_MERCURY_MOD, ONLY : ADD_HgP_WD

USE DEPO_MERCURY_MOD, ONLY : ADD_Hg2_SNOWPACK

USE ErrCode_Mod

USE ERROR_MOD

USE GET_NDEP_MOD, ONLY: SOIL_WETDEP
USE Input_Opt_Mod, ONLY: OptInput
USE Species_Mod, ONLY: Species
USE State_Chm_Mod, ONLY: ChmState
USE State_Met_Mod, ONLY: MetState
USE TIME_MOD, ONLY: GET_TS_DYN
USE UnitConv_Mod

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

LOGICAL, INTENT(IN) :: LS ! =T for large-scale precip

! =F for convective precip

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input options

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

Precipitation fields:

Layer	Formation of New Precip	Precipitation falling down	- Top of A+m
LM	QQ(L,I,J) 	PDOWN(LM,I,J)	= lop of Atm.
LM-1	QQ(L,I,J) V	PDOWN(LM-1,I,J) VV	-
	 I	 I	

	V	V	
3	QQ(L,I,J)	PDOWN(3,I,J)	
	I	I	
2	V QQ(L,I,J)	PDOWN(2,I,J)	
2	ψω(L,1,3)		
	· 	·	
1	QQ(L,I,J)	PDOWN(1,I,J)	
]	
==========	:=====\========	:======V======= (Ground

Where:

- (a) New formation forming in grid box (I,J,L) = QQ(L,I,J)
- (b) Precip coming in thru top of layer L = PDOWN(L+1,I,J)
- (c) Precip going out thru bottom of layer L = PDOWN(L, I,J)

Rainout:

=======

Rainout occurs when there is more precipitation in grid box (I,J,L) than in grid box (I,J,L+1). In other words, rainout occurs when the amount of rain falling through the bottom of grid box (I,J,L) is more than the amount of rain coming in through the top of grid box (I,J,L).

Soluble gases/aerosols are incorporated into the raindrops and are completely removed from grid box (I,J,LLPAR). There is no evaporation and "resuspension" of aerosols during a rainout event.

For large-scale (a.k.a. stratiform) precipitation, the first order rate constant for rainout in the grid box (I,J,L=LLPAR) (cf. Eq. 12, Jacob et al, 2000) is given by:

and the areal fraction of grid box (I,J,L=LLPAR) that is actually experiencing large-scale precipitation (cf. Eq. 11, Jacob et al, 2000) is given by:

Where:

L + W = condensed water content in cloud = 1.5e-6 [cm3 H2O/cm3 air]

Q = QQ = rate of precipitation formation [cm3 H2O / cm3 air / s]

For convective precipitation, $K_RAIN = 5.0e-3$ [s^-1], and the expression for F' (cf. Eq. 13, Jacob et al, 2000) becomes:

Where:

Q = QQ = rate of precipitation formation [cm3 H2O/cm3 air/s]

FMAX = maximum value for F'
= 0.3

DT = dynamic time step from the CTM [s]

TAU = duration of rainout event = 1800 s (30 min)

L + W = condensed water content in cloud = 2.0e-6 [cm3 H2O/cm3 air]

 K_RAIN and F' are needed to compute the fraction of species in grid box (I,J,L=LLPAR) lost to rainout. This is done in module routine RAINOUT.

Washout:

======

Washout occurs when we have evaporation (or no precipitation at all) at grid box (I,J,L), but have rain coming down from grid box (I,J,L+1).

- 02 Apr 1999 H. Liu, I. Bey, R. Yantosca Initial version
- (1) WETDEP should be called twice, once with LS = .TRUE. and once with LS = .FALSE. This will handle both large-scale and convective precipitation. (bmy, 2/28/00)
- (2) Call subroutine ${\tt MAKE_QQ}$ to construct the ${\tt QQ}$ and ${\tt PDOWN}$ precipitation

- fields before calling WETDEP. (bmy, 2/28/00)
- (3) Since we are working with an (I,J) column, the ordering of the loops goes J-I-L-N. Dimension arrays DSTT, PDOWN, QQ to take advantage of this optimal configuration (bmy, 2/28/00)
- (4) Use double-precision exponents to force REAL(fp) accuracy (e.g. 1e+0_fp, bmy, 2/28/00)
- (5) Diagnostics ND16, ND17, ND18, and ND39 use allocatable arrays from "diag_mod.f" (bmy, bey, 3/14/00)
- (6) WETDEP only processes soluble tracers and/or aerosols, as are defined in the NSOL and IDWETD arrays (bmy, 3/14/00)
- (7) Add kludge to prevent wet deposition in the stratosphere (bmy, 6/21/00)
- (8) Removed obsolete code from 10/27/00 (bmy, 12/21/00)
- (9) Remove IREF, JREF -- they are obsolete (bmy, 9/27/01)
- (10) Removed obsolete commented out code from 9/01 (bmy, 10/24/01)
- (11) Replaced all instances of IM with IIPAR and JM with JJPAR, in order to prevent namespace confusion for the new TPCORE (bmy, 6/25/02)
- (12) Now reference BXHEIGHT from "dao_mod.f". Also references routine GEOS_CHEM_STOP from "error_mod.f". Also fix ND39 diagnostic so that the budget of tracer lost to wetdep is closed. Now bundled into "wetscav_mod.f". Now only save to AD16, AD17, AD18, AD39 if L<=LD16, L<=LD17, L<=LD18, and L<=LD39 respectively; this avoids out-of-bounds array errors. Updated comments, cosmetic changes. (qli, bmy, 11/26/02)
- (13) References IDTS02, IDTS04 from "tracerid_mod.f". S02 in sulfate chemistry is wet-scavenged on the raindrop and converted to S04 by aqueous chem. If evaporation occurs then S02 comes back as S04. (rjp, bmy, 3/23/03)
- (14) Now use function GET_TS_DYN() from "time_mod.f" (bmy, 3/27/03)
- (15) Now parallelize over outermost J-loop. Also move internal routines LS_K_RAIN, LS_F_PRIME, CONV_F_PRIME, and SAFETY to the module, since we cannot call internal routines from w/in a parallel loop. (bmy, 3/18/04)
- (16) Now references STT & N_TRACERS from "tracer_mod.f". Also now make DSTT a 4-d internal array so as to facilitate -C checking on the SGI platform. (bmy, 7/20/04)
- (17) Now references IDTHg2 from "tracerid_mod.f". Now pass the amt of Hg2 wet scavenged out of the column to "ocean_mercury_mod.f" via routine ADD_Hg2_WD. (sas, bmy, 1/19/05)
- (18) Bug fix: replace line that can cause numerical blowup with a safer analytical expression. (bmy, 2/23/05)
- (19) Block out parallel loop with #ifdef statements for SGI_MIPS compiler. For some reason this causes an error. (bmy, 5/5/05)
- (20) Now use function IS_Hg2 to determine if a tracer is a tagged Hg2 tracer. Now also pass N to ADD_Hg2_WD. Now references LDYNOCEAN from "logical_mod.f". Now do not call ADD_Hg2_WD if we are not using the dynamic ocean model. (eck, sas, cdh, bmy, 2/27/06)
- (21) Eliminate unnecessary variables XDSTT, L_PLUS_W. Also zero all unused variables for each grid box. (bmy, 5/24/06)
- (22) Redimension DSTT with NSOL instead of NSOLMAX. In many cases, NSOL is

```
running at 2x25 or greater resolution. (bmy, 1/31/08)
(23) Remove reference to SGI_MIPS (bmy, 7/8/09)
16 Sep 2010 - R. Yantosca - Added ProTeX headers
27 May 2011 - R. Yantosca - Now pass F_RAINOUT to DO_WASHOUT_ONLY
25 Aug 2014 - M. Sulprizio- Now accept Input_Opt as an argument
02 Apr 2015 - E. Lundgren - Move tracer unit conversion from kg/kg to kg
                            to within this routine
04 Jun 2015 - E. Lundgren - Now accept am_I_Root and RC as arguments
09 Jun 2015 - R. Yantosca - Now deposit Hg2, HgP to snowpack regardless of
                            whether the dynamic ocean is used
22 Sep 2015 - E. Lundgren - Tracer units now converted to kg/m2 from kg/kg
22 Apr 2016 - R. Yantosca - Now get Is_Hg2, Is_HgP from species database
25 Apr 2016 - R. Yantosca - Now get the Hg category # from species database
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected
                            species ID from State_Chm%Map_Advect.
30 Jun 2016 - R. Yantosca - Replace STT with Spc and DSTT with DSpc
05 Jul 2016 - R. Yantosca - Now replace IDWETD with State_Chm%Map_Wetdep
05 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code
05 Aug 2016 - R. Yantosca - Remove reference to Spc, it's not needed
```

less than NSOLMAX and this will help to save memory especially when

4.2.18 wetdep_merra

USE CMN_SIZE_MOD

Subroutine WETDEP_MERRA computes the downward mass flux of species due to washout and rainout of aerosols and soluble species in a column. This subroutine implements a new algorithm in which the precipitation fields come directly from the MERRA archive.

INTERFACE:

```
SUBROUTINE WETDEP_MERRA( am_I_Root, Input_Opt, State_Met, & State_Chm, RC, LS)
```

USES:

```
USE CMN_DIAG_MOD
USE DEPO_MERCURY_MOD,
                        ONLY : ADD_Hg2_WD
USE DEPO_MERCURY_MOD,
                        ONLY : ADD_HgP_WD
USE DEPO_MERCURY_MOD,
                        ONLY : ADD_Hg2_SNOWPACK
USE ErrCode_Mod
USE ERROR_MOD
USE Input_Opt_Mod,
                        ONLY : OptInput
USE State_Chm_Mod,
                        ONLY : ChmState
USE State_Met_Mod,
                        ONLY : MetState
USE TIME_MOD,
                        ONLY : GET_TS_DYN
USE Species_Mod,
                        ONLY : Species
USE UnitConv_Mod
```

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

LOGICAL, INTENT(IN) :: LS ! =T for large-scale precip

! =F for convective precip

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input options

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

Precipitation fields:

Layer	Formation of New Precip	Top of Atm	
LM		 PDOWN(LM,I,J) 	TOP OI ACM.
LM-1	Ì	PDOWN(LM-1,I,J) V	- -
	 V	 V	_
3	QQ(L,I,J) 	PDOWN(3,I,J) 	
2	V	PDOWN(2,I,J) 	
1	Ì	PDOWN(1,I,J) V	== Ground

Where:

- (a) New formation forming in grid box (I,J,L) = QQ(L,I,J)
- (b) Precip coming in thru top of layer L = PDOWN(L+1,I,J)
- (c) Precip going out thru bottom of layer L = PDOWN(L, I,J)

Rainout:

======

Rainout occurs when there is more precipitation in grid box (I,J,L) than

in grid box (I,J,L+1). In other words, rainout occurs when the amount of rain falling through the bottom of grid box (I,J,L) is more than the amount of rain coming in through the top of grid box (I,J,L).

Soluble gases/aerosols are incorporated into the raindrops and are completely removed from grid box (I,J,LLPAR). There is no evaporation and "resuspension" of aerosols during a rainout event.

For large-scale (a.k.a. stratiform) precipitation, the first order rate constant for rainout in the grid box (I,J,L=LLPAR) (cf. Eq. 12, Jacob et al, 2000) is given by:

and the areal fraction of grid box (I,J,L=LLPAR) that is actually experiencing large-scale precipitation (cf. Eq. 11, Jacob et al, 2000) is given by:

Where:

L + W = condensed water content in cloud = 1.5e-6 [cm3 H2O/cm3 air]

$$Q = QQ = rate of precipitation formation [cm3 H2O / cm3 air / s]$$

For convective precipitation, $K_RAIN = 5.0e-3$ [s^-1], and the expression for F' (cf. Eq. 13, Jacob et al, 2000) becomes:

Where:

Q = QQ = rate of precipitation formation[cm3 H2O/cm3 air/s]

FMAX = maximum value for F'

= 0.3

DT = dynamic time step from the CTM [s]

TAU = duration of rainout event

= 1800 s (30 min)

L + W = condensed water content in cloud = 2.0e-6 [cm3 H20/cm3 air]

K_RAIN and F' are needed to compute the fraction of species in grid box (I,J,L=LLPAR) lost to rainout. This is done in module routine RAINOUT.

Washout:

=======

Washout occurs when we have evaporation (or no precipitation at all) at grid box (I,J,L), but have rain coming down from grid box (I,J,L+1).

- 20 Sep 2010 R. Yantosca Initial version, based on WETDEP
- 28 Sep 2010 H. Amos Now define Q, QDOWN directly from MERRA met
- 08 Oct 2010 R. Yantosca Adjusted OpenMP do loop
- 09-Dec-2010 H. Amos Added PDOWN(L+1) > 0 to criterion for IS_WASHOUT 09-Dec-2010 H. Amos SAFETY now prints PDOWN(L+1) instead of PDOWN(L) 31-Dec-2010 H. Amos Clean up code, remove obsolete code
- Added comments 31-Dec-2010 - H. Amos
- 27 May 2011 R. Yantosca Now pass F_RAINOUT to DO_WASHOUT_ONLY
- 25 Aug 2014 M. Sulprizio- Now accept Input_Opt as an argument
- 01 Apr 2015 L. Zhang - Don't do wetdep in nested-grid buffer zone
- 02 Apr 2015 E. Lundgren Move tracer unit conversion from kg/kg to kg to within this routine
- 04 Jun 2015 E. Lundgren Now accept am_I_Root and RC as arguments
- 09 Jun 2015 R. Yantosca Now deposit Hg2, HgP to snowpack regardless of whether the dynamic ocean is used
- Added option to scale convective fraction of 04 Mar 2016 - C. Keller large-scale precip.
- 22 Apr 2016 R. Yantosca Now get Is_Hg2, Is_HgP from species database
- 25 Apr 2016 R. Yantosca Now get the Hg category # from species database
- 29 Apr 2016 R. Yantosca Don't initialize pointers in declaration stmts
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.
- 30 Jun 2016 R. Yantosca Replace STT with Spc and DSTT with DSpc
- 01 Jul 2016 R. Yantosca Now rename species DB object ThisSpc to SpcInfo
- 05 Jul 2016 R. Yantosca Now replace IDWETD with State_Chm%Map_Wetdep

```
05 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code 05 Aug 2016 - R. Yantosca - Remove reference to Spc, it's not needed
```

4.2.19 ls_k_rain

Function LS_K_RAIN computes K_RAIN, the first order rainout rate constant for large-scale (a.k.a. stratiform) precipitation.

INTERFACE:

```
FUNCTION LS_K_RAIN( Q ) RESULT( K_RAIN )
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: Q     ! Rate of precipitation formation
! [cm3 H2O/cm3 air/s]
```

RETURN VALUE:

```
REAL(fp) :: K_RAIN ! 1st order rainout rate constant [1/s]
```

REVISION HISTORY:

```
18 Mar 2004 - R. Yantosca - Initial version
```

- (1) Now made into a MODULE routine since we cannot call internal routines from w/in a parallel loop. Updated comments. (bmy, 3/18/04)
- 16 Sep 2010 R. Yantosca Added ProTeX headers
- 23 Oct 2015 R. Yantosca Now use parameter COND_WATER_CONTENT

4.2.20 ls_f_prime

Function LS_F_PRIME computes F', the fraction of the grid box that is precipitating during large scale (a.k.a. stratiform) precipitation.

INTERFACE:

```
FUNCTION LS_F_PRIME( Q, K_RAIN ) RESULT( F_PRIME )
```

INPUT PARAMETERS:

```
\mbox{REAL(fp), INTENT(IN)} \ :: \ \mbox{Q} \qquad \qquad ! \ \mbox{Rate of precipitation formation}
```

! [cm3 H2O/cm3 air/s]

REAL(fp), INTENT(IN) :: K_RAIN ! 1st order rainout rate constant [1/s]

REMARKS:

```
REAL(fp) :: F_PRIME ! Fraction of grid box undergoing
```

! large-scale precipitation [unitless]

REVISION HISTORY:

```
18 Mar 2004 - R. Yantosca - Initial version
(1 ) Now made into a MODULE routine since we cannot call internal routines
     from w/in a parallel loop. Updated comments. (bmy, 3/18/04)
16 Sep 2010 - R. Yantosca - Added ProTeX headers
23 Oct 2015 - R. Yantosca - Now use COND_WATER_CONTENT parameter
```

4.2.21 conv_f_prime

Function CONV_F_PRIME computes F', the fraction of the grid box that is precipitating during convective precipitation.

INTERFACE:

```
FUNCTION CONV_F_PRIME( Q, K_RAIN, DT ) RESULT( F_PRIME )
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: Q ! Rate of precipitation formation ! [cm3 H2O/cm3 air/s]

REAL(fp), INTENT(IN) :: K_RAIN ! 1st order rainout rate constant [1/s] REAL(fp), INTENT(IN) :: DT ! Wet deposition timestep [s]

RETURN VALUE:

REAL(fp) :: F_PRIME ! Frac. of grid box undergoing
```

REVISION HISTORY:

```
18 Mar 2004 - R. Yantosca - Initial version
(1 ) Now made into a MODULE routine since we cannot call internal routines
     from w/in a parallel loop. Updated comments. (bmy, 3/18/04)
16 Sep 2010 - R. Yantosca - Added ProTeX headers
```

! convective precipitation [unitless]

4.2.22 do_rainout_only

Subroutine DO_RAINOUT_ONLY removes species by rainout.

INTERFACE:

```
SUBROUTINE DO_RAINOUT_ONLY( am_I_Root, LS, I, J, L, & IDX, ERRMSG, F_RAINOUT, & K_RAIN, DT, DSpc, & Input_Opt, State_Met, State_Chm, & RC
```

USES:

! Diagnostic flags USE CMN_DIAG_MOD USE CMN_SIZE_MOD ! Size parameters ! ND16 diag array USE DIAG_MOD, ONLY: AD16 USE DIAG_MOD, ! ND17 diag array ONLY: AD17 #if defined(BPCH_DIAG) USE DIAG_MOD, ONLY: AD39 ! ND39 diag array #endif USE DIAG_MOD, ONLY : CT16 ! ND16 diag counter USE DIAG_MOD, ONLY: CT17 ! ND17 diag counter USE ERROR_MOD, ONLY : IT_IS_NAN ! Test for NaN USE GET_NDEP_MOD, ONLY : SOIL_WETDEP ! Wet deposited species USE Input_Opt_Mod, ONLY : OptInput ! Input options type USE State_Chm_Mod, ONLY : ChmState ! Chemistry State type USE State_Met_Mod, ONLY : MetState ! Met State type #if defined(TOMAS) USE TOMAS_MOD, ONLY: IBINS, ICOMP, AQOXID USE TOMAS_MOD, ONLY: GETFRACTION ONLY : ADO5 USE DIAG_MOD, #endif

INPUT PARAMETERS:

LOGICAL, :: am_I_Root ! Are we on root CPU? INTENT(IN) ! =T denotes LS precip LOGICAL, INTENT(IN) :: LS ! Longitude index INTEGER, INTENT(IN) :: I INTENT(IN) :: J ! Latitude index INTEGER, ! Level index INTEGER, INTENT(IN) :: L INTENT(IN) :: IDX ! ND38 index INTEGER, REAL(fp), :: F_RAINOUT ! Fraction of grid box INTENT(IN) ! undergoing rainout ! Rainout constant REAL(fp), INTENT(IN) :: K_RAIN ! Rainout timestep [s] REAL(fp), INTENT(IN) :: DT CHARACTER(LEN=*), INTENT(IN) :: ERRMSG ! Error message ! Input options TYPE(OptInput), INTENT(IN) :: Input_Opt TYPE(MetState), INTENT(IN) :: State_Met ! Met State object

INPUT/OUTPUT PARAMETERS:

REAL(fp), INTENT(INOUT) :: DSpc(:,:,:,:) ! Accumulator array [kg] TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

The modifications for the MERRA met fields require calling this same

sequence of code more than once. The expedient solution was to just move the relevant code into this subroutine.

An IF statement in WETDEP decides if this rainout is to be done (and thus if this routine will be called. The criteria for rainout is:

FOR MERRA MET FIELDS:

There is rainout if there is new precip formation in the grid box (i.e. DQRLSAN(I,J,L) > 0) and the fraction of the grid box experiencing rainout (i.e. $F_RAINOUT$) is greater than or equal to the fraction of the grid box directly overhead experiencing precip (i.e. FTOP).

-- Helen Amos (9/10/10)

FOR ALL OTHER MET FIELDS:

We use a simple test: if the rainout fraction in this grid box (i.e. $F_RAINOUT$) is nonzero, do rainout. Don't compare to the grid box immediately above us (i.e. FTOP).

REVISION HISTORY:

```
16 Sep 2010 - R. Yantosca - Initial version
25 Aug 2014 - M. Sulprizio- Now accept Input_Opt as an argument
22 Sep 2015 - E. Lundgren - Input STT is now in kg/m2 (prev kg)
24 Sep 2015 - E. Lundgren - Now pass am_I_Root and RC as arguments
29 Sep 2015 - E. Lundgren - Now pass State_Chm as argument and use
local pointer for STT array [kg/m2]
30 Jun 2016 - R. Yantosca - Replace STT with Spc and DSTT with DSpc
05 Jul 2016 - R. Yantosca - Now replace IDWETD with State_Chm%Map_WetDep
```

4.2.23 do_washout_only

Subroutine DO_WASHOUT_ONLY removes species by washout.

The modifications for the MERRA met fields require calling this same sequence of code more than once. The expedient solution was to just move the relevant code into this this subroutine.

INTERFACE:

SUBROUTINE	DO_WASHOUT_ONLY(am_I_Root,	LS,	I, J, L,	
&		IDX,	ERRMSG,	QDOWN,	
&		Q,	$F_{WASHOUT}$,	F_RAINOUT,	
&		DT,	PDOWN,	DSpc,	
&		<pre>Input_Opt,</pre>	State_Met,	State_Chm,	
&		RC,	REEVAP)	

USES:

```
USE CMN_DIAG_MOD
                                                      ! Diagnostic flags
     USE CMN_SIZE_MOD
                                                      ! Size parameters
                                                      ! ND16 diag array
     USE DIAG_MOD,
                             ONLY : AD16
     USE DIAG_MOD,
     USE DIAG_MOD,
                            ONLY: AD17
                                                     ! ND17 diag array
                                                      ! ND18 diag array
                             ONLY : AD18
#if defined( BPCH_DIAG )
     USE DIAG_MOD,
                             ONLY: AD39
                                                      ! ND39 diag array
#endif
     USE DIAG_MOD,
                             ONLY: CT16
                                                     ! ND16 diag counter
     USE DIAG_MOD,
                             ONLY : CT17
                                                     ! ND17 diag counter
     USE DIAG_MOD,
                             ONLY : CT18
                                                     ! ND18 diag counter
     USE ErrCode_Mod
     USE ERROR_MOD
     USE GET_NDEP_MOD,
                             ONLY : SOIL_WETDEP
                                                      ! Wet deposited species
                        ONLY : OptInput
ONLY : ChmState
                                                      ! Input options
     USE Input_Opt_Mod,
     USE State_Chm_Mod,
                                                     ! Chemistry State object
     USE State_Met_Mod,
                                                     ! Met State object
                             ONLY : MetState
#if defined( TOMAS )
                         ONLY : IBINS, ICOMP, AQOXID
     USE TOMAS_MOD,
     USE DIAG_MOD,
                           ONLY : ADO5
#endif
```

INPUT PARAMETERS:

LOGICAL,	INTENT(IN)	::	am_I_Root	!	Are we on the root CPU?
LOGICAL, OPTIONAL,	INTENT(IN)	::	REEVAP	!	Do re-evaporation?
LOGICAL,	INTENT(IN)	::	LS	!	=T denotes LS precip
INTEGER,	INTENT(IN)	::	I	!	Longitude index
INTEGER,	INTENT(IN)	::	J	!	Latitude index
INTEGER,	INTENT(IN)	::	L	!	Level index
INTEGER,	INTENT(IN)	::	IDX	!	ND38 index
CHARACTER(LEN=*),	INTENT(IN)	::	ERRMSG	!	Error message
REAL(fp),	INTENT(IN)	::	QDOWN	!	Precip leaving thru
				!	bottom of box (I,J,L)
REAL(fp),	INTENT(IN)	::	Q	!	Precip forming or
				!	evaporating
				!	in box (I,J,L)
REAL(fp),	INTENT(IN)	::	F_WASHOUT	!	Fraction of grid box
				!	undergoing washout
REAL(fp),	INTENT(IN)	::	F_RAINOUT	!	Fraction of grid box
				!	undergoing rainout
REAL(fp),	INTENT(IN)	::	DT	!	Rainout timestep [s]
REAL(fp),	INTENT(IN)	::	PDOWN(:,:,:)	!	Precip
TYPE(OptInput),	INTENT(IN)	::	Input_Opt	!	Input options
<pre>TYPE(MetState),</pre>	INTENT(IN)	::	State_Met	!	Met State object

INPUT/OUTPUT PARAMETERS:

REAL(fp), INTENT(INOUT) :: DSpc(:,:,:,:) ! Accumulator array

! [kg/m2]

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

A fraction ALPHA of the raindrops falling down from grid box (I,J,L+1) to grid box (I,J,L) will evaporate along the way. ALPHA is given by:

We assume that a fraction ALPHA2 = 0.5 * ALPHA of the previously rained-out aerosols and HNO3 coming down from level (I,J,L+1) will evaporate and re-enter the atmosphere in the gas phase in grid box (I,J,L). This process is called "resuspension".

For non-aerosol species, the amount of previously rained out mass coming down from grid box (I,J,L+1) to grid box (I,J,L) is figured into the total mass available for washout in grid box (I,J,L). We therefore do not have to use the fraction ALPHA2 to compute the resuspension.

NOTE from Hongyu Liu about ALPHA (hyl, 2/29/00)

If our QQ field was perfect, the evaporated amount in grid box (I,J,L) would be at most the total rain amount coming from above (i.e. PDOWN(I,J,L+1)). But this is not true for the MOISTQ field we are using. Sometimes the evaporation in grid box (I,J,L) can be more than the rain amount from above. The reason is our "evaporation" also includes the effect of cloud detrainment. For now we cannot find a way to distinguish between the two. We then decided to release aerosols in both the detrained air and the evaporated air.

Therefore, we should use this term in the numerator:

```
-QQ(I,J,L) * BXHEIGHT(I,J,L)
```

instead of the term:

PDOWN(L+1)-PDOWN(L)

Recall that in make_qq.f we have restricted PDOWN to positive values, otherwise, QQ would be equal to PDOWN(L+1)-PDOWN(L).

Update (V. Shah 6/29/16)

For GEOS-FP, MERRA and MERRA2 met fields we use the following term in the numerator instead:

REEVAP(L,I,J) * BXHEIGHT(I,J,L)

```
16 Sep 2010 - R. Yantosca - Initial version
20 Sep 2010 - R. Yantosca - Update definition of ALPHA if we are doing
                            partial re-evaporation.
28 Sep 2010 - H. Amos
                          - Now check for NaN's with function IT_IS_NAN
31 Dec 2010 - H. Amos
                          - new variable, TK, for temperature
26 May 2011 - R. Yantosca - Bug fix: Only apply the error trap for the
                            condition WASHFRAC < 1d-3 for MERRA met
25 May 2011 - Q. Wang
                          - new variable, TF, for total precip fraction
25 May 2011 - Q. Wang
                          - Also pass F_RAINOUT via the arg list
25 May 2011 - Q. Wang
                          - Correct the washfrac to make sure that washout
                            is applied the area of F_washout instead of
                            total area of (F_washout+F_rainout)
27 May 2011 - R. Yantosca - Added comments, readjusted IF statements to
                            avoid floating-point problems
                          - Replace logical AER with KIN to emphasize that
16 Aug 2011 - H. Amos
                            washout is either modeled as a kinetic process
                            or an equilibrium process
                          - Replaced all met field arrays with State_Met
09 Nov 2012 - M. Payer
                            derived type object
26 Sep 2013 - R. Yantosca - Renamed GEOS_57 Cpp switch to GEOS_FP
25 Aug 2014 - M. Sulprizio- Now accept Input_Opt as an argument
04 Feb 2015 - M. Sulprizio- Fix calculation of WETLOSS for non-aerosol
                            tracers (C. Friedman)
20 May 2015 - M. Sulprizio- Remove WASHFRAC < 1D-3 error trap for MERRA
                            following recommendation by Viral Shah
04 Jun 2015 - E. Lundgren - Now accept am_I_Root and RC as arguments
22 Sep 2015 - E. Lundgren - Incoming tracer units are now [kg/m2]
29 Sep 2015 - E. Lundgren - Now use local pointer for STT array [kg/m2]
30 Jun 2016 - R. Yantosca - Replace STT with Spc and DSTT with DSpc
05 Jul 2016 - R. Yantosca - Replace IDWETD with State_Chm%Map_WetDep
```

4.2.24 do_complete_reevap

Subroutine DO_COMPLETE_REEVAP re-evaporates all of the soluble species back into the atmosphere.

INTERFACE:

```
SUBROUTINE DO_COMPLETE_REEVAP( am_I_Root, LS, I, J, L, & IDX, ERRMSG, DT, & DSpc, Input_Opt, State_Met, & State_Chm, RC )
```

USES:

```
USE CMN_DIAG_MOD
                                                       ! Diagnostic flags
     USE CMN_SIZE_MOD
                                                       ! Size parameters
     USE DIAG_MOD,
                                                       ! ND16 diag array
                              ONLY: AD16
     USE DIAG_MOD,
                                                       ! ND17 diag array
                              ONLY: AD17
     USE DIAG_MOD,
                                                       ! ND18 diag array
                              ONLY: AD18
#if defined( BPCH_DIAG )
     USE DIAG_MOD,
                              ONLY: AD39
                                                       ! ND39 diag array
#endif
     USE DIAG_MOD,
                              ONLY : CT16
                                                       ! ND16 diag counter
     USE DIAG_MOD,
                              ONLY : CT17
                                                       ! ND17 diag counter
     USE DIAG_MOD,
                                                       ! ND18 diag counter
                              ONLY: CT18
     USE ERROR_MOD
     USE GET_NDEP_MOD,
                              ONLY : SOIL_WETDEP
                                                       ! Wet deposited species
     USE Input_Opt_Mod,
                              ONLY : OptInput
     USE State_Chm_Mod,
                              ONLY : ChmState
     USE State_Met_Mod,
                              ONLY : MetState
#if defined( TOMAS )
     USE TOMAS_MOD,
                             ONLY: IBINS, ICOMP, AQOXID
                              ONLY: ADO5
     USE DIAG_MOD,
#endif
```

INPUT PARAMETERS:

```
LOGICAL,
                 INTENT(IN)
                               :: am_I_Root
                                                ! Are we on the root CPU?
LOGICAL,
                                                ! =T denotes LS precip
                 INTENT(IN)
                               :: LS
                                                ! Longitude index
INTEGER,
                 INTENT(IN)
                               :: I
                               :: J
                                                ! Latitude index
INTEGER,
                 INTENT(IN)
                 INTENT(IN) :: L
                                                ! Level index
INTEGER,
INTEGER,
                 INTENT(IN)
                               :: IDX
                                               ! ND38 index
CHARACTER(LEN=*), INTENT(IN)
                               :: ERRMSG
                                               ! Error message
                               :: DT
                                                ! Rainout timestep [s]
REAL(fp),
                 INTENT(IN)
                                                ! Input options
TYPE(OptInput),
                 INTENT(IN)
                               :: Input_Opt
TYPE(MetState),
                               :: State_Met
                                                ! Meteorology State obj
                 INTENT(IN)
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object REAL(fp), INTENT(INOUT) :: DSpc(:,:,:,:) ! Accumulator array ! [kg/m2]
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

The modifications for the MERRA met fields require calling this same sequence of code more than once. The expedient solution was to just move the relevant code into this this subroutine.

REVISION HISTORY:

```
16 Sep 2010 - R. Yantosca - Initial version

22 Sep 2015 - E. Lundgren - Incoming tracer units are now kg/m2 (prev kg)

24 Sep 2015 - E. Lundgren - Now pass am_I_Root and RC as arguments and local pointer for STT array [kg/m2]

30 Sep 2015 - E. Lundgren - Now pass Input_Opt for use in TOMAS AQOXID

30 Jun 2016 - R. Yantosca - Replace STT with Spc and DSTT with DSpc

05 Jul 2016 - R. Yantosca - Replace IDWETD with State_Chm%Map_WetDep
```

4.2.25 do_washout_at_sfc

USE DIAG_MOD,

Subroutine DO_WASHOUT_AT_SFC washes out the species at the surface.

INTERFACE:

```
SUBROUTINE DO_WASHOUT_AT_SFC( am_I_Root, LS,
                                                           I, J, L,
                                     IDX,
                                                ERRMSG,
                                                           QDOWN,
      &
                                                DT,
                                                           DSpc,
                                     Input_Opt, State_Met, State_Chm,
      &
      &
USES:
       USE CMN_DIAG_MOD
                                                        ! Diagnostic flags
       USE CMN_SIZE_MOD
                                                        ! Size parameters
      USE DIAG_MOD,
                               ONLY : AD16
                                                        ! ND16 diag array
      USE DIAG_MOD,
                               ONLY : AD17
                                                        ! ND17 diag array
      USE DIAG_MOD,
                               ONLY : AD18
                                                        ! ND18 diag array
 #if defined( BPCH_DIAG )
      USE DIAG_MOD,
                               ONLY : AD39
                                                        ! ND39 diag array
 #endif
                                                        ! ND16 diag counter
      USE DIAG_MOD,
                               ONLY : CT16
                                                        ! ND17 diag counter
      USE DIAG_MOD,
                              ONLY : CT17
```

ONLY : CT18

! ND18 diag counter

```
USE ErrCode_Mod
USE ERROR_MOD,
                       ONLY : IT_IS_NAN
                                                ! Test for NaN
USE GET_NDEP_MOD,
                       ONLY : SOIL_WETDEP
                                                ! Wet deposited species
USE Input_Opt_Mod,
                      ONLY : OptInput
                                                ! Input options
                       ONLY : ChmState
                                                ! Chm State object
USE State_Chm_Mod,
USE State_Met_Mod,
                       ONLY : MetState
                                                ! Met State object
```

INPUT PARAMETERS:

LOGICAL,	INTENT(IN)	::	am_I_Root	!	Are we on the root CPU?
LOGICAL,	INTENT(IN)	::	LS	!	=T denotes LS precip
INTEGER,	INTENT(IN)	::	I	!	Longitude index
INTEGER,	INTENT(IN)	::	J	!	Latitude index
INTEGER,	INTENT(IN)	::	L	!	Level index
INTEGER,	INTENT(IN)	::	IDX	!	ND38 index
CHARACTER(LEN=*),	INTENT(IN)	::	ERRMSG	!	Error message
REAL(fp),	INTENT(IN)	::	QDOWN	!	Precip leaving thru
				!	bottom of box (I,J,L)
REAL(fp),	INTENT(IN)	::	F	!	Fraction of grid box
				!	undergoing precip
REAL(fp),	INTENT(IN)	::	DT	!	Rainout timestep [s]
TYPE(OptInput),	INTENT(IN)	::	Input_Opt	!	Input options
TYPE(MetState),	INTENT(IN)	::	State_Met	!	Met State object

INPUT/OUTPUT PARAMETERS:

```
REAL(fp), INTENT(INOUT) :: DSpc(:,:,:,:) ! Accumulator array
```

! [kg/m2]

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

Assume all of the species precipitating down from grid box (I,J,L=2) to grid box (I,J,L=1) gets washed out in grid box (I,J,L=1).

The modifications for the MERRA met fields require calling this same sequence of code more than once. The expedient solution was to just move the relevant code into this this subroutine.

```
16 Sep 2010 - R. Yantosca - Initial version

09 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met derived type object

25 Aug 2014 - M. Sulprizio- Now accept Input_Opt as an argument

04 Jun 2015 - E. Lundgren - Now accept am_I_Root and RC as arguments

22 Sep 2015 - E. Lundgren - Tracer units are now kg/m2 (prev kg)
```

```
29 Sep 2015 - E. Lundgren - Now use local pointer for STT array [kg/m2] 30 Jun 2016 - R. Yantosca - Replace STT with Spc and DSTT with DSpc 05 Jul 2016 - R. Yantosca - Now replace IDWETD with State_Chm%Map_Wetdep
```

4.2.26 safety

Subroutine SAFETY stops the run with debug output and an error message if negative species are found.

INTERFACE:

	SUBROUTINE	SAFETY(I,	J,	L,	N,
ě	k		Α,	LS,	PDOWN,	QQ,
ě	k		ALPHA,	ALPHA2,	RAINFRAC,	WASHFRAC,
ě	દ		MASS_WASH,	MASS_NOWASH,	WETLOSS,	GAINED,
ě	&		LOST,	DSpc,	Spc)	

USES:

```
USE CMN_SIZE_MOD
USE ERROR_MOD, ONLY : GEOS_CHEM_STOP
```

INPUT PARAMETERS:

```
! Arguments
LOGICAL,
                  INTENT(IN) :: LS
                  INTENT(IN) :: I
INTEGER,
INTEGER,
                  INTENT(IN) :: J
INTEGER,
                  INTENT(IN) :: L
                  INTENT(IN) :: N
INTEGER,
CHARACTER(LEN=*), INTENT(IN) :: A
REAL(fp),
                  INTENT(IN) :: PDOWN
REAL(fp),
                  INTENT(IN) :: QQ
REAL(fp),
                  INTENT(IN) :: ALPHA
                  INTENT(IN) :: ALPHA2
REAL(fp),
REAL(fp),
                  INTENT(IN) :: RAINFRAC
                  INTENT(IN) :: WASHFRAC
REAL(fp),
REAL(fp),
                  INTENT(IN) :: MASS_WASH
REAL(fp),
                  INTENT(IN) :: MASS_NOWASH
REAL(fp),
                  INTENT(IN) :: WETLOSS
REAL(fp),
                  INTENT(IN) :: GAINED
REAL(fp),
                  INTENT(IN) :: LOST
REAL(fp),
                  INTENT(IN) :: DSpc(LLPAR)
REAL(fp),
                  INTENT(IN) :: Spc(LLPAR)
```

```
18 Mar 2004 - R. Yantosca - Initial version
```

(1) Now made into a MODULE routine since we cannot call internal routines from w/in a parallel loop. Updated comments. (bmy, 3/18/04)

16 Sep 2010 - R. Yantosca - Added ProTeX headers

4.2.27 get_vud

Function GET_VUD returns the vertical updraft velocity in m/s at location I, J, L.

INTERFACE:

```
FUNCTION GET_VUD( State_Met, I, J, L ) RESULT( VUD )
```

USES:

USE DAO_MOD, ONLY : IS_WATER
USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

```
TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INTEGER, INTENT(IN) :: I, J, L ! Location

RETURN VALUE:

REAL(fp) :: VUD ! Vertical updraft velocity in m/s.

REVISION HISTORY:

```
12 Feb 2015 - C. Keller - Initial version
```

26 Feb 2015 - E. Lundgren - Remove dependency on pressure_mod since not used.

27 Jun 2016 - C. Keller - Use VUD_DEFINED instead of ESMF_ compiler switch.

4.2.28 get_f

Function GET_F returns the scavenged fraction at location I, J, L and for the given rate constant K.

INTERFACE:

```
FUNCTION GET_F( State_Met, I, J, L, K ) RESULT( F )
```

USES:

USE DAO_MOD, ONLY : IS_WATER USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

RETURN VALUE:

```
REAL(fp) :: F ! Fraction of species scavenged ! out of the updraft [1]
```

REVISION HISTORY:

```
12 Feb 2015 - C. Keller - Initial version
26 Feb 2015 - E. Lundgren - Remove dependency on pressure_mod since not used.
25 Jun 2015 - M. Sulprizio- Now pass FF as an optional argument for aerosols
25 Sep 2015 - R. Yantosca - Remove FF; we scale Kc in F_AEROSOL now.
```

4.2.29 init_wetscay

Subroutine INIT_WETSCAV initializes updraft velocity, cloud liquid water content, cloud ice content, and mixing ratio of water fields, which are used in the wet scavenging routines.

INTERFACE:

```
SUBROUTINE INIT_WETSCAV( am_I_Root, Input_Opt, State_Chm, RC )
```

USES:

```
USE ErrCode_Mod

USE Error_Mod

USE Input_Opt_Mod, ONLY : OptInput

USE Species_Mod, ONLY : Species

USE State_Chm_Mod, ONLY : ChmState

USE State_Chm_Mod, ONLY : Ind_
```

INPUT PARAMETERS:

USE CMN_Size_Mod

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

```
03 Sep 2015 - R. Yantosca - Split off from the old INIT_WETSCAV. We now just allocate arrays here. Arrays are assigned values from State_Met in SETUP_WETSCAV.
```

```
03 Sep 2015 - R. Yantosca - Also initialize IDWETD here; this makes routine
WETDEPID obsolete, so we can remove it.

22 Sep 2015 - R. Yantosca - Bug fix: only define the IDWETD array if
wetdep or drydep is turned on. Also only
print info if wetdep is turned on.

29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts

20 Jun 2016 - R. Yantosca - Now define species IDs in the init phase
```

4.2.30 setup_wetscav

Subroutine SETUP_WETSCAV initializes updraft velocity, cloud liquid water content, cloud ice content, and mixing ratio of water fields, which are used in the wet scavenging routines.

INTERFACE:

```
SUBROUTINE SETUP_WETSCAV( am_I_Root, Input_Opt, & State_Met, State_Chm, RC )
```

USES:

```
USE CMN_Size_Mod

USE ErrCode_Mod

USE Error_Mod, ONLY : Alloc_Err

USE Input_Opt_Mod, ONLY : OptInput

USE PhysConstants, ONLY : AIRMW

USE State_Chm_Mod, ONLY : ChmState

USE State_Met_Mod, ONLY : MetState

USE UnitConv_Mod
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

```
23 Feb 2000 - R. Yantosca - Initial version
```

- (1) References "e_ice.f" -- routine to compute Eice(T).
- (2) Vud, CLDLIQ, CLDICE, $C_{\rm H20}$ are all independent of tracer, so we can compute them once per timestep, before calling the cloud

- convection and wet deposition routines.
- (3) Set C_H2O = 0 below -120 Celsius. E_ICE(T) has a lower limit of -120 Celsius, so temperatures lower than this will cause a stop with an error message. (bmy, 6/15/00)
- (4) Replace {IJL}GLOB with IIPAR, JJPAR, LLPAR. Also rename PW to P. Remove IREF, JREF, these are obsolete. Now reference IS_WATER from "dao_mod.f" to determine water boxes.
- (5) Removed obsolete code from 9/01. Updated comments and made cosmetic changes. (bmy, 10/24/01)
- (6) Now use routine GET_PCENTER from "pressure_mod.f" to compute the pressure at the midpoint of grid box (I,J,L). Also removed P and SIG from the argument list (dsa, bdf, bmy, 8/20/02)
- (7) Now reference T from "dao_mod.f". Updated comments. Now allocate Vud, C_H2O, CLDLIQ and CLDICE here on the first call. Now references ALLOC_ERR from "error_mod.f". Now set H2O2s and SO2s to the initial values from for the first call to COMPUTE_F. Now call WETDEPID on the first call to initialize the wetdep index array. (bmy, 1/27/03)
- (8) Now references STT from "tracer_mod.f". Also now we call WETDEPID from "input_mod.f" (bmy, 7/20/04)
- (9) Now references new function E_ICE, which is an analytic function of Kelvin temperature instead of Celsius. (bmy, 3/7/05)
- 16 Sep 2010 R. Yantosca Added ProTeX headers
- 18 Oct 2012 R. Yantosca Removed DEVEL from #ifdef statement, now use EXTERNAL_GRID || EXTERNAL_FORCING
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 26 Feb 2015 E. Lundgren Replace GET_PCENTER with State_Met%PMID_DRY.
 Remove dependency on pressure_mod.
- 28 Apr 2015 E. Lundgren Change PMID_DRY to PMID for Dalton's Law.
- 13 Aug 2015 E. Lundgren Incoming tracer units are now kg/kg dry air
- 03 Sep 2015 R. Yantosca Now allocate IDWETD
- 03 Sep 2015 R. Yantosca Now move array allocation into INIT_WETSCAV
- 22 Sep 2015 R. Yantosca Bug fix: now initialize H2O2s and SO2s on the first call. This was done in INIT_WETSCAV, but that is now called before the restart file is read from disk.
- 23 Sep 2015 R. Yantosca Now accept State_Chm as an argument
- 29 Apr 2016 R. Yantosca Don't initialize pointers in declaration stmts
- 23 Jun 2016 R. Yantosca Remove reference to tracerid_mod.F
- 30 Jun 2016 R. Yantosca Remove instances of STT and State_Chm%TRACERS
- 04 Jul 2016 M. Yannetti Replace TCVV with species db MW and phys constant
- 05 Aug 2016 R. Yantosca Remove temporary tracer-removal code

4.2.31 cleanup_wetscav

Subroutine CLEANUP_WETSCAV deallocates all module arrays.

INTERFACE:

SUBROUTINE CLEANUP_WETSCAV

REVISION HISTORY:

```
23 Feb 2000 - R. Yantosca - Initial version
16 Sep 2010 - R. Yantosca - Added ProTeX headers
03 Sep 2015 - R. Yantosca - Now deallocate IDWETD
```

5 Boundary layer mixing modules

These modules contain routines to perform the boundary layer mixing.

5.1 Fortran: Module Interface mixing_mod.F90

Module mixing_mod.F90 is a wrapper module for the PBL mixing in GEOS-Chem.

INTERFACE:

PR.TVATE.

```
MODULE MIXING_MOD
```

USES:

```
USE PRECISION_MOD

IMPLICIT NONE
```

PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: INIT_MIXING
PUBLIC :: DO_MIXING
PUBLIC :: DO_TEND
```

PRIVATE MEMBER FUNCTIONS:

REVISION HISTORY:

```
04 Mar 2015 - C. Keller - Initial version.
```

5.1.1 init_mixing

Subroutine INIT_MIXING initialized the pbl mixing wrapper module.

INTERFACE:

```
SUBROUTINE INIT_MIXING (am_I_Root, Input_Opt, State_Met, State_Chm, RC)
```

USES:

```
USE ERROR_MOD, ONLY : ERROR_STOP
USE Input_Opt_Mod, ONLY : OptInput
```

USE PBL_MIX_MOD, ONLY : COMPUTE_PBL_HEIGHT

USE PBL_MIX_MOD, ONLY : DO_PBL_MIX
USE State_Met_Mod, ONLY : MetState
USE State_Chm_Mod, ONLY : ChmState
USE VDIFF_MOD, ONLY : DO_PBL_MIX_2

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root ! root CPU?

TYPE(OptInput), INTENT(IN ) :: Input_Opt ! Input opts
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Met state
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry state
```

INTEGER, INTENT(INOUT) :: RC ! Failure or success

!REMARKS

(A) While all dry deposition rates are calculated either in DO_PBL_MIX2 or DO_TEND, settling of aerosols is still computed in the dust/seasalt modules.

REVISION HISTORY:

```
04 Mar 2015 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Now also call COMPUTE_PBL_HEIGHT so that we populate PBL quantities w/ the initial met
```

5.1.2 do_mixing

Subroutine DO₋MIXING performs the PBL mixing.

INTERFACE:

```
SUBROUTINE DO_MIXING ( am_I_Root, Input_Opt, State_Met, State_Chm, RC )
```

USES:

```
USE ErrCode_Mod

USE ERROR_MOD, ONLY : GC_Error

USE Input_Opt_Mod, ONLY : OptInput

USE PBL_MIX_MOD, ONLY : DO_PBL_MIX

USE State_Met_Mod, ONLY : MetState

USE State_Chm_Mod, ONLY : ChmState
```

USE UnitConv_Mod

USE VDIFF_MOD, ONLY : DO_PBL_MIX_2

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root ! root CPU? TYPE(OptInput), INTENT(IN ) :: Input_Opt ! Input opts
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Met state
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry state
INTEGER, INTENT(INOUT) :: RC ! Failure or success
!REMARKS
```

(A) While all dry deposition rates are calculated either in DO_PBL_MIX2 or DO_TEND, settling of aerosols is still computed in the dust/seasalt modules.

REVISION HISTORY:

```
04 Mar 2015 - C. Keller - Initial version

12 Aug 2015 - E. Lundgren - Input tracer units are now [kg/kg] and are converted to [v/v] for mixing

30 Sep 2014 - E. Lundgren - Move unit conversion for DO_TEND to DO_TEND

30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

08 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code
```

5.1.3 do_tend

Subroutine DO₋TEND adds the species tendencies (dry deposition and emissions) to the species array.

INTERFACE:

```
SUBROUTINE DO_TEND ( am_I_Root, Input_Opt, State_Met, & State_Chm, OnlyAbovePBL, RC, DT )
```

USES:

```
USE CHEMGRID_MOD,
                        ONLY : GET_CHEMGRID_LEVEL
USE CMN_DIAG_MOD,
                        ONLY: ND44
USE CMN_SIZE_MOD,
                        ONLY : IIPAR,
                                        JJPAR,
                                                 LLPAR
USE DRYDEP_MOD,
                        ONLY : DEPSAV
USE ErrCode_Mod
USE ERROR_MOD,
                        ONLY : ERROR_STOP, SAFE_DIV
USE GET_NDEP_MOD,
                        ONLY : SOIL_DRYDEP
USE HCO_INTERFACE_MOD,
                        ONLY: GetHcoVal, GetHcoDiagn
USE Input_Opt_Mod,
                        ONLY : OptInput
                        ONLY : GET_FRAC_UNDER_PBLTOP
USE PBL_MIX_MOD,
USE PhysConstants,
                        ONLY: AVO
USE Species_Mod,
                        ONLY : Species
USE State_Met_Mod,
                        ONLY : MetState
```

```
USE State_Chm_Mod,
                            ONLY : ChmState
    USE TIME_MOD,
                            ONLY : GET_TS_DYN, GET_TS_CONV, GET_TS_CHEM
    USE State_Chm_Mod,
                            ONLY : Ind_
    USE UnitConv_Mod
#if defined( BPCH_DIAG )
   USE DIAG_MOD,
                            ONLY: AD44
#endif
#if defined( NC_DIAG )
    USE HCO_ERROR_MOD
    USE HCO_INTERFACE_MOD, ONLY : HcoState, GetHcoID
    USE HCO_DIAGN_MOD,
                            ONLY : Diagn_Update
#endif
#if defined( USE_TEND )
    USE TENDENCIES_MOD
#endif
```

INPUT PARAMETERS:

```
LOGICAL,
                                        :: am_I_Root
                                                        ! root CPU?
                 INTENT(IN )
TYPE(OptInput),
                                         :: Input_Opt
                 INTENT(IN
                             )
                                                        ! Input opts
TYPE(MetState), INTENT(IN
                                        :: State_Met
                                                        ! Met state
                             )
LOGICAL,
                 INTENT(IN
                             )
                                         :: OnlyAbovePBL ! Only above PBL?
REAL(fp),
                 INTENT(IN
                             ), OPTIONAL :: DT
                                                        ! Time step [s]
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry state INTEGER, INTENT(INOUT) :: RC ! Failure or success
```

```
04 Mar 2015 - C. Keller
                          - Initial version
09 Mar 2015 - R. Yantosca - Bug fix: Use the drydep ID number instead of the
                            tracer number to index the AD44 drydep array
09 Mar 2015 - R. Yantosca - Bug fix: Remove an IF ( L1 == 1 ) block where
                            we define DRYDEPID. This isn't needed here.
                          - Now exchange PARANOX loss fluxes via HEMCO
10 Apr 2015 - C. Keller
                            diagnostics.
12 Jun 2015 - R. Yantosca - Bug fix in SAFE_DIV: the denominator was
                            arranged wrongly. Now corrected.
18 Jun 2015 - C. Keller
                          - Now restrict all emissions to chemistry grid
                            if UCX=false.
30 Sep 2015 - E. Lundgren - Now convert locally to kg/m2 for area-independent
                            compatibility between tracer units and flux
22 Mar 2016 - C. Keller
                          - Bug fix: make sure drydep velocities are written
                            to diagnostics if emissions are zero.
16 Mar 2016 - E. Lundgren - Exclude specialty simulations in restriction of
                            all emissions to chemistry grid if UCX=false
                          - Make sure PARANOx fluxes are applied to tracers.
29 Feb 2016 - C. Keller
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
```

```
25 May 2016 - E. Lundgren - Replace input_opt%TRACER_MW_KG with species database field emMW_g (emitted species g/mol)

16 Jun 2016 - C. Miller - Now define species ID's with the Ind_ function

17 Jun 2016 - R. Yantosca - Only define species ID's on the first call

30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

01 Jul 2016 - R. Yantosca - Now rename species DB object ThisSpc to SpcInfo

19 Jul 2016 - R. Yantosca - Now bracket tendency calls with #ifdef USE_TEND
```

5.2 Fortran: Module Interface pbl_mix_mod.F

Module PBL_MIX_MOD contains routines and variables used to compute the planetary boundary layer (PBL) height and to mix tracers underneath the PBL top.

INTERFACE:

MODULE PBL_MIX_MOD

USES:

```
USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

IMPLICIT NONE
PRIVATE
```

PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: CLEANUP_PBL_MIX

PUBLIC :: DO_PBL_MIX

PUBLIC :: GET_FRAC_OF_PBL

PUBLIC :: GET_FRAC_UNDER_PBLTOP

PUBLIC :: GET_PBL_MAX_L

PUBLIC :: GET_PBL_TOP_hPa

PUBLIC :: GET_PBL_TOP_L

PUBLIC :: GET_PBL_TOP_M

PUBLIC :: GET_PBL_TOP_M

PUBLIC :: GET_PBL_THICK

PUBLIC :: INIT_PBL_MIX

PUBLIC :: COMPUTE_PBL_HEIGHT

#if defined ( DEVEL )

PUBLIC :: PBL_TOP_L, PBL_TOP_M

#endif
```

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: TURBDAY

```
11 Feb 2005 - R. Yantosca - Initial version
(1 ) Now modified for GCAP and GEOS-5 met fields (bmy, 5/24/05)
(2 ) Remove reference to "CMN" and XTRA2. (bmy, 8/30/05)
(3 ) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
(4 ) Add INIT_PBL_MIX and COMPUTE_PBL_HEIGHT as PUBLIC routines (lin, 5/29/09)
(5 ) Extend tracers for APM simulation (GanLuo, 2010)
28 Feb 2012 - R. Yantosca - Removed support for GEOS-3
28 Feb 2012 - R. Yantosca - Added ProTeX headers
01 Mar 2012 - R. Yantosca - Now reference new grid_mod.F90
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
19 Nov 2014 - M. Yannetti - Added PRECISION_MOD
23 Jun 2016 - R. Yantosca - Remove references to APM code; it is no longer compatible with the FlexChem implementation
```

5.2.1 do_pbl_mix

Subroutine DO_PBL_MIX is the driver routine for planetary boundary layer mixing. The PBL layer height and related quantities are always computed. Complete mixing of tracers underneath the PBL top is toggled by the DO_TURBDAY switch.

INTERFACE:

```
SUBROUTINE DO_PBL_MIX( am_I_Root, DO_TURBDAY, Input_Opt, & State_Met, State_Chm, RC )
```

USES:

```
USE ErrCode_Mod

USE Input_Opt_Mod, ONLY : OptInput

USE State_Met_Mod, ONLY : MetState

USE State_Chm_Mod, ONLY : ChmState

USE TIME_MOD, ONLY : GET_TS_CONV

#if defined(USE_TEND)

USE TENDENCIES_MOD

#endif
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Root CPU?

LOGICAL, INTENT(IN) :: DO_TURBDAY ! =T means call TURBDAY

! for full PBL mixing

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

INPUT/OUTPUT PARAMETERS:

REVISION HISTORY:

```
11 Feb 2005 - R. Yantosca - Initial version

07 Sep 2011 - G. Luo - Add modifications for APM

28 Feb 2012 - R. Yantosca - Added ProTeX headers

25 Mar 2013 - M. Payer - Now pass State_Chm object via the arg list

22 Aug 2014 - R. Yantosca - Now declare State_Met INTENT(INOUT)

30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

06 Jul 2016 - R. Yantosca - Now pass State_Chm and am_I_Root to TURBDAY

19 Jul 2016 - R. Yantosca - Now bracket tendency calls with #ifdef USE_TEND

08 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code
```

5.2.2 compute_pbl_height

Subroutine COMPUTE_PBL_HEIGHT computes the PBL height and other related quantities.

INTERFACE:

```
SUBROUTINE COMPUTE_PBL_HEIGHT( State_Met )
```

USES:

```
USE CMN_SIZE_MOD ! Size parameters
USE ERROR_MOD, ONLY : ERROR_STOP
USE PhysConstants ! Scale height
USE State_Met_Mod, ONLY : MetState
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met   ! Meteorology State object
```

```
11 Feb 2005 - R. Yantosca - Initial version
(1 ) Now modified for GEOS-5 and GCAP met fields (swu, bmy, 5/25/05)
(2 ) Remove reference to "CMN" and XTRA2 -- they're obsolete. Also do not force BLTOP, BLTHIK to minimum values for GEOS-STRAT met fields. (bmy, 8/30/05)
(3 ) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
28 Feb 2012 - R. Yantosca - Removed support for GEOS-3
28 Feb 2012 - R. Yantosca - Added ProTeX headers
09 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met derived type object
```

```
22 Aug 2014 - R. Yantosca - Now declare State_Met INTENT(INOUT)
26 Feb 2015 - E. Lundgren - Replace GET_PEDGE with State_Met%PEDGE.
Remove dependency on pressure_mod.
```

5.2.3 turbday

! Subroutine TURBDAY executes the GEOS-Chem boundary layer mixing algorithm (full PBL mixing).

INTERFACE:

```
SUBROUTINE TURBDAY( am_I_root, Input_Opt, & State_Met, State_Chm, RC )
```

USES:

```
USE CMN_DIAG_MOD
USE CMN_SIZE_MOD
```

USE DIAG_MOD, ONLY : TURBFLUP

USE ErrCode_Mod

USE Input_Opt_Mod, ONLY : OptInput
USE PhysConstants, ONLY : AIRMW
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState
USE TIME_MOD, ONLY : GET_TS_CONV

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root
TYPE(OptInput), INTENT(IN) :: Input_Opt
TYPE(MetState), INTENT(IN) :: State_Met
```

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC

REMARKS:

Original subroutine by Dale Allen, Univ of MD.

- 30 Jan 1998 I. Bey, R. Yantosca Initial version
- (1) TURBDAY is written in Fixed-Form Fortran 90. Also use F90 syntax for declarations (bmy, 4/1/99).
- (2) New tracer concentrations are returned in TC.
- (3) PS(I,J) is ACTUAL surface pressure and not Psurface PTOP
- (4) Change in tracer in kg is now stored in DTC(I,J,L,N). This makes it easier to compute diagnostic quantities. The new mixing ratio is computed as TC(I,J,L,N) = TC(I,J,L,N) + DTC(I,J,L,N) / AD(I,J,L).
- (5) XTRA2(*,*,5) is the height of the PBL in # of layers. So if the PBL top is located in the middle of the 3rd sigma layer at (I,J)

- the value of XTRA2(I,J,5) would be 2.5. The XTRA2 variable is used by the HCTM drydep subroutines...it really is a historical holdover.
- (6) Restore the following NDxx diagnostics: (a) ND63 : Mass balance (CNVUPP) (b) ND15 : Mass change due to mixing in the boundary layer
- (7) Now pass TCVV and NCONV for the mass flux diagnostics. Also updated comments and cleaned up a few things. (bey, bmy, 11/10/99)
- (8) Remove PTOP and XNUMOL from the arg list. PTOP is now a parameter in "CMN_SIZE". XNUMOL is no longer used in TURBDAY. (bmy, 2/10/00)
- (9) Also removed obsolete ND63 diagnostics and updated comments. (bmy, 4/12/00)
- (10) Now use NTRC instead of NNPAR to dimension variables TC, TCVV, DTC, and DTCSUM (bmy, 10/17/00).
- (11) Removed obsolete code from 10/17/00 (bmy, 12/21/00)
- (12) If the PBL depth is very small (or zero), then assume a PBL depth of 2 mb -- this prevents NaN's from propagating throughout the code. Also updated comments & made cosmetic changes. (bmy, 3/9/01)
- (13) DTCSUM was declared twice but wasn't used. Elminate declarations to DTCSUM. (bmy, 7/16/01)
- (14) XTRA2(IREF, JREF, 5) is now XTRA2(I, J). Also updated comments.

 Also remove IREF, JREF and some debug output. (bmy, 9/25/01)
- (15) Removed obsolete commented out code from 9/01 (bmy, 10/24/01)
- (16) Now takes in P=PS-PTOP instead of PS. Redimension SIGE to (1:LLPAR+1).
- (17) Renamed PS to PZ so as not to conflict w/ the existing P variable.

 Now pass P-PTOP thru PZ, in order to ensure that P and AD are

 consistent w/ each other. Added parallel DO-loops. Updated comments,

 cosmetic changes. Now print a header to stdout on the first call,

 to confirm that TURBDAY has been called. (bmy, 4/11/02)
- (18) Now use GET_PEDGE from "pressure_mod.f" to compute the pressure at the bottom edge of grid box (I,J,L). Deleted obsolete code from 4/02. Removed PZ, SIGE from the argument list, since we now compute pressure from GET_PEDGE. (dsa, bdf, bmy, 8/22/02)
- (19) Now reference AD, PBL from "dao_mod.f". Now removed DXYP from the arg list, use GET_AREA_M2 from "grid_mod.f" instead. Now removed NCONV, ALPHA_d, ALPHA_n from the arg list. Now no longer reference SUNCOS. Now set A(:,:)=1 day & nite; we assume full mixing all the time regardless of SUNCOS. Updated comments, cosmetic changes. (bmy, 2/11/03)
- (20) Now can handle PBL field in meters for GEOS-4/fvDAS. Also the atmospheric scale height from CMN_GCTM. (bmy, 6/23/03)
- (21) Now bundled into "pbl_mix_mod.f". Broke off the part which computes PBL height and related quantities into COMPUTE_PBL_HEIGHT. (bmy, 2/15/05)
- 28 Feb 2012 R. Yantosca Added ProTeX headers
- 2 Mar 2012 R. Yantosca Remove reference to GET_AREA_M2
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object

```
15 Jul 2015 - C. Keller - Added tendencies module
06 Jul 2016 - R. Yantosca - Now pass State_Chm and am_I_Root as args
so that we can loop over advected species
25 Jul 2016 - M. Yannetti - Now takes in State_Chm to access spec db
```

5.2.4 get_frac_of_pbl

Function GET_FRAC_OF_PBL returns the fraction of grid box (I,J,L) that lies within the planetary boundary layer.

INTERFACE:

```
FUNCTION GET_FRAC_OF_PBL( I, J, L ) RESULT( FRAC )
```

USES:

```
USE CMN_SIZE_MOD  ! Size parameters
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I, J, L ! Lon, lat, lev indices
```

RETURN VALUE:

```
REAL(fp) :: FRAC ! Fraction of box (I,J,L) in the PBL
```

REVISION HISTORY:

```
11 Feb 2005 - R. Yantosca - Initial version
28 Feb 2012 - R. Yantosca - Added ProTeX headers
```

5.2.5 get_frac_under_pbltop

Function GET_FRAC_UNDER_PBLTOP returns the fraction of grid box (I,J,L) that lies underneath the planetary boundary layer top.

INTERFACE:

```
FUNCTION GET_FRAC_UNDER_PBLTOP( I, J, L ) RESULT( FRAC )
```

USES:

```
USE CMN_SIZE_MOD ! Size parameters
```

INPUT PARAMETERS:

```
{\tt INTEGER,\ INTENT(IN)\ ::\ I,\ J,\ L\quad !\ Lon,\ lat,\ level\ indices}
```

RETURN VALUE:

REAL(fp) :: FRAC ! Fraction of box (I,J,L) below PBL top

REVISION HISTORY:

```
11 Feb 2005 - R. Yantosca - Initial version
28 Feb 2012 - R. Yantosca - Added ProTeX headers
```

$5.2.6 \quad get_pbl_max_l$

Function GET_PBL_MAX_L returns the model level at the highest part of the planetary boundary layer.

INTERFACE:

```
FUNCTION GET_PBL_MAX_L() RESULT( TOP )
```

RETURN VALUE:

```
INTEGER :: TOP ! Highest extent of PBL [model levels]
```

REVISION HISTORY:

```
11 Feb 2005 - R. Yantosca - Initial version
28 Feb 2012 - R. Yantosca - Added ProTeX headers
```

5.2.7 get_pbl_top_hpa

Function GET_PBL_TOP_hPa returns the planetary boundary layer top [hPa] at a given GEOS-Chem surface location (I,J).

INTERFACE:

```
FUNCTION GET_PBL_TOP_hPa( I, J ) RESULT( TOP )
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I, J ! Lon and lat indices
```

RETURN VALUE:

```
REAL(fp) :: TOP ! PBL top [hPa]
```

```
11 Feb 2005 - R. Yantosca - Initial version
28 Feb 2012 - R. Yantosca - Added ProTeX headers
```

5.2.8 get_pbl_top_l

Function GET_PBL_TOP_L returns the planetary boundary layer top [model levels] at a given GEOS-Chem surface location (I,J).

INTERFACE:

```
FUNCTION GET_PBL_TOP_L( I, J ) RESULT( TOP )
```

USES:

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I, J ! Lon and lat indices
```

RETURN VALUE:

```
REAL(fp) :: TOP ! PBL top [model levels]
```

REVISION HISTORY:

```
11 Feb 2005 - R. Yantosca - Initial version
28 Feb 2012 - R. Yantosca - Added ProTeX headers
```

$5.2.9 \quad get_pbl_top_m$

Function GET_PBL_TOP_m returns the planetary boundary layer top [m] at a given GEOS-CHEM surface location (I,J).

INTERFACE:

```
FUNCTION GET_PBL_TOP_m( I, J ) RESULT( TOP )
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I, J ! Lon and lat indices
```

RETURN VALUE:

```
REAL(fp) :: TOP ! PBL top [m]
```

```
11 Feb 2005 - R. Yantosca - Initial version
28 Feb 2012 - R. Yantosca - Added ProTeX headers
```

5.2.10

Function GET_PBL_THICK returns the thickness of the PBL at a given surface location (I,J).

INTERFACE:

```
FUNCTION GET_PBL_THICK( I, J ) RESULT( THICK )
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I, J  ! Lon and lat indices
```

RETURN VALUE:

```
REAL(fp) :: THICK ! PBL thickness [hPa]
```

REVISION HISTORY:

```
11 Feb 2005 - R. Yantosca - Initial version
28 Feb 2012 - R. Yantosca - Added ProTeX headers
```

$5.2.11 \quad init_pbl_mix$

Subroutine INIT_PBL_MIX allocates and zeroes module arrays

INTERFACE:

SUBROUTINE INIT_PBL_MIX

USES:

```
USE CMN_SIZE_MOD
USE ERROR_MOD, ONLY : ALLOC_ERR
```

REVISION HISTORY:

5.2.12 cleanup_pbl_mix

Subroutine CLEANUP_PBL_MIX allocates and zeroes module arrays.

INTERFACE:

SUBROUTINE CLEANUP_PBL_MIX

REVISION HISTORY:

```
11 Feb 2005 - R. Yantosca - Initial version
28 Feb 2012 - R. Yantosca - Added ProTeX headers
```

5.3 Fortran: Module Interface vdiff_mod.F90

Module VDIFF_MOD includes all routines for the non-local PBL mixing scheme.

INTERFACE:

MODULE VDIFF_MOD

USES:

```
USE CMN_DIAG_MOD, ONLY : ND15, ND44 ! Diagnostics USE CMN_SIZE_MOD, ONLY : IIPAR, JJPAR, LLPAR ! Grid dimensions
USE CMN_SIZE_MOD, ONLY : plev => LLPAR
                                                      ! # of levels
                     ONLY : DEBUG_MSG
USE ERROR_MOD,
                                                      ! Routine for debug output
USE PhysConstants
                                                      ! Physical constants
USE PRECISION_MOD
                                                      ! For GEOS-Chem Precision(fp)
USE VDIFF_PRE_MOD, ONLY : PCNST
                                                      ! N_TRACERS
USE VDIFF_PRE_MOD, ONLY : LPRT
                                                       ! Debug print?
                                                       ! Do PBL mixing?
USE VDIFF_PRE_MOD, ONLY : LTURB
IMPLICIT NONE
PRIVATE
```

PUBLIC MEMBER FUNCTIONS:

```
public :: DO_PBL_MIX_2
!PRIVATE DATA MEMBERS:
save
integer :: plevp
real(fp), parameter ::
     cpair = 1004.64e+0_{fp},
                                  &
     latvap = 2.5104e+06_fp,
                                  &
     rhoh2o = 1.e+3_fp,
     tfh2o = 273.16e+0_fp,
                                  &
     rair = Rd,
                                  &
     rh2o = Rv,
                                  &
     gravit = g0,
```

```
zvir = rh2o/rair - 1.,
      cappa = Rd/cpair,
      r_g = Rd / g0
 ! Obsolete variables and variables that are now defined with global params
 ! (ewl, 1/7/16)
 real(fp), parameter ::
      rearth = 6.37122e+6_{fp}, & ! not used
       cpwv = 1.81e + 3_{fp},
                                   & ! not used
      ra = 1.e+0_fp/rearth, & ! not used

epsilo = 0.622e+0_fp, & ! not used

latice = 3.336e+5_fp, & ! not used

rair = 287.04e+0_fp, & ! now use global Rd

rh2o = 461.e+0_fp, & ! now use global Rv

gravit = 9.80616e+0_fp, & ! now use global g0
      cappa = rair/cpair, & ! now use global Rd
      r_g = rair / gravit, & ! now use global Rd and g0
  ... pbl constants
 ! These are constants, so use PARAMETER tag
real(fp), parameter :: &
      betam = 15.e+0_fp, & ! constant in wind gradient expression
     betas = 5.e+0_fp, &! constant in surface layer gradient expression
      betah = 15.e+0_fp, & ! constant in temperature gradient expression
      fak = 8.5e+0_fp, &! constant in surface temperature excess
      fakn = 7.2e+0_fp, &! constant in turbulent prandtl number
      ricr = .3e+0_fp, & ! critical richardson number
      sffrac = .1e+0_fp, & ! surface layer fraction of boundary layer
                .4e+0_fp ! von karmans constant
 ! These are assigned later, so we can't use the PARAMETER tag
real(fp) ::
                       & ! gravitational acceleration
      g,
                       & ! 1/3 power in wind gradient expression
      onet,
      ccon,
                       & ! fak * sffrac * vk
                       & ! betam * sffrac
      binm,
                          ! betah * sffrac
      binh
  ... constants used in vertical diffusion and pbl
______
real(fp) :: &
                       ! minimum kneutral*f(ri)
real(fp), allocatable :: ml2(:) ! mixing lengths squaredB
real(fp), allocatable :: qmincg(:) ! min. constituent concentration
```

! counter-gradient term

REMARKS:

The non-local PBL mixing routine VDIFF modifies the specific humidity, (State_Met%SPHU) field. Therefore, we must pass State_Met as an argument to DO_PBL_MIX_2 and VDIFFDR with INTENT(INOUT).

Because logical_mod.F and tracer_mod.F have been superseded by Input_Opt, we now use VDIFF_PRE_MOD to supply values

```
(1 ) This code is modified from mo_vdiff.F90 in MOZART-2.4. (lin, 5/14/09)
07 Oct 2009 - R. Yantosca - Added CVS Id Tag
                          - Modified ND15 to account for all mixing
24 Sep 2010 - J. Lin
                            processes but not dry deposition and emissions.
17 Dec 2010 - R. Yantosca - Declare constants w/ the PARAMETER attribute
20 Dec 2010 - R. Yantosca - Bug fixes for the parallelization
02 Mar 2011 - R. Yantosca - Bug fixes for PGI compiler: these mostly
                            involve explicitly using "D" exponents
25 Mar 2011 - R. Yantosca - Corrected bug fixes noted by Jintai Lin
08 Feb 2012 - R. Yantosca - Add modifications for GEOS-5.7.2 met
22 Jun 2012 - R. Yantosca - Now use pointers to flip arrays in vertical
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
24 Jun 2014 - R. Yantosca - Now get PCNST from vdiff_pre_mod.F90
24 Nov 2014 - M. Yannetti - Added PRECISION_MOD
07 Jan 2016 - E. Lundgren - Replace hard-coded physical params w/ global and
                            remove unused parameters
22 Jun 2016 - M. Yannetti - Replace TCVV with species db MW and phys constant
29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90
```

5.3.1 pbinti

Subroutine PBINTI initializes time independent variables of pbl package

INTERFACE:

```
subroutine pbinti( gravx )
```

USES:

implicit none

INPUT PARAMETERS:

```
real(fp), intent(in) :: gravx    ! acceleration of gravity
```

REVISION HISTORY:

```
02 Mar 2011 - R. Yantosca - Bug fixes for PGI compiler: these mostly involve explicitly using "D" exponents
```

5.3.2 vdiff

Subroutine vdiff is the driver routine to compute vertical diffusion of momentum, moisture, trace constituents and potential temperature.

INTERFACE:

```
subroutine vdiff( lat,
                                                                 &
                             ip,
                                        uwnd,
                                                    vwnd,
                 tadv,
                             pmid,
                                        pint,
                                                    rpdel_arg,
                 rpdeli_arg, ztodt,
                                        zm_arg,
                                                    shflx_arg,
                                                                 &
                                                    pblh_arg,
                 sflx,
                             thp_arg,
                                        as2,
                                                                 &
                 kvh_arg,
                             kvm_arg,
                                        tpert_arg,
                                                    qpert_arg,
                                                                 &
                                        wvflx_arg,
                                                    plonl,
                 cgs_arg,
                             shp,
                                                                 &
                 Input_Opt,
                             State_Met, State_Chm,
                                                    taux_arg,
                                                                 &
                 tauy_arg,
                             ustar_arg )
```

USES:

```
USE DIAG_MOD, ONLY : TURBFLUP
USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState
```

implicit none

INPUT PARAMETERS:

```
integer, intent(in) :: lat, ip ! latitude index, long tile index
integer, intent(in) :: plonl ! number of local longitudes
real(fp), intent(in) :: &
```

```
! 2 delta-t
         ztodt
    real(fp), intent(in) :: &
         uwnd(:,:,:),
                                   ! u wind input
                             &
         ! v wind input
         tadv(:,:,:),
                           &
                                   ! temperature input
                          &
&
&
         pmid(:,:,:),
                                   ! midpoint pressures
         pint(:,:,:),
                                   ! interface pressures
                                   ! 1./pdel (thickness bet interfaces)
         rpdel_arg(:,:,:),
         rpdeli_arg(:,:,:), & ! 1./pdeli (thickness bet midpoints)
zm_arg(:,:,:), & ! midpoint geoptl height above sfc
shflx_arg(:,:), & ! surface sensible heat flux (w/m2)
                             &
         sflx(:,:,:),
                                   ! surface constituent flux (kg/m2/s)
         wvflx_arg(:,:)
                                   ! water vapor flux (kg/m2/s)
    TYPE(OptInput), INTENT(IN) :: Input_Opt   ! Input Options object
    TYPE(MetState), INTENT(IN) :: State_Met
                                              ! Meteorology State object
INPUT/OUTPUT PARAMETERS:
    real(fp), intent(inout) :: &
         as2(:,:,:,:),
                             &
                                   ! moist, tracers after vert. diff
         shp(:,:,:),
                                   ! specific humidity (kg/kg)
                             &
         thp_arg(:,:,:)
                                   ! pot temp after vert. diffusion
    TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
OUTPUT PARAMETERS:
    real(fp), intent(out) ::
         kvh_arg(:,:,:),
                            & ! coefficient for heat and tracers
         kvm_arg(:,:,:),
                                   ! coefficient for momentum
                             &
         ! convective temperature excess
                                   ! convective humidity excess
         cgs_arg(:,:,:)
                                   ! counter-grad star (cg/flux)
    real(fp), optional, intent(inout) :: &
         taux_arg(:,:),
                            &
                                   ! x surface stress (n)
         tauy_arg(:,:),
                                   ! y surface stress (n)
                             &
         ustar_arg(:,:)
                                   ! surface friction velocity
    real(fp), intent(inout) :: pblh_arg(:,:) ! boundary-layer height [m]
```

REMARKS:

Free atmosphere diffusivities are computed first; then modified by the boundary layer scheme; then passed to individual parameterizations modiff, qvdiff.

The free atmosphere diffusivities are based on standard mixing length forms for the neutral diffusivity multiplied by functions of Richardson number. $k = 1^2 * |dv/dz| * f(ri). \label{eq:kappa}$ The same functions are used for momentum, potential temperature, and constitutents.

```
The stable Richardson num function (ri>0) is taken from Holtslag and Beljaars (1989), ECMWF proceedings. f = 1 / (1 + 10*ri*(1 + 8*ri)). The unstable richardson number function (ri<0) is taken from ccm1. f = sqrt(1 - 18*ri)
```

REVISION HISTORY:

5.3.3 pbldif

Subroutine PBLDIF computes the atmospheric boundary layer. The nonlocal scheme determines eddy diffusivities based on a diagnosed boundary layer height and a turbulent velocity scale. Also, countergradient effects for heat and moisture, and constituents are included, along with temperature and humidity perturbations which measure the strength of convective thermals in the lower part of the atmospheric boundary layer.

References:

1. Holtslag, A. A. M., and B. A. Boville, 1993: Local versus nonlocal boundary-layer diffusion in a global climate model, J. Clim., 6, 1825-1842.

INTERFACE:

```
subroutine pbldif( th
                                                         ,v, &
                                      ,z
                                               ,u
                            ,q
                            ,pmid
                                      ,kvf
                                               ,cflx
                                                         ,shflx, &
                            ,kvh, &
                    kvm
                                                ,pblh
                                                         ,tpert, &
                    cgh
                            ,cgq
                                      ,cgs
                                               ,plonl, &
                    qpert
                            ,wvflx
                                      ,cgsh
                                      ,ustar )
                    taux
                            ,tauy
```

USES:

implicit none

INPUT PARAMETERS:

```
integer, intent(in) :: &
  plonl
    real(fp), intent(in) :: &
         th(plon1,plev), &
                                  ! potential temperature [k]
         q(plonl,plev), &
                                  ! specific humidity [kg/kg]
         z(plonl,plev), &
                                ! height above surface [m]
         u(plon1,plev), &
                                 ! windspeed x-direction [m/s]
         v(plonl,plev), &
                                  ! windspeed y-direction [m/s]
         t(plon1,plev), &
                                  ! temperature (used for density)
         pmid(plon1,plev), &
                                  ! midpoint pressures
         kvf(plon1,plevp), &
                                ! free atmospheric eddy diffsvty [m2/s]
                                  ! surface constituent flux (kg/m2/s)
         cflx(plon1,pcnst), &
         wvflx(plon1), &
                                  ! water vapor flux (kg/m2/s)
         shflx(plon1)
                                  ! surface heat flux (w/m2)
INPUT/OUTPUT PARAMETERS:
    real(fp), optional, intent(inout) :: &
         taux(plon1), &
                                ! x surface stress (n)
         tauy(plon1), &
                                ! y surface stress (n)
         ustar(plon1)
                                 ! surface friction velocity
    OUTPUT PARAMETERS:
    real(fp), intent(out) :: &
         kvm(plon1,plevp), &
                                ! eddy diffusivity for momentum [m2/s]
         kvh(plonl,plevp), &
                                ! eddy diffusivity for heat [m2/s]
                               ! counter-gradient term for heat [k/m]
         cgh(plonl,plevp), &
         cgq(plonl,plevp,pcnst), & ! counter-gradient term for constituents
         cgsh(plonl,plevp), &
                                ! counter-gradient term for sh
         cgs(plon1,plevp), & ! counter-gradient star (cg/flux)
                                 ! convective temperature excess
         tpert(plon1), &
         qpert(plon1)
                                 ! convective humidity excess
REVISION HISTORY:
   02 Mar 2011 - R. Yantosca - Bug fixes for PGI compiler: these mostly
                             involve explicitly using "D" exponents
```

5.3.4 qvdiff

Subroutine QVDIFF solve vertical diffusion eqtn for constituent with explicit srfc flux.

INTERFACE:

USES:

implicit none

INPUT PARAMETERS:

INPUT/OUTPUT PARAMETERS:

```
real(fp), intent(inout) :: &
    ze(plonl,plev) ! term in tri-diag. matrix system
```

OUTPUT PARAMETERS:

```
real(fp), intent(out) :: &
     qp1(plonl,plev,ncnst) ! final constituent
```

REMARKS:

```
Procedure for solution of the implicit equation follows: Richtmyer and Morton (1967,pp 198-199)
```

REVISION HISTORY:

```
02 Mar 2011 - R. Yantosca - Bug fixes for PGI compiler: these mostly involve explicitly using "D" exponents
```

5.3.5 vdiffar

Subroutine VDIFFAR is the driver routine to compute vertical diffusion of trace constituents using archived coefficients for cgs and kvh. This is a gutted version of vdiff.

INTERFACE:

USES:

implicit none

INPUT PARAMETERS:

```
integer, intent(in) :: lat
                                   ! latitude index
    integer, intent(in) :: plonl
                                   ! lon tile dim
    real(fp), intent(in) :: &
         ztodt , &
                                   ! 2 delta-t
         tadv(:,:,:), &
                               ! temperature input
         pmid(:,:,:), &
                           ! midpoint pressures
         pint(:,:,:), &
                           ! interface pressures
                                  ! 1./pdel (thickness bet interfaces)
         rpdel_arg(:,:,:), &
         rpdeli_arg(:,:,:), &
                                  ! 1./pdeli (thickness bet midpoints)
         sflx(:,:,:), &
                            ! surface constituent flux (kg/m2/s)
         kvh_arg(:,:,:), &
                                 ! coefficient for heat and tracers
         cgs_arg(:,:,:)
                                 ! counter-grad star (cg/flux)
INPUT/OUTPUT PARAMETERS:
    real(fp), intent(inout) :: &
         as2(:,:,:)
                          ! moist, tracers after vert. diff
REVISION HISTORY:
    02 Mar 2011 - R. Yantosca - Bug fixes for PGI compiler: these mostly
                               involve explicitly using "D" exponents
5.3.6 pbldifar
Subroutine PBLDIFAR is a modified version of pbldif which only calculates cgq given cgs.
INTERFACE:
  SUBROUTINE PBLDIFAR( t, pmid, cflx, cgs, cgq, plonl )
USES:
     implicit none
INPUT PARAMETERS:
     integer, intent(in) :: &
         plonl
    real(fp), intent(in) :: &
         t(plon1,plev), &
                                 ! temperature (used for density)
         pmid(plon1,plev), &
                                 ! midpoint pressures
         cflx(plonl,pcnst), &
                                 ! surface constituent flux (kg/m2/s)
         cgs(plonl,plevp)
                                 ! counter-gradient star (cg/flux)
OUTPUT PARAMETERS:
    real(fp), intent(out) :: &
         cgq(plon1,plevp,pcnst) ! counter-gradient term for constituents
```

02 Mar 2011 - R. Yantosca - Bug fixes for PGI compiler: these mostly

involve explicitly using "D" exponents

5.3.7 vdinti

Subroutine VDINTI initializes time independent fields for vertical diffusion. Calls initialization routine for boundary layer scheme.

INTERFACE:

SUBROUTINE VDINTI

USES:

```
USE ERROR_MOD, ONLY : ALLOC_ERR
USE PRESSURE_MOD, ONLY : GET_AP, GET_BP
```

REVISION HISTORY:

implicit none

```
02 Mar 2011 - R. Yantosca - Bug fixes for PGI compiler: these mostly involve explicitly using "D" exponents
```

5.3.8 vdiffdr

Subroutine VDIFFDR calculates the vertical diffusion on a latitude slice of data.

- 1. The dummy argument as 2 is in vv. (lin, 06/04/08)
- 2. TCVV and TRACER_MW_KG assume 12 g/mol for all HCs. Thus, when using them to convert units of HCs to be the inputs for vdiffdr, the converted units are NOT kg/kg for concentrations and kg/m2/s for surface flux. However, since the units for both inputs are consistent, there should not be any problem. (lin, 06/04/08)

INTERFACE:

```
SUBROUTINE VDIFFDR( am_I_Root, Input_Opt, State_Met, State_Chm )
```

USES:

```
USE DAO_MOD,
                            ONLY : IS_ICE, IS_LAND
    USE DEPO_MERCURY_MOD,
                            ONLY: ADD_Hg2_DD, ADD_HgP_DD
    USE DEPO_MERCURY_MOD,
                            ONLY: ADD_Hg2_SNOWPACK
#if defined( BPCH_DIAG )
    USE DIAG_MOD,
                            ONLY: AD44
#endif
    USE DRYDEP_MOD,
                            ONLY: DEPSAV
    USE GET_NDEP_MOD,
                            ONLY : SOIL_DRYDEP
    USE GLOBAL_CH4_MOD,
                            ONLY : CH4_EMIS
    USE GC_GRID_MOD,
                            ONLY: GET_AREA_M2
    USE Input_Opt_Mod,
                            ONLY : OptInput
    USE MERCURY_MOD,
                            ONLY : HG_EMIS
    USE OCEAN_MERCURY_MOD,
                            ONLY: Fg !hma
```

USE OCEAN_MERCURY_MOD, ONLY : OMMFP => Fp

USE OCEAN_MERCURY_MOD, ONLY : LHg2HalfAerosol !cdh

USE PBL_MIX_MOD, ONLY : GET_PBL_TOP_m, COMPUTE_PBL_HEIGHT, &

GET_PBL_MAX_L, GET_FRAC_UNDER_PBLTOP

USE Species_Mod, ONLY : Species
USE State_Chm_Mod, ONLY : ChmState
USE State_Chm_Mod, ONLY : Ind_
USE State_Met_Mod, ONLY : MetState

USE TIME_MOD, ONLY : GET_TS_CONV, GET_TS_EMIS, GET_TS_CHEM

#if defined(USE_TEND)

USE TENDENCIES_MOD

#endif

! HEMCO update

USE HCO_INTERFACE_MOD, ONLY : GetHcoID, GetHcoVal, GetHcoDiagn

#if defined(NC_DIAG)

USE ERROR_MOD, ONLY : ERROR_STOP
USE HCO_INTERFACE_MOD, ONLY : HcoState
USE HCO_ERROR_MOD, ONLY : HCO_SUCCESS
USE HCO_DIAGN_MOD, ONLY : Diagn_Update

#endif

implicit none

INPUT/OUTPUT PARAMETERS:

! is this the root CPU?

LOGICAL, INTENT(IN) :: am_I_Root

! Input options object

TYPE(OptInput), INTENT(IN) :: Input_Opt

! Meteorology State object

TYPE(MetState), INTENT(INOUT) :: State_Met

! Chemistry State object

TYPE(ChmState), INTENT(INOUT) :: State_Chm

REMARKS:

- (1) Need to declare the Meteorology State object (State_MET) with INTENT(INOUT). This is because VDIFF will modify the specific humidity field. (bmy, 11/21/12)
- (2) VDIFF also archives drydep fluxes to the soil NOx emissions module (by calling routine SOIL_DRYDEP) and to the ND44 diagnostic.
- (3) As of July 2016, we assume that all of the advected species are listed first in the species database. This is the easiest way to pass a slab

to the TPCORE routine. This may change in the future. (bmy, 7/13/16)

```
(1) Calls to vdiff and vdiffar are now done with full arrays as arguments.
      (ccc, 11/19/09)
04 Jun 2010 - C. Carouge - Updates for mercury simulations with GTMM
25 Aug 2010 - R. Yantosca - Treat MERRA in the same way as GEOS-5
24 Sep 2010 - J. Lin
                          - Move ND15 to vdiff.
21 Dec 2010 - R. Yantosca - Add logical flags for different sim types
21 Dec 2010 - R. Yantosca - Now call ITS_A_FULLCHEM_SIM instead of
                            relying on NCS == 0
22 Dec 2010 - C. Carouge - Combine array flipping w/ unit conversion
                            to save on operations
02 Mar 2011 - R. Yantosca - Bug fixes for PGI compiler: these mostly
                            involve explicitly using "D" exponents
                          - Use MERRA land fraction information
26 Apr 2011 - J. Fisher
25 Oct 2011 - H. Amos
                          - bring Hg2 gas-particle partitioning code into
                            v9-01-02
08 Feb 2012 - R. Yantosca - Treat GEOS-5.7.2 in the same way as MERRA
01 Mar 2012 - R. Yantosca - Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
22 Jun 2012 - R. Yantosca - Now use pointers to flip arrays in vertical
09 Nov 2012 - M. Payer
                          - Replaced all met field arrays with State_Met
                            derived type object
18 Jun 2013 - M. Payer - Add emissions for offline aerosol simulation
01 Aug 2013 - R. Yantosca - Now pass Input_Opt via the arg list
01 Aug 2013 - J. Lin
                          - Modified for Rn-Pb-Be simulation
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
26 Sep 2013 - R. Yantosca - Renamed GEOS_57 Cpp switch to GEOS_FP
06 Jun 2014 - R. Yantosca - Fix parallelization error in the HEMCO
                            modifications: Hold TOPMIX, TEMPBL private
06 Jun 2014 - R. Yantosca - Wrap some debug printout in #if defined(DEBUG)
25 Jun 2014 - R. Yantosca - Now get N_MEMBERS from input_mod.F
16 Oct 2014 - C. Keller
                          - Bug fix: now add deposition rates instead of
                            overwriting them.
26 Feb 2015 - E. Lundgren - Replace GET_PEDGE and GET_PCENTER with
                            State_Met%PEDGE and State_Met%PMID.
                            Remove dependency on pressure_mod.
                            Use virtual temperature in hypsometric eqn.
                          - Now exchange PARANOX loss fluxes via HEMCO
10 Apr 2015 - C. Keller
                            diagnostics.
25 Jan 2016 - E. Lundgren - Update netcdf drydep flux diagnostic
22 Apr 2016 - R. Yantosca - Now get Hg info from species database
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
26 May 2016 - E. Lundgren - Replace input_opt TRACER_MW_KG with species
                            database field emMW_g (emitted species molec wt)
                          - Now define species ID's with the Ind_ function
16 Jun 2016 - K. Yu
17 Jun 2016 - R. Yantosca - Only define species ID's on the first call
```

```
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

01 Jul 2016 - R. Yantosca - Now rename species DB object ThisSpc to SpcInfo
13 Jul 2016 - R. Yantosca - Now use NA as loop index for advected species and ND as loop index for drydep species

19 Jul 2016 - R. Yantosca - Now bracket tendency calls with #ifdef USE_TEND

27 Jul 2016 - R. Yantosca - Bug fix: set nDrydep=0 if drydep is turned off
04 Aug 2016 - M. Yannetti - Replace TCVV with species db MW and phys constant
08 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code
```

5.3.9 do_pbl_mix_2

Subroutine DO_PBL_MIX_2 is the driver routine for planetary boundary layer mixing. The PBL layer height and related quantities are always computed. Mixing of tracers underneath the PBL top is toggled by the DO_TURBDAY switch.

INTERFACE:

```
SUBROUTINE DO_PBL_MIX_2( am_I_Root, DO_VDIFF, Input_Opt, & State_Met, State_Chm, RC )
```

USES:

```
USE DAO_MOD, ONLY : AIRQNT USE ERROR_MOD, ONLY : DEBUG_MSG
```

USE ErrCode_Mod

USE Input_Opt_Mod, ONLY : OptInput
USE PBL_MIX_MOD, ONLY : INIT_PBL_MIX

USE PBL_MIX_MOD, ONLY : COMPUTE_PBL_HEIGHT

USE State_Chm_Mod, ONLY : ChmState USE State_Met_Mod, ONLY : MetState

USE TIME_MOD, ONLY : ITS_TIME_FOR_EMIS

IMPLICIT NONE

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

LOGICAL, INTENT(IN) :: DO_VDIFF ! Switch which turns on PBL
```

! mixing of tracers
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met   ! Meteorology State object
TYPE(ChmState), INTENT(INOUT) :: State_Chm   ! Chemistry State object
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

```
11 Feb 2005 - R. Yantosca - Initial version
21 Dec 2010 - R. Yantosca - Now only call SETEMIS for fullchem simulations
22 Dec 2010 - R. Yantosca - Bug fix: print debug output only if LPRT=T
05 Mar 2013 - R. Yantosca - Add am_I_root, Input_Opt, RC arguments
05 Mar 2013 - R. Yantosca - Now call SETEMIS with am_I_Root, Input_Opt, RC
05 Mar 2013 - R. Yantosca - Now use Input_Opt%ITS_A_FULLCHEM_SIM
25 Mar 2013 - M. Payer - Now pass State_Chm object via the arg list
01 Aug 2013 - R. Yantosca - Now pass the Input_Opt object to VDIFFDR
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
22 Aug 2014 - R. Yantosca - Renamed DO_TURBDAY to DO_VDIFF for clarity
16 Nov 2015 - E. Lundgren - Update air quantities after VDIFFDR call
since specific humidity is updated
13 Jul 2016 - R. Yantosca - Remove STT, we can point to State_Chm%Species
in the VDIFFDR routine directly
```

5.4 Fortran: Module Interface vdiff_pre_mod.F90

Module VDIFF_PRE_MOD contains variables used in VDIFF_MOD.

INTERFACE:

MODULE VDIFF_PRE_MOD

USES:

IMPLICIT NONE

PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: Init_VDIFF_PRE
PUBLIC :: Cleanup_VDIFF_PRE
PUBLIC :: Set_VDIFF_VALUES

PUBLIC DATA MEMBERS:

LOGICAL, PUBLIC :: LPRT ! Passes LPRT to vdiff_mod
LOGICAL, PUBLIC :: LTURB ! Passes LTURB to vdiff_mod
INTEGER, PUBLIC :: PCNST ! Passes N_TRACERS to vdiff_mod

```
01 Jun 2009 - C. Carouge & J. Lin - Initial version
07 Oct 2009 - R. Yantosca - Added CVS Id tag
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
24 Jun 2014 - R. Yantosca - Now add PCNST as a module variable
```

24 Jun 2014 - R. Yantosca - Add routine SET_VDIFF_VALUES, since we need to pass N_TRACERS, LPRT, LTURB to vdiff_mod.F90 now that logical_mod.F, tracer_mod.F are gone.

24 Jun 2014 - R. Yantosca - Renamed to vdiff_pre_mod.F90

24 Nov 2014 - M. Yannetti - Added PRECISION_MOD

30 Jun 2016 - M. Sulprizio- Remove NCS, NDRYDEP, ND15, ND44, IIPAR, JJPAR since they are not used anymore

5.4.1 init_vdiff_pre

Subroutine INIT_VDIFF_PRE allocates all module arrays.

INTERFACE:

```
SUBROUTINE Init_VDIFF_PRE( am_I_Root, RC )
```

USES:

USE ErrCode_Mod

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC     ! Success or failure?
```

REMARKS:

Need to add error-checking on the allocation statements, so that we exit the code upon error.

REVISION HISTORY:

5.4.2 cleanup_vdiff_pre

Subroutine CLEANUP_VDIFF_PRE deallocates all module arrays.

INTERFACE:

```
SUBROUTINE Cleanup_VDIFF_PRE( am_I_Root, RC )
```

USES:

USE ErrCode_Mod

IMPLICIT NONE

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC     ! Success or failure?
```

REMARKS:

REVISION HISTORY:

```
19 Nov 2012 - R. Yantosca - Initial version
```

5.4.3 set_vdiff_values

Subroutine SET_VDIFF_VALUES initializes the PCNST value, which is the number of advected species. This is needed in vdiff_mod.F90.

INTERFACE:

```
SUBROUTINE Set_VDIFF_VALUES( am_I_Root, Input_Opt, State_Chm, RC )
```

USES:

```
USE ErrCode_Mod
```

USE Input_Opt_Mod, ONLY : OptInput USE State_Chm_Mod, ONLY : ChmState

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REMARKS:

This routine has to be called after routine READ_INPUT_FILE.

```
24 Jun 2014 - R. Yantosca - Initial version
```

6 Dry deposition modules

These modules contain routines to remove species from the atmosphere by dry deposition. Related modules compute the land cover that is used by the dry deposition routines.

6.1 Fortran: Module Interface drydep_mod.F

Module DRYDEP_MOD contains variables and routines for the GEOS-Chem dry deposition scheme.

INTERFACE:

MODULE DRYDEP_MOD

USES:

```
USE CMN_SIZE_MOD
                                                 ! Size parameters
      USE CMN_DIAG_MOD
                                                 ! Diag counters & flags
      USE DAO_MOD
                                                 ! Met field subroutines
#if defined( BPCH_DIAG )
      USE DIAG_MOD,
                          ONLY: AD44
                                                 ! Diagnostic arrays
#endif
      USE ERROR_MOD
                                                 ! Error handling routines
      USE GC_GRID_MOD,
                                                 ! Grid box surface areas [cm2]
                          ONLY : GET_AREA_CM2
      USE PBL_MIX_MOD
                                                 ! Boundary layer quantities
      USE TIME_MOD,
                          ONLY : GET_TS_CHEM
                                                 ! Chemistry timestep
      defined( TOMAS )
#if
      USE TOMAS_MOD
                                                 ! For TOMAS microphysics
#endif
      USE PhysConstants
                                                 ! Physical constants
      USE PRECISION_MOD
                                                 ! For GEOS-Chem Precision (fp)
      IMPLICIT NONE
      PRIVATE
```

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: CLEANUP_DRYDEP
PUBLIC :: DO_DRYDEP
PUBLIC :: INIT_DRYDEP
PUBLIC :: INIT_WEIGHTSS

PUBLIC DATA MEMBERS:

PUBLIC :: DEPNAME
PUBLIC :: DEPSAV
PUBLIC :: NUMDEP
PUBLIC :: NTRAIND

PUBLIC :: IDEP, IRGSS, IRAC, IRCLS

PUBLIC :: IRGSO, IRLU, IRI, IRCLO, DRYCOEFF

PUBLIC :: NDVZIND ! MSL -> For MPI broadcasting in GCHP

REMARKS:

References:

- (1) Baldocchi, D.D., B.B. Hicks, and P. Camara, "A canopy stomatal resistance model for gaseous deposition to vegetated surfaces", Atmos. Environ. 21, 91-101, 1987.
- (2) Brutsaert, W., "Evaporation into the Atmosphere", Reidel, 1982.
- (3) Businger, J.A., et al., "Flux-profile relationships in the atmospheric surface layer", J. Atmos. Sci., 28, 181-189, 1971.
- (4) Dwight, H.B., "Tables of integrals and other mathematical data", MacMillan, 1957.
- (5) Guenther, A., and 15 others, A global model of natural volatile organic compound emissions, J. Geophys. Res., 100, 8873-8892, 1995.
- (6) Hicks, B.B., and P.S. Liss, "Transfer of SO2 and other reactive gases across the air-sea interface", Tellus, 28, 348-354, 1976.
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- (13) Wesely, M.L, "Improved parameterizations for surface resistance to gaseous dry deposition in regional-scale numerical models", Environmental Protection Agency Report EPA/600/3-88/025, Research Triangle Park (NC), 1988.
- (14) Wesely, M. L., Parameterization of surface resistance to gaseous dry deposition in regional-scale numerical models. Atmos. Environ., 23 1293-1304, 1989.
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- (16) Karl, T., Harley, P., Emmons, L., Thornton, B., Guenther, A., Basu, C., Turnipseed, A., and Jardine, K.: Efficient Atmospheric Cleansing of Oxidized Organic Trace Gases by Vegetation, Science, 330, 816-819, 10.1126/science.1192534, 2010.

REVISION HISTORY:

27 Jan 2003 - R. Yantosca - Moved standalone routines into this module

- (1) Bug fix: Do not assume NO2 is the 2nd drydep species. This causes a mis-indexing for CANOPYNOX. Now archive ND44 diagnostic in kg for Radon runs in routine DRYFLXRnPbBe; convert to kg/s in diag3.f (bmy, 1/27/03)
- (2) Now references "grid_mod.f" and the new "time_mod.f". Renamed DRYDEP routine to DO_DRYDEP for consistency w/ other drivers called from the MAIN program. (bmy, 2/11/03)
- (3) Added error check in DRYFLX for SMVGEAR II (bmy, 4/28/03)
- (4) Added drydep of N2O5. Now added PBLFRAC array, which is the fraction of each level below the PBL top. Also now compute drydep throughout the entire PBL, in order to prevent short-lived species such as HNO3 from being depleted in the shallow GEOS-3 surface layer. (rjp, bmy, 7/21/03)
- (5) Bug fix for GEOS-4 in DRYFLXRnPbBe (bmy, 12/2/03)
- (6) Now made CFRAC, RADIAT local variables in DO_DRYDEP (bmy, 12/9/03)
- (7) Now enclose AD44 in !\$OMP CRITICAL block for drydep flux (bmy, 3/24/04)
- (8) Now handle extra carbon & dust tracers (rjp, tdf, bmy, 4/1/04)
- (9) Added routines AERO_SFCRS1, AERO_SFCRSII. Increased MAXDEP to 25. Now handles extra carbon & dust tracers. (rjp, tdf, bmy, 4/1/04)
- (10) Increased MAXDEP to 26. Added A_RADI and A_DEN module variables.

 Other modifications for size-resolved drydep. (rjp, bec, bmy, 4/20/04)
- (11) Increased MAXDEP to 35 and handle extra SOA tracers (rjp, bmy, 7/13/04)
- (12) Now references "logical_mod.f", "directory_mod.f", and "tracer_mod.f" (bmy, 7/20/04)
- (13) Add Hg2, HgP as drydep tracers (eck, bmy, 12/8/04)
- (14) Updated for AS, AHS, LET, NH4aq, SO4aq (cas, bmy, 1/6/05)
- (15) Now references "pbl_mix_mod.f". Removed PBLFRAC array. (bmy, 2/22/05)
- (16) Now include SO4s, NITs tracers. Now accounts for hygroscopic growth of seasalt aerosols when computing aerodynamic resistances. (bec, bmy, 4/13/05)
- (17) Now modified for GEOS-5 and GCAP met fields (bmy, 5/25/05)
- (18) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (19) Now change Reynold's # criterion from 1 to 0.1 in DEPVEL. Also change Henry's law constant for Hg2. Also increase MAXDEP from 35 to 37. (eck, djj, bmy, 2/1/06)
- (20) Bug fix in INIT_DRYDEP (bmy, 4/17/06)
- (21) Now bundle function DIFFG into "drydep_mod.f". Also updated for SOG4 and SOA4 tracers. Bug fix in INIT_DRYDEP. (dkh, bmy, 5/24/06)
- (22) Fix typo in INIT_DRYDEP (dkh, bmy, 6/23/06)
- (23) Add H2 and HD as drydep tracers. Added subroutine DRYFLXH2HD for H2HD offline sim (phs, 9/18/07)
- (24) Extra error check for small RH in AERO_SFCRII (phs, 6/11/08)
- (25) Added 15 more dry deposition species (tmf, 7/31/08)
- (26) Modify dry depostion to follow the non-local PBL scheme. (lin, ccc, 5/29/09)
- (27) Minor bug fix in mol wts for ALPH, LIMO (bmy, 10/19/09)
- (28) Change MAXDEP from 50 to 81 (win, 7/14/09)
- (28a) modified to use Zhang 2001 for all non-size resolved aerosols (hotp)

- (29) Add aromatics SOA (dkh)
- (30) Add new species. Some tracers give 2 deposition species: ISOPN-> ISOPNB and ISOPND. (fp)
- (31) Updates for mercury simulation (ccc, 5/17/10)
- (32) Add POPs (eck, 9/20/10)
- (33) Increase MAXDEP to 51 for dicarbonyls simulation. (ccc, 10/8/10)
- 01 Aug 2011 J. Fisher Set aerosol dry deposition velocity to 0.03 cm/s over snow and ice based on Nilsson & Rannik, 2001
- 21 Dec 2011 M. Payer Updates for sea salt (jaegle 5/11/11)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 10 Jan 2012 M. Payer Update to use local surface pressure
- 01 Mar 2012 R. Yantosca Now reference new grid_mod.F90
- 26 Mar 2012 R. Yantosca Now reference CMN_SIZE_MOD at the top of module
- 26 Mar 2012 R. Yantosca Replace NNTYPE, NNPOLY, NNVEGTYPE w/ the values NTYPE, NPOLY, NVEGTYPE from CMN_SIZE
- 26 Mar 2012 R. Yantosca Now retire MODIN and RDDRYCF; read drydep inputs from a netCDF file w/ routine READ_DRYDEP_INPUTS
- 26 Mar 2012 R. Yantosca Reorganize module USE statements for clarity
- 09 Apr 2012 R. Yantosca Now replace IJREG, IJLAND, IJUSE, XYLAI arrays with IREG, ILAND, IUSE, XLAI.
- 31 Jul 2012 R. Yantosca Modifications for grid-independence
- 11 Dec 2012 M. Long Now call READ_DRYDEP_INPUTS from INIT_DRYDEP
- 11 Dec 2012 R. Yantosca Now call INIT_WEIGHTSS from INIT_DRYDEP
- 13 Dec 2012 R. Yantosca Remove reference to obsolete CMN_DEP_mod.F
- 26 Feb 2013 R. Yantosca Now use Input_Opt fields where possible
- 13 Aug 2013 M. Sulprizio- Add modifications for updated SOA and SOA + semivolatile POA simulations (H. Pye)
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 12 Sep 2013 M. Sulprizio- Add modifications for acid uptake on dust aerosols (T.D. Fairlie)
- 29 Jan 2014 R. Yantosca Now set MAXDEP=105 for all simulations. For TOMAS we had MAXDEP=100; this is close enough.
- 23 Jun 2014 R. Yantosca Removed references to logical_mod.F
- 25 Jul 2014 R. Yantosca Removed reference to commsoil_mod.F
- 12 Nov 2014 M. Yannetti Added PRECISION_MOD, changed REAL*8 to REAL(fp)
- 26 Feb 2015 E. Lundgren Replace GET_PEDGE with State_Met%PEDGE
- 03 Mar 2015 C. Keller Disabled DRYFLX. Now done in mixing_mod.F90
- 15 Jun 2015 R. Yantosca Disabled DRYFLXRnPbBe, also done in mixing_mod
- 01 Oct 2015 R. Yantosca Remove DVZ_MINVAL function
- 01 Oct 2015 R. Yantosca Added PRIVATE flag ID_ACET
- 06 Jan 2016 E. Lundgren Use global physical parameters
- 13 Jul 2016 R. Yantosca Remove DRYHgO, DRYHgP, DRYHgP ID flags
- 13 Jul 2016 R. Yantosca Also make NDVZIND a local variable for now
- 29 Nov 2016 R. Yantosca grid_mod.F90 is now gc_grid_mod.F90

6.1.1 do_drydep

Subroutine DO_DRYDEP is the driver for the GEOS-CHEM dry deposition scheme. DO_DRYDEP calls DEPVEL to compute deposition velocities [m/s], which are then converted to [cm/s]. Drydep frequencies are also computed. (lwh, gmg, djj, 1989, 1994; bmy, 2/11/03, 5/25/05)

INTERFACE:

```
SUBROUTINE DO_DRYDEP( am_I_Root, Input_Opt, State_Met, State_Chm, RC )
```

USES:

```
USE ErrCode_Mod

USE HCO_ERROR_MOD

USE HCO_INTERFACE_MOD, ONLY : HcoState

USE HCO_DIAGN_MOD, ONLY : Diagn_Update

USE Input_Opt_Mod, ONLY : OptInput

USE Species_Mod, ONLY : Species

USE State_Chm_Mod, ONLY : ChmState

USE State_Met_Mod, ONLY : MetState

USE UnitConv_Mod
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REMARKS:

NOTE: Modeled aerosol dry deposition velocities over snow and ice surfaces in the Arctic are much higher than estimated from measured values (e.g., Ibrahim et al. [1983]; Duan et al. [1988]; Nilsson and Rannik [2001]). We will impose a dry deposition velocity of 0.03 cm/s for all aerosols over snow and ice surfaces. (Jenny Fisher, 01 Aug 2011) References (see full citations above):

```
(1 ) Wesely, M. L., 1989
```

(2) Jacob, D.J., and S.C. Wofsy, 1990

REVISION HISTORY:

(1) Remove SUNCOS, USTAR, AZO, OBK from the arg list; now reference these as well as AD and T from "dao_mod.f". Cleaned up code and updated

- comments. Now only order tracer numbers into NTRAIND on the first call. Now force double-precision with "D" exponents. Now also reference IDTNOX, IDTOX, etc. from "tracerid_mod.f". Bundled into "drydep_mod.f" (bmy, 11/19/02)
- (2) Now make sure that the PBL depth (THIK) is greater than or equal to the thickness of the first layer. Now initialize PBLFRAC array on each call. (rjp, bmy, 7/21/03)
- (3) Now declare CFRAC, RADIAT, AZO, USTAR as local variables, which are returned by METERO. CFRAC and RADIAT have also been deleted from "CMN_DEP". (bmy, 12/9/03)
- (4) Now use explicit formula for IJLOOP to allow parallelization.

 Also reference LPRT from "logical_mod.f" (bmy, 7/20/04)
- (5) Now use routines from "pbl_mix_mod.f" to get PBL quantities, instead of re-computing them here. Removed PBLFRAC array. Removed reference to "pressure_mod.f". Removed reference to header file CMN. Parallelize DO-loops. (bmy, 2/22/05)
- (6) Now define RHB as a local array, which is defined in METERO and then passed to DEPVEL. (bec, bmy, 4/13/05)
- (7) Now dimension AZO for GEOS or GCAP met fields. Remove obsolete variables. (swu, bmy, 5/25/05)
- (8) Remove reference to TRACERID_MOD, it's not needed (bmy, 10/3/05)
- 01 Aug 2011 J. Fisher Set aerosol dry deposition velocity to 0.03 cm/s over snow and ice based on Nilsson & Rannik, 2001
- 15 Aug 2011 R. Yantosca Now reference IDTxxx flags from tracerid_mod.f
- 07 Oct 2011 R. Yantosca Rename SUNCOS30 to SUNCOS_MID, which is the cos(SZA) at the midpt of the chemistry timestep
- 22 Dec 2011 M. Payer Added ProTeX headers
- 10 Jan 2012 M. Payer Added local surface pressure
- 26 Mar 2012 R. Yantosca Now read drydep inputs from a netCDF file via routine READ_DRYDEP_INPUTS
- 26 Mar 2012 R. Yantosca Remove calls to obsolete MODIN, RDDRYCF routines
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 28 Nov 2012 R. Yantosca Now make SUNCOS_MID a local array of size MAXIJ, populated from State_Met%SUNCOSmid
- 11 Dec 2012 R. Yantosca Now do not call READ_DRYDEP_INPUTS and INIT_WEIGHTSS when using the ESMF environment
- 11 Dec 2012 R. Yantosca Remove FIRST variable, as we now read inputs from disk in routine INIT_DRYDEP
- 12 Dec 2012 R. Yantosca Now pass State_Met to DEPVEL
- 26 Feb 2013 R. Yantosca Now use Input_Opt fields where possible. This facilitates connection to the GEOS-5 GCM.
- 31 May 2013 R. Yantosca Now pass Input_Opt & State_Chm to DEPVEL
- 15 Jan 2015 R. Yantosca Add new netCDF diagnostics structure
- 12 Aug 2015 E. Lundgren Tracer units are now [kg/kg]
- 01 Oct 2015 R. Yantosca Remove DVZ_MINVAL; now use species database

```
to set the minimum drydep velocity for aerosols

01 Oct 2015 - R. Yantosca - Now use species database to set Vd for aerosols over snow/ice; combine with the prior update to enforce a minimum Vd for aerosol species

01 Oct 2015 - R. Yantosca - Remove references to tracerid_mod.F (except for TOMAS for now)

21 Jan 2016 - E. Lundgren - Update netcdf diagnostics for drydep trcr names
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
17 May 2016 - M. Sulprizio- Remove IJLOOP and change dimension of arrays from (MAXIJ) to (IIPAR, JJPAR)

18 Jul 2016 - M. Sulprizio- Remove special handling for ISOPN and MVKN for ND44 netCDF diagnostic. Family tracers have been eliminated.
```

6.1.2 metero

Subroutine METERO calculates meteorological constants needed for the dry deposition velocity module. (lwh, gmg, djj, 1989, 1994; bmy, 10/3/05)

INTERFACE:

```
SUBROUTINE METERO( State_Met, CZ1, TCO, OBK, CFRAC, & RADIAT, AZO, USTR, ZH, LSNOW, & RHB, PRESSU, W10, SUNCOS_MID )
```

USES:

USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

OUTPUT PARAMETERS:

```
LOGICAL, INTENT(OUT) :: LSNOW (IIPAR, JJPAR)
                                               ! Flag for denoting snow/ice
REAL(f8), INTENT(OUT) :: CZ1
                                               ! Midpt ht of 1st model lev
                                (IIPAR, JJPAR)
                                               ! [m]
REAL(f8), INTENT(OUT) :: TCO
                                (IIPAR, JJPAR)
                                               ! Grid box sfc temp [K]
                                               ! Monin-Obhukov length [m]
REAL(f8), INTENT(OUT) :: OBK
                                (IIPAR, JJPAR)
REAL(f8), INTENT(OUT) :: CFRAC (IIPAR, JJPAR)
                                               ! Column cloud fraction
                                               ! [unitless]
REAL(f8), INTENT(OUT) :: RADIAT(IIPAR, JJPAR)
                                               ! Solar radiation @ ground
                                               ! [W/m2]
REAL(f8), INTENT(OUT) :: RHB
                                               ! Rel humidity at sfc
                                (IIPAR, JJPAR)
                                               ! [unitless]
REAL(f8), INTENT(OUT) :: USTR (IIPAR, JJPAR)
                                               ! Friction velocity [m/s]
REAL(f8), INTENT(OUT) :: ZH
                                (IIPAR, JJPAR)
                                               ! PBL height [m]
REAL(f8), INTENT(OUT) :: PRESSU(IIPAR, JJPAR)
                                               ! Local surface press [Pa]
```

REAL(f8), INTENT(OUT) :: W10 (IIPAR, JJPAR) ! 10 meter windspeed [m/s] REAL(f8), INTENT(OUT) :: SUNCOS_MID(IIPAR, JJPAR) ! COS(SZA) @ midpt of ! current chem timestep

! Dimension AZO for GCAP or GEOS met fields (swu, bmy, 5/25/05) #if defined(GCAP)

REAL(f8), INTENT(OUT) :: AZO(NTYPE) ! Roughness heights, by landtype #else

 $\mathtt{REAL}(\mathtt{f8})$, $\mathtt{INTENT}(\mathtt{OUT}) :: \mathtt{AZO}(\mathtt{IIPAR},\mathtt{JJPAR}) \; ! \; \mathtt{Roughness} \; \mathtt{heights}$, by $\mathtt{grid} \; \mathtt{box} \; \mathtt{\#endif}$

REMARKS:

References (see full citations above):

- (1) Wesely, M. L., 1989.
- (2) Jacob, D.J., and S.C. Wofsy, 1990

- (1) Now reference GET_PEDGE from "pressure_mod.f". Now reference T from "dao_mod.f". Removed obsolete code & comments, and added new documentation header. Now force double precision with "D" exponents. Now compute OBK here as well. Bundled into F90 module "drydep_mod.f" (bmy, 11/20/02)
- (2) Now reference CLDFRC, RADSWG, ZO, USTAR from "dao_mod.f". Also now pass CFRAC, RADIAT, AZO, USTR back to the calling routine via the arg list. (bmy, 12/9/03)
- (3) Now use explicit formula for IJLOOP to allow parallelization (bmy, 7/20/04)
- (4) Now compute ZH and LSNOW here instead of w/in DO_DRYDEP. Parallelize DO-loops. Now use BXHEIGHT from "dao_mod.f" instead of computing the thickness of the 1st level here. Remove reference to "pressure_mod.f". Remove reference to T from "dao_mod.f". Now reference ALBD from "dao_mod.f" (bmy, 2/22/05)
- (5) Now references RH from "dao_mod.f". Now passes relative humidity from the surface layer back via RHB argument. (bec, bmy, 4/13/05)
- (6) Now call GET_OBK from "dao_mod.f" to get the M-O length for both GEOS or GCAP met fields. Remove local computation of M-O length here. Also now dimension AZO appropriately for GCAP or GEOS met fields. Remove obsolete variables. (swu, bmy, 5/25/05)
- (7) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (8) Move XLTMMP function to module MEGANUT_MOD. (ccc, 11/20/09)
- (9) Add sea level pressure and 10m windspeed as arguments (jaegle 5/11/11)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 10 Jan 2012 M. Payer Added local surface pressure
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object

```
28 Nov 2012 - R. Yantosca - Add SUNCOS_MID to the argument list and populate that with State_Met%SUNCOSmid
21 Oct 2013 - R. Yantosca - Bug fix: need to hold SP private in OMP loop
25 Jul 2014 - R. Yantosca - Now remove reference to function SFCWINDSQR
17 May 2016 - M. Sulprizio- Remove IJLOOP and change dimension of output arrays from (MAXIJ) to (IIPAR, JJPAR)
```

6.1.3 depvel

Subroutine DEPVEL computes the dry deposition velocities using a resistance-in-series model.

INTERFACE:

SUBROUTINE	DEPVEL(<pre>am_I_Root,</pre>	<pre>Input_Opt,</pre>	State_Met,	State_Chm,	
&		RADIAT,	TEMP,	SUNCOS,		
&		FO,	HSTAR,	XMW,	AIROSOL,	
&		USTAR,	CZ1,	OBK,	CFRAC,	
&		ZH,	LSNOW,	DVEL,	ZO,	
&		RHB,	PRESSU,	W10,	RC)

USES:

```
USE Drydep_Toolbox_Mod, ONLY : BioFit
USE ErrCode_Mod
USE ERROR_MOD
USE Input_Opt_Mod, ONLY : OptInput
USE Species_Mod, ONLY : Species
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

```
INTENT(IN) :: am_I_Root
                                              ! Are we on the root CPU?
TYPE(OptInput), INTENT(IN) :: Input_Opt
                                              ! Input Options object
TYPE(MetState), INTENT(IN) :: State_Met
                                              ! Meteorology state object
REAL(f8), INTENT(IN) :: RADIAT (IIPAR, JJPAR) ! Solar radiation [W/m2]
REAL(f8), INTENT(IN) :: TEMP
                               (IIPAR, JJPAR) ! Temperature [K]
REAL(f8), INTENT(IN) :: SUNCOS (IIPAR, JJPAR) ! Cosine of solar zenith angle
LOGICAL, INTENT(IN) :: AIROSOL(NUMDEP)
                                              ! =T denotes aerosol species
REAL(f8), INTENT(IN) :: FO
                                              ! React. factor for oxidation
                               (NUMDEP)
                                              ! of biological substances
                                              ! Henry's law constant
REAL(f8), INTENT(IN) :: HSTAR (NUMDEP)
REAL(f8), INTENT(IN) :: XMW
                               (NUMDEP)
                                              ! Molecular weight [kg/mol]
                               (IIPAR, JJPAR) ! Friction velocity [m/s]
REAL(f8), INTENT(IN) :: USTAR
REAL(f8), INTENT(IN) :: CZ1
                               (IIPAR, JJPAR) ! Alt @ which Vd is computed
                                              ! [m]
```

```
REAL(f8), INTENT(IN) :: OBK
                                     (IIPAR, JJPAR) ! Monin-Obhukov length [m]
      REAL(f8), INTENT(IN) :: CFRAC (IIPAR, JJPAR) ! Surface cloud fraction
      REAL(f8), INTENT(IN) :: ZH
                                     (IIPAR, JJPAR) ! Roughness height [m]
      REAL(f8), INTENT(IN) :: RHB
                                     (IIPAR, JJPAR) ! Relative humidity [%]
      REAL(f8), INTENT(IN) :: PRESSU (IIPAR, JJPAR) ! Surface pressure [hPa]
      REAL(f8), INTENT(IN) :: W10
                                     (IIPAR, JJPAR) ! Wind speed @ 10m altitude
                                                   ! [m/s]
INPUT/OUTPUT PARAMETERS:
       TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
OUTPUT PARAMETERS:
       INTEGER, INTENT(OUT) :: RC
                                                   ! Success or failure?
       REAL(f8), INTENT(OUT) :: DVEL(IIPAR, JJPAR, NUMDEP) ! Drydep velocity [m/s]
REMARKS:
    Need as landtype input for each grid square (I,J); see CMN_DEP_mod.F
       IREG(I,J)
                      - # of landtypes in grid square
       ILAND(I,J,LDT) - Land type ID for element LDT =1, IREG(I,J)
                         (could be from any source - mapped to deposition
                         surface ID in input unit 65)
       IJUSE(I,J,LDT) - Fraction ((per mil) of gridbox area occupied by
                        land type element LDT
   Need as leaf area index; see CMN_DEP_mod.F
      XLAI(I,J,LDT) - Leaf Area Index of land type element LDT
   Need as meteorological input for each grid square(I,J) (passed):
      RADIAT(I,J)
                     - Solar radiation in W m-2
      TEMP(I,J)
                     - Surface air temperature in K
       SUNCOS(I,J)
                     - Cosine of solar zenith angle
      LSNOW(I,J)
                     - Logical for snow and sea ice
      RHB(I,J)
                     - Relative humidity at the surface
      PRESSU(I,J)
                     - Local surface pressure
      W10(I,J)
                     - 10m wind speed
   Need as input for each species K (passed):
                     - reactivity factor for oxidation of biological substances
      FO(K)
                     - Henry's Law constant
      HSTAR(K)
                     - Molecular weight (kg/mole) of species K
      XMW(K)
                       (used to calculate molecular diffusivities)
       AIROSOL(K)
                     - LOGICAL flag (T = aerosol species;
                                     F = gas-phase species)
   Also need to call the following subroutines to read drydep input data:
      READ_DRYDEP_INPUTS
                            - (in this module) Reads in Olson land type
                              indices, dry deposition land type indices,
```

default roughness heights, and polynomial coefficients. (This supersedes MODIN, RDDRYCF) COMPUTE_OLSON_LANDMAP - (in olson_landmap_mod.F90). Reads in the Olson land types at native resolution and re-bins them on-the-fly to the GEOS-Chem grid resolution. (This supersedes RDLAND) - reads Leaf Area Indices from files "lai**.global" "rdlai.f" Some variables used in the subroutine (passed): LRGERA(I,J) T -> stable atmosphere; a high aerodynamic resistance (RA=1.E4 m s-1) is imposed; else RA is calculated - Friction velocity (m s-1) USTAR(I,J)CZ1(I,J)- Altitude (m) at which deposition velocity is computed OBK(I,J)- Monin-Obukhov length (m): set to 1.E5 m under neutral conditions - Fractional cloud cover CFRAC(I,J)- Mixing depth (m) ZH(I,J)Some variables used in the subroutine: MAXDEP - the maximum number of species for which the dry deposition calculation is done ZO(LDT) - Roughness height (m) for specific surface type indexed RSURFC(K,LDT) - Bulk surface resistance (s m-1) for species K to surface LDT C1X(K) - Total resistance to deposition (s m-1) for species K

Returned:

DVEL(I,J,K) - Deposition velocity (m s-1) of species K

References:

Baldocchi, D.D., B.B. Hicks, and P. Camara, A canopy stomatal resistance model for gaseous deposition to vegetated surfaces, Atmos. Environ. 21, 91-101, 1987.

Brutsaert, W., Evaporation into the Atmosphere, Reidel, 1982.

Businger, J.A., et al., Flux-profile relationships in the atmospheric surface layer, J. Atmos. Sci., 28, 181-189, 1971.

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Guenther, A., and 15 others, A global model of natural volatile organic compound emissions, J. Geophys. Res., 100, 8873-8892, 1995.

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** Version 3.7 4/20/04 -- Now also do drydep of SEASALT aerosol tracers ** Version 3.8 4/13/05 -- Accounts for hygroscopic growth of SEASALT

** Version 3.9.1 11/17/05 -- change Reynolds # criterion from 1 to 0.1

of 1000 hPa

surfaces

09 Apr 2012 - R. Yantosca - Remove reference to CMN_VEL_mod.F

13 Dec 2012 - R. Yantosca - Now get XLAI from State_Met

** Version 3.9

11 May 2011 - L. Jaegle

22 Dec 2011 - M. Payer

10 Jan 2012 - M. Payer

an input argument.

- Added ProTeX headers

09 Apr 2012 - R. Yantosca - Remove IJREG, IJLAND, IJUSE, XYLAI arrays and

09 Apr 2012 - R. Yantosca - Now use INTENT(IN), INTENT(OUT) for arguments 30 Jul 2012 - R. Yantosca - Now accept am_I_Root as an argument when

12 Dec 2012 - R. Yantosca - Now get ILAND, IUSE, IREG from State_Met

aerosol tracers. DUST aerosol tracers do not grow hygroscopically. Added RHB as

- Updated to use actual Sea level pressure instead

- Modified to used Slinn & Slinn (1980) over Ocean

5/25/05 -- Now restore GISS-specific code for GCAP model

- Updated to use local surface pressure

replace w/ IREG, ILAND, IUSE, XLAI

running with the traditional driver main.F

```
06 Mar 2013 - H. Amos
                          - Merge C. Friedman's PAH code
 31 May 2013 - R. Yantosca - Now pass State_Chm, for TOMAS
 14 Jun 2013 - R. Yantosca - Now use Input_Opt%ITS_A_POPS_SIM
 29 Aug 2013 - R. Yantosca - Bug fix: Skip to the next species if unless
                            HSTAR>O and XMW>O, or AIROSOL=t. This avoids
                            a floating-point invalid condition.
 12 Sep 2013 - M. Sulprizio- Add modifications for acid uptake on dust
                            aerosols (T.D. Fairlie)
 28 Jan 2014 - R. Yantosca - For TOMAS, don't hold A_RADI and A_DEN PRIVATE
 19 May 2014 - C. Keller
                          - Now call BIOFIT from drydep_toolbox_mod.F\
 12 Aug 2015 - E. Lundgren - Now accept am_I_Root and RC as input args
 12 Aug 2015 - E. Lundgren - Now pass am_I_Root and RC to AERO_DIADEN
                            to enable unit conversion in that routine
 22 Sep 2015 - R. Yantosca - Now use NUMDEP instead of MAXDEP for arrays
 15 Mar 2016 - C. Keller
                          - Prevent very small numbers of CORR1 and ZOOBK
 29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
 17 May 2016 - M. Sulprizio- Remove IJLOOP and change dimension of arrays
                            from (MAXIJ) to (IIPAR, JJPAR); Also remove NPTS
                            input argument
**************************
  Changes from Version 3.2 to Version 3.3:
  * We now suppress dry deposition over aerodynamically smooth
                                                                 ***
    surfaces. The previous algorithm yielded negative numbers
    when u* was very small (due to the logarithm going negative).
    See the comments below for more information.
                                                                 ***
  * Now eliminate obsolete variables ZLMO and SIH from the code.
                                                                 ***
  * Obsolete comments have been updated or removed.
                                                                 ***
*****************************
  Changes from version 3.1 to version 3.2:
                                                                 ***
  * In unstable atmospheres with |ZLMO| < ZO, as can happen
                                                                 ***
   occasionally under very low wind conditions with tall canopies, ***
   application of Monin-Obukhov similarity yields negative values
   for RA. This was a problem in version 3.1. In fact,
                                                                 ***
   Monin-Obukhov similarity does not apply under such conditions,
                                                                 ***
   so we now set RA to zero and let the boundary
   resistance RB define the overall aerodynamic resistance.
                                                          Since ***
   RB varies inversely with U* it will impose a large aerodynamic
   resistance under very low wind conditions.
  * The range of applicability of stability correction functions
   to Monin-Obukhov similarity has been extended to
   -2.5 < z/zMO < 1.5, based on Figure 2 of Businger et al. [1971].***
   The range used to be -1 < z/zMO < 1 in version 3.1.
*****************************
```

6.1.4 diffg

Subroutine DIFFG calculates the molecular diffusivity [m2/s] in air for a gas X of molecular weight XM [kg] at temperature TK [K] and pressure PRESS [Pa]. (bmy, 5/16/06)

INTERFACE:

```
FUNCTION DIFFG( TK, PRESS, XM ) RESULT( DIFF_G )
```

INPUT PARAMETERS:

```
REAL(f8), INTENT(IN) :: TK ! Temperature [K]
REAL(f8), INTENT(IN) :: PRESS ! Pressure [Pa]
REAL(f8), INTENT(IN) :: XM ! Molecular weight of gas [kg]
```

REMARKS:

We specify the molecular weight of air (XMAIR) and the hard-sphere molecular radii of air (RADAIR) and of the diffusing gas (RADX). The molecular radius of air is given in a Table on p. 479 of Levine [1988]. The Table also gives radii for some other molecules. Rather than requesting the user to supply a molecular radius we specify here a generic value of 2.E-10 m for all molecules, which is good enough in terms of calculating the diffusivity as long as molecule is not too big.

REVISION HISTORY:

```
    (1) Originally was a standalone function; now bundled into drydep_mod.f.
        Also now force REAL(f8) precision with D exponents. Now use F90
        style syntax and updated comments. (bmy, 5/16/06)
    22 Dec 2011 - M. Payer - Added ProTeX headers
    O6 Jan 2016 - E. Lundgren - Now use global physical parameters
```

${\bf 6.1.5} \quad {\bf read_drydep_inputs}$

Subroutine READ_DRYDEP_INPUTS reads inputs for the dry deposition module corresponding to either the Olson 1992 (GEOS-Chem default) or Olson 2001 (planned replacement for Olson 1992) land map.

INTERFACE:

```
SUBROUTINE READ_DRYDEP_INPUTS( am_I_Root, Input_Opt,
                                  DRYCOEFF, IOLSON,
&
                                                        IDEP,
&
                                  IWATER,
                                             NWATER,
                                                        IZO,
                                  IDRYDEP,
&
                                             IRI,
                                                        IRLU,
                                             IRGSS,
                                                        IRGSO,
&
                                  IRAC,
&
                                  IRCLS,
                                             IRCLO,
                                                        IVSMAX,
                                  RC )
&
```

USES:

```
USE ErrCode_Mod
      USE Input_Opt_Mod,
                          ONLY : OptInput
      ! Modules for netCDF read
      USE m_netcdf_io_open
      USE m_netcdf_io_get_dimlen
      USE m_netcdf_io_read
      USE m_netcdf_io_readattr
      USE m_netcdf_io_close
      include "netcdf.inc"
INPUT PARAMETERS:
      LOGICAL,
                    INTENT(IN) :: am_I_Root ! Is this the root CPU?
      TYPE(OptInput), INTENT(IN) :: Input_Opt  ! Input Options object
OUTPUT PARAMETERS:
      I-----
      ! DRYCOEFF : Baldocchi polynomial coeffs
                : Olson land type indices (+1)
      ! IOLSON
      ! IDEP
                : Mapping: Olson ==> drydep ID
      ! IWATER : Olson types that represent water
      ! NWATER : Number of Olson types that are water
      ! IZO
              : Default ZO (routgness height) for each Olson land type
      ! IDRYDEP : Dry deposition land type indices
                      resistance for drydep
      ! IRI : RI
      ! IRLU
              : RLU resistance for drydep
      ! IRAC
              : RAC resistance for drydep
      ! IRGSS : RGSS resistance for drydep
      ! IRGSO : RGSO resistance for drydep
      ! IRCLS : RCLS resistance for drydep
      ! IRCLO : RCLO resistance for drydep
      ! IVSMAX : Max drydep velocity (for aerosol) perr drydep land type
      !-----
      REAL(fp), INTENT(OUT) :: DRYCOEFF(NPOLY
      INTEGER, INTENT(OUT) :: IOLSON (NVEGTYPE )
      INTEGER, INTENT(OUT) :: IDEP
                                   (NVEGTYPE )
      INTEGER, INTENT(OUT) :: IWATER (NVEGTYPE )
      INTEGER, INTENT(OUT) :: NWATER
      INTEGER, INTENT(OUT) :: IZO
                                   (NVEGTYPE )
      INTEGER, INTENT(OUT) :: IDRYDEP (NDRYDTYPE)
      INTEGER, INTENT(OUT) :: IRI
                                   (NDRYDTYPE)
      INTEGER, INTENT(OUT) :: IRLU
                                   (NDRYDTYPE)
      INTEGER, INTENT(OUT) :: IRAC
                                   (NDRYDTYPE)
      INTEGER, INTENT(OUT) :: IRGSS (NDRYDTYPE)
      INTEGER, INTENT(OUT) :: IRGSO
                                   (NDRYDTYPE)
```

(NDRYDTYPE)

INTEGER, INTENT(OUT) :: IRCLS

```
INTEGER, INTENT(OUT) :: IRCLO (NDRYDTYPE)
INTEGER, INTENT(OUT) :: IVSMAX (NDRYDTYPE)
! Success or failure flag
INTEGER, INTENT(OUT) :: RC
```

REMARKS:

Routine READ_DRYDEP_INPUTS replaces routines MODIN (which read the ASCII file "drydep.table") and RDDRYCF (which read the ASCII file "drydep.coef").

READ_DRYDEP_INPUTS was generated from the Perl script "ncCodeRead", which is part of the NcdfUtilities package (with subsequent hand-editing).

Assumes that you have:

- (1) A netCDF library (either v3 or v4) installed on your system
- (2) The NcdfUtilities package (from Bob Yantosca) source code

REVISION HISTORY:

```
26 Mar 2012 - R. Yantosca - Initial version

03 Feb 2014 - M. Sulprizio- Change the internal resistance for coniferous forests to match the internal resistance for deciduous forests when using the Olson 2001 land map (skim, 1/27/14)

18 Dec 2014 - R. Yantosca - Now read DRYCOEFF at REAL*8 precision and then cast to flexible precision

13 Mar 2015 - R. Yantosca - Replace DATA_DIR_1x1 w/ CHEM_INPUTS_DIR
```

6.1.6 aero_sfcrsii

Function AERO_SFCRSII computes the aerodynamic resistance of seasalt aerosol species according to Zhang et al 2001. We account for hygroscopic growth of the seasalt aerosol particles. (rjp, tdf, bec, bmy, 4/1/04, 6/11/08)

INTERFACE:

```
FUNCTION AERO_SFCRSII( K, II, PRESS, TEMP, USTAR, RHB,
& W10, Input_Opt ) RESULT(RS)
```

USES:

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: K ! Drydep species index (range: 1-NUMDEP)
INTEGER, INTENT(IN) :: II ! Surface type index of GEOS-CHEM
REAL(f8), INTENT(IN) :: PRESS ! Pressure [kPa] (1 mb=100 Pa=0.1 kPa)
REAL(f8), INTENT(IN) :: TEMP ! Temperature [K]
```

```
REAL(f8), INTENT(IN) :: USTAR ! Friction velocity [m/s]
REAL(f8), INTENT(IN) :: RHB ! Relative humidity (fraction)
REAL(f8), INTENT(IN) :: W10 ! 10 m windspeed [m/s]
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

RETURN VALUE:

REAL(f8) :: RS ! Surface resistance for particles [s/m]

REMARKS:

Do computations internally with REAL*8 (8-byte) floating-point precision, in order to avoid a loss of precision.

REVISION HISTORY:

- (1) Updated comments. Also now force double precision w/ "D" exponents. (bmy, 4/1/04)
- (2) Now limit relative humidity to [tiny(real(f8)),0.99] range for DLOG argument (phs, 6/11/08)
- (3) Bug fixes to the Gerber (1985) growth function (jaegle 5/11/11)
- (4) Update growth function to Lewis and Schwartz (2006) and density calculation based on Tang et al. (1997) (bec, jaegle 5/11/11)
- (5) Updates of sea salt deposition over water to follow the Slinn & Slinn (1980) formulation over water surface. Described in Jaegle et al. (ACP, 11, 2011) (jaegle 5/11/11)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 14 Jun 2013 R. Yantosca Now pass Input_Opt via the arg list
- 06 Jan 2015 E. Lundgren Use global physical parameters

6.1.7 init_weightss

Subroutine INIT_WEIGHTSS calculates the volume size distribution of sea-salt. This only has to be done once. We assume that sea-salt is the combination of a coarse mode and accumulation model log-normal distribution functions. The resulting arrays are: DMID = diameter of bin and SALT_V = dV/dln(D) [in um3]. (jaegle 5/11/11)

INTERFACE:

```
SUBROUTINE INIT_WEIGHTSS( Input_Opt )
```

USES:

INPUT PARAMETERS:

```
TYPE(OptInput), INTENT(IN) :: Input_Opt
```

REVISION HISTORY:

```
11 May 2011 - L. Jaegle - Initial version
22 Dec 2011 - M. Payer - Added ProTeX headers
14 Jun 2013 - R. Yantosca - Now accept Input_Opt via tha argument list
06 Jan 2016 - E. Lundgren - Use global physical parameters
```

6.1.8 dust_sfcrsi

Function DUST_SFCRSI computes the aerodynamic resistance of dust aerosol species according to Seinfeld et al 96. We do not consider hygroscopic growth of the dust aerosol particles. (rjp, tdf, bmy, bec, 4/1/04, 4/15/05)

INTERFACE:

```
FUNCTION DUST_SFCRSI( K, II, PRESS, TEMP, USTAR ) RESULT( RS )
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: K    ! Drydep species (range: 1-NUMDEP)
INTEGER, INTENT(IN) :: II    ! Surface type index of GEOS-CHEM
REAL(f8), INTENT(IN) :: PRESS    ! Pressure [kPa]
REAL(f8), INTENT(IN) :: TEMP    ! Temperature [K]
REAL(f8), INTENT(IN) :: USTAR    ! Friction velocity [m/s]
```

RETURN VALUE:

```
REAL(f8) :: RS ! Surface resistance for particles [s/m]
```

REVISION HISTORY:

- (1) Updated comments. Also now force double precision w/ "D" exponents. (bmy, 4/1/04)
- (2) Renamed to DUST_SFCRSII, since this will only be used to compute aerodynamic resistance of dust aerosols. (bec, bmy, 4/15/05)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 06 Jan 2016 E. Lundgren Use global physical paramters

6.1.9 adust_sfcrsii

Function ADUST_SFCRSII computes the aerodynamic resistance of non-size resolved aerosol according to Zhang et al 2001. We do not consider the hygroscopic growth of the aerosol particles. (rjp, tdf, bec, bmy, 4/1/04, 4/15/05)

This routine is used for all aerosols except dust, sulfate, and seasalt (hotp 7/31/09)

INTERFACE:

FUNCTION ADUST_SFCRSII(K, II, PRESS, TEMP, USTAR) RESULT(RS)

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: K   ! Drydep species index (range: 1-NUMDEP)
INTEGER, INTENT(IN) :: II   ! Surface type index of GEOS-CHEM
REAL(f8), INTENT(IN) :: PRESS ! Pressure [kPa] (1 mb = 100 Pa = 0.1 kPa)
REAL(f8), INTENT(IN) :: TEMP   ! Temperature [K]
REAL(f8), INTENT(IN) :: USTAR ! Friction velocity [m/s]
```

RETURN VALUE:

```
REAL(f8) :: RS ! Surface resistance for particles [s/m]
```

REVISION HISTORY:

- (1) Updated comments. Also now force double precision w/ "D" exponents. (bmy, 4/1/04)
- (2) Renamed to DUST_SFCRSII, since this will only be used to compute aerodynamic resistance of dust aerosols. (bec, bmy, 4/15/05)
- (3) Modified hotp for non size resolved aerosols. This is just DUST_SFCRSII renamed and the diameter and density fixed. (hotp 7/12/07)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 06 Jan 2016 E. Lundgren Use global physical parameters

6.1.10 dust_sfcrsii

Function DUST_SFCRSII computes the aerodynamic resistance of dust aerosol species according to Zhang et al 2001. We do not consider the hygroscopic growth of the aerosol particles. (rjp, tdf, bec, bmy, 4/1/04, 4/15/05)

INTERFACE:

```
FUNCTION DUST_SFCRSII( K, II, PRESS, TEMP, USTAR, DIAM, DEN )
& RESULT( RS )
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: K    ! Drydep species index (range: 1-NUMDEP)
INTEGER, INTENT(IN) :: II    ! Surface type index of GEOS-CHEM
REAL(f8), INTENT(IN) :: PRESS    ! Pressure [kPa]
REAL(f8), INTENT(IN) :: TEMP    ! Temperature [K]
REAL(f8), INTENT(IN) :: USTAR    ! Friction velocity [m/s]
REAL(f8), INTENT(IN) :: DIAM    ! Particle diameter [m]
REAL(f8), INTENT(IN) :: DEN    ! Particle density [kg/m3]
```

RETURN VALUE:

```
REAL(f8) :: RS ! Surface resistance for particles [s/m]
```

REVISION HISTORY:

- (1) Updated comments. Also now force double precision w/ "D" exponents. (bmy, 4/1/04)
- (2) Renamed to DUST_SFCRSII, since this will only be used to compute aerodynamic resistance of dust aerosols. (bec, bmy, 4/15/05)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 31 Jan 2014 R. Yantosca Now pass DIAM and DEN as arguments so as to avoid parallelization errors when using the TOMAS microphysics package.
- 06 Jan 2016 E. Lundgren Use global physical parameters

6.1.11 init_drydep

Subroutine INIT_DRYDEP initializes certain variables for the GEOS-CHEM dry deposition subroutines. (bmy, 11/19/02, 10/19/09)

INTERFACE:

```
SUBROUTINE INIT_DRYDEP( am_I_Root, Input_Opt, State_Chm, RC )
```

USES:

```
USE ErrCode_Mod
```

USE Input_Opt_Mod, ONLY : OptInput
USE Species_Mod, ONLY : Species
USE State_Chm_Mod, ONLY : ChmState
USE State_Chm_Mod, ONLY : Ind_

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?!

INPUT/OUTPUT PARAMETERS:

```
TYPE(OptInput), INTENT(INOUT) :: Input_Opt   ! Input Options object
TYPE(ChmState), INTENT(INOUT) :: State_Chm   ! Chemistry_State object
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REMARKS:

We now know how many drydep species there are before INIT_DRYDEP is called. This allows us to get rid of MAXDEP. NUMDEP should be equal to State_Chm%nDryDep, otherwise there is an error. Also note: we need to use the actual molecular weights instead of the emitted molecular weights. These are necessary for the Schmidt # computation.

- (1) Added N2O5 as a drydep tracer, w/ the same drydep velocity as HNO3. Now initialize PBLFRAC array. (rjp, bmy, 7/21/03)
- (2) Added extra carbon & dust aerosol tracers (rjp, tdf, bmy, 4/1/04)
- (3) Added seasalt aerosol tracers. Now use A_RADI and A_DEN to store radius & density of size-resolved tracers. Also added fancy output. (bec, rjp, bmy, 4/26/04)
- (3) Now handles extra SOA tracers (rjp, bmy, 7/13/04)
- (4) Now references LDRYD from "logical_mod.f" and N_TRACERS, SALA_REDGE_um, and SALC_REDGE_um from "tracer_mod.f" (bmy, 7/20/04)
- (5) Included Hg2, HgP tracers (eck, bmy, 12/14/04)
- (6) Included AS, AHS, LET, NH4aq, SO4aq tracers (cas, bmy, 1/6/05)
- (7) Remove reference to PBLFRAC array -- it's obsolete (bmy, 2/22/05)
- (8) Included SO4s, NITs tracers (bec, bmy, 4/13/05)
- (9) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (10) Now set Henry's law constant to 1.0d+14 for Hg2. Now use ID_Hg2, ID_HgP, and ID_Hg_tot from "tracerid_mod.f". Bug fix: split up compound IF statements into separate 2 IF statements for ID_Hg2, ID_HgP to avoid seg faults. (eck, cdh, bmy, 4/17/06)
- (11) Now also initialize SOG4, SOA4 drydep species. Bug fix: Remove 2nd "IF (IS_Hg) THEN" statement. (dkh, bmy, 5/24/06)
- (12) Bug fix: fix TYPO in IF block for IDTSOA4 (dkh, bmy, 6/23/06)
- (13) Included H2/HD tracers for offline H2-HD sim (phs, 9/18/07)
- (14) Add dicarbonyl chemistry species (tmf, ccc, 3/6/09)
- (15) Minor bug fix: ALPH, LIMO should have molwt = 136.23, not 136 even (bmy, 10/19/09)
- (16) Add TOMAS aerosol NK1-NK30 and H2SO4 to drydep list (win, 7/14/09)
- 15 Dec 2011 M. Payer Update OVOC drydep according to Karl et al. 2010 and add drydep for MVK and MACR. (J. Mao)
- 21 Dec 2011 M. Payer Add allocation for size distribution of sea salt SALT_V and DMID (jaegle, 5/11/11)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 14 Mar 2013 M. Payer Replace NOx and Ox with NO2 and O3 as part of removal of NOx-Ox partitioning
- 12 Jun 2013 R. Yantosca Bug fix: now only copy NUMDEP values to Input_Opt%NDVZIND and Input_Opt%DEPNAME
- 14 Jun 2013 R. Yantosca Now replace fields from tracer_mod.F with fields from Input_Opt
- 13 Aug 2013 M. Sulprizio- Add modifications for updated SOA and SOA + semivolatile POA simulations (H. Pye)
- 29 Aug 2013 R. Yantosca Assign XMW=118d-3 to RIP and IEPOX. This now prevents XMW=0e+0_f8 from being passed to function DIFFG, where it is in the denominator.
- 04 Sep 2013 R. Yantosca Improve printout of drydep species
- 12 Sep 2013 M. Sulprizio- Add modifications for acid uptake on dust

```
aerosols (T.D. Fairlie)

15 Jan 2015 - R. Yantosca - Now save NTRAIND to Input_Opt%NTRAIND

08 Jul 2015 - E. Lundgren - Add marine organic aerosols (B.Gantt, M.Johnson)

22 Sep 2015 - R. Yantosca - Now allocate internal variables that used to be of size MAXDEP.

30 Sep 2015 - R. Yantosca - DD_A_Density is renamed to Density

30 Sep 2015 - R. Yantosca - DD_A_Radius is renamed to Radius

14 Dec 2015 - R. Yantosca - Now use actual MW (MW_g) instead of emitted MW (EmMW_g) to define the XMW array

20 Jun 2016 - R. Yantosca - Now define a couple of species ID flags here as module variables on the first call

18 Jul 2016 - M. Sulprizio- Remove special handling for ISOPN and MVKN. Family tracers have been eliminated.
```

6.1.12 cleanup_drydep

Subroutine CLEANUP_DRYDEP deallocates all module arrays. (bmy, 2/27/03, 2/22/05)

INTERFACE:

SUBROUTINE CLEANUP_DRYDEP

REVISION HISTORY:

- (1) Remove reference to PBLFRAC array; it's obsolete (bmy, 2/22/05)
- (2) Added SALT_V and DMID (jaegle, 5/11/11)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 22 Sep 2015 R. Yantosca Now deallocate arrays that were formerly sized to MAXDEP.

6.2 Fortran: Module Interface modis_lai_mod.F90

Module MODIS_LAI_MOD reads the MODIS LAI and CHLR data at native resolution (either 0.25×0.25 or 0.5×0.5 , in netCDF format) and rebins them to the proper GEOS-Chem LAI and CHLR arrays. CHLR data is only read if marine organic aerosol tracers are enabled. This module eliminates the need for the following GEOS-Chem modules, routines, and data files:

- lai mod.F
- readlai.F
- rdlai.F
- findmon.F
- The lai*.global input files

• CMN_VEL_mod.F

INTERFACE:

MODULE Modis_Lai_Mod

USES:

USE CMN_SIZE_Mod ! Size parameters

USE Error_Mod ! Error checking routines

USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

USE Mapping_Mod ! Mapping weights & areas

USE Time_Mod ! EXPAND_DATE

IMPLICIT NONE

PRIVATE

PUBLIC DATA MEMBERS:

REAL(fp), PUBLIC, POINTER :: GC_LAI(:,:) ! DailyLAI, G-C grid REAL(fp), PUBLIC, POINTER :: GC_CHLR(:,:) ! DailyCHLR, G-C grid

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: Read_Modis_Lai
PUBLIC :: Compute_Modis_Lai
PUBLIC :: Find_Lai_Month
PUBLIC :: Init_Modis_Lai
PUBLIC :: Cleanup_Modis_Lai

PRIVATE MEMBER FUNCTIONS:

PUBLIC :: Read_Modis
PUBLIC :: Compute_Modis

PRIVATE :: RoundOff

REMARKS:

Functionality of this module:

If you are using the Olson 1992 land map, then this module will pick the MODIS LAI data at 0.5 x 0.5 native resolution. This is because the legacy code assumed a direct correspondence between the Olson 1992 land map and the MODIS LAI data. Similarly, if you are using the Olson 2001 land map, then this module will pick the MODIS LAI data at 0.25 x 0.25 resolution.

Follows the same algorithm as in the IDL codes used to regrid MODIS LAI data (regridmodis_lai_v5.pro; contact GEOS-Chem Support team).

Historical background of how LAI data have been used in GEOS-Chem:

.

Note that GEOS-Chem (as of April 2012) uses LAI data from two separate sources. The dry deposition and soil NOx modules rely on the data from "lai*.global" ASCII files. These files (which are pre-processed offline by IDL codes) are generated for each specific GEOS-Chem grid configuration (e.g. 4x5, 2x25, 0.5x0.666 nested grids). These files are read from disk by routine RDLAI, which saves the LAI data into the XLAI and XYLAI arrays. XLAI and XYLAI store the leaf area index as a function of Olson land type (cf Olson 1992 land map).

However, the MEGAN biogenic emissions code relies on LAI data stored at 1x1 resolution stored in bpch format. These binary files are read by routine RDISOLAI (and other underlying routines in lai_mod.F), and are regridded on-the-fly to the current GEOS-Chem grid resolution.

Therefore, these two sources of LAI data present an inconsistency that should be resolved. Also, for the Grid-Indpendent GEOS-Chem project, we must move away from ASCII files (which prevent interfacing with external GCMs). We also cannot assume any particular horizontal grid, since that is now to be specified at the start of the simulation.

Also, to facilitate simulations at ultra-fine horizontal resolution, we will eventually adopt the Olson 2001 land map, which has a native resolution of 0.25×0.25 degrees, and likewise use an updated version of the MODIS LAI data at 0.25×0.25 resolution.

To resolve these issues, we have created a new module (modis_lai_mod.F90) which reads from the MODIS LAI data in netCDF format at the native resolution and then regrids the LAI data to GEOS-Chem resolution on-the-fly. The XLAI array is populated for backwards compatibility with the existing legacy codes. The LAI arrays used for MEGAN (ISOLAI, PMISOLAI, MISOLAI, and NMISOLAI) are now replaced by arrays GC_LAI, GC_LAI_PM, GC_LAI_CM, and GC_LAI_NM) from modis_lai_mod.F.

We have validated that the new scheme generates identical XLAI arrays w/r/t the old scheme. The arrays GC_LAI etc. differ from the ISOLAI etc. arrays slightly (but generally agree to within 0.001). This is due to the fact that the ISOLAI arrays were regridded from 1 x 1 native resolution, but now we are regridding from much finer resolution (either 0.5 x 0.5 or 0.25 x 0.25).

NOTES:

- (1) At the present time, we have removed all references to the obsolete XYLAI array and its parent module CMN_VEL_mod.F.
- (2) At the present time, we have not yet disabled the RDISOLAI function. We will do so in the future, and will validate this with a separate benchmark.
- (3) As of December 2012, XLAI and XLAI2 have been moved out of obsolete module Headers/CMN_DEP_mod.F and are now carried as part of the

Meteorology State object (State_Met). This modification was made to facilitate the Grid-Independent GEOS-Chem (GIGC) project.

-- Bob Yantosca (geos-chem-support@as.harvard.edu), 13 Dec 2012 (4) The previous, current, and next month LAI values (GC_LAI_PM, GC_LAI_CM, GC_LAI_NM) were only used for MEGAN. In the HEMCO implementation, MEGAN only needs GC_LAI as input, so all the other GC_LAI arrays were removed. This also makes MODIS_LAI_PM obsolete (ckeller, 10/9/2014).

LAI arrays and where they are (or will be) used in GEOS-Chem:

```
    (1) State_Met%XLAI --> Used in dry deposition routine DEPVEL
    (2) State_Met%XLAI2 --> Used to compute XLAI
    (3) XYLAI --> %%% OBSOLETE: REMOVED, NOW REPLACED BY XLAI %%%
    (4) GC_LAI --> Intended replacement for ISOLAI (from lai_mod.F)
    (5) GC_LAI_PM --> Intended replacement for PMISOLAI (from lai_mod.F)
```

--> Intended replacement for MISOLAI (from lai_mod.F)

--> Intended replacement for NMISOLAI (from lai_mod.F)

(7) GC_LAI_NM REVISION HISTORY:

(6) GC_LAI_CM

```
03 Apr 2012 - R. Yantosca - Initial version
05 Apr 2012 - R. Yantosca - Added descriptive comments
09 Apr 2012 - R. Yantosca - Fixed error in ROUNDOFF function that caused numbers to be rounded up incorrectly.
09 Apr 2012 - R. Yantosca - Changed variables to REAL(fp)
09 Apr 2012 - R. Yantosca - Now set MODIS_START and MODIS_END depending on which version of MODIS LAI we are using
13 Dec 2012 - R. Yantosca - Remove reference to obsolete CMN_DEP_mod.F;
XLAI, XLAI2 now are carried in State_Met
23 Jun 2014 - R. Yantosca - Removed references to logical_mod.F
09 Oct 2014 - C. Keller - Removed GC_LAI_PM, GC_LAI_CM, GC_LAI_NM and MODIS_LAI_PM.
17 Nov 2014 - M. Yannetti - Added PRECISION_MOD
07 Jul 2015 - E. Lundgren - Now also read and compute MODIS chlorophyll-a
(B. Gantt, M. Johnson). Use separate end years.
```

6.2.1 read_modis_lai

Subroutine READ_MODIS_LAI is the wrapper routine to read the MODIS LAI from disk in netCDF format for the current month, and for next month. If enabled, MODIS CHLR is also read in the same way as LAI.

INTERFACE:

SUBROUTINE Read_Modis_Lai(am_I_Root, Input_Opt, yyyy, mm, wasModisRead, RC)

USES:

```
USE ErrCode_Mod
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INTEGER, INTENT(IN) :: yyyy ! Year for LAI data

INTEGER, INTENT(IN) :: mm ! Month for LAI data
```

OUTPUT PARAMETERS:

```
LOGICAL, INTENT(OUT) :: wasModisRead ! Was LAI data just read in?
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REVISION HISTORY:

```
03 Apr 2012 - R. Yantosca - Initial version
05 Apr 2012 - R. Yantosca - Renamed arg "doMonthly" to "wasModisRead"
05 Jun 2013 - R. Yantosca - Bug fix, use "mm" for current month index
20 Jun 2014 - R. Yantosca - Now accept am_I_Root, Input_Opt, RC
09 Oct 2014 - C. Keller - MODIS_LAI_PM not needed anymore.
05 Mar 2015 - R. Yantosca - Now read data w/r/t ExtData/CHEM_INPUTS
07 Jul 2015 - E. Lundgren - Generalized to read either LAI or CHLR
08 Jul 2015 - E. Lundgren - Now read LAI and CHLR data. Abstracted read code to new routine Read_Modis.
```

6.2.2 read_modis

Subroutine READ_MODIS reads the MODIS LAI or CHLR from disk (in netCDF format) for the current month, and for next month.

INTERFACE:

```
SUBROUTINE Read_Modis( am_I_Root, ReadLAI, nc_tmpl, Input_Opt, & yyyy, mm, wasModisRead, RC )
```

USES:

include "netcdf.inc" ! netCDF settings & parameters

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

LOGICAL, INTENT(IN) :: ReadLAI ! T for LAI, F to read CHLR

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

CHARACTER(LEN=255), INTENT(IN) :: nc_tmpl

INTEGER, INTENT(IN) :: yyyy ! Year for LAI data

INTEGER, INTENT(IN) :: mm ! Month for LAI data
```

OUTPUT PARAMETERS:

```
LOGICAL, INTENT(OUT) :: wasModisRead ! Was data just read in?
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REVISION HISTORY:

```
07 Jul 2015 - E. Lundgren - Initial version, containing legacy Read_Modis_Lai code plus modifications to read CHLR
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
```

6.2.3 compute_modis_lai

Subroutine COMPUTE_MODIS_LAI is the wrapper routine to compute the daily MODIS leaf area indices for GEOS-Chem directly from the native grid resolution (0.25 x 0.25 or 0.5 x 0.5). If marine organic aerosol tracers are used, then daily MODIS chlorophyll is also computed.

INTERFACE:

```
SUBROUTINE Compute_Modis_Lai( am_I_Root, Input_Opt, State_Met, & doy, mm, mapping, & wasModisRead, RC )
```

USES:

```
USE ErrCode_Mod
USE Input_Opt_Mod, ONLY : OptInput
USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INTEGER, INTENT(IN) :: doy ! Day of year

INTEGER, INTENT(IN) :: mm ! Month for LAI data

TYPE(MapWeight), POINTER :: mapping(:,:) ! "fine" -> "coarse" grid map

LOGICAL, INTENT(IN) :: wasModisRead ! Was LAI data just read in?
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met  ! Meteorology State object
```

OUTPUT PARAMETERS:

INTENT(OUT) :: RC

! Success or failure?

REVISION HISTORY: 03 Apr 2012 - R. Yantosca - Initial version 05 Apr 2012 - R. Yantosca - Renamed arg "doMonthly" to "wasModisRead" 09 Apr 2012 - R. Yantosca - Changed variables to REAL(fp) 09 Apr 2012 - R. Yantosca - Now follows same algorithm as rdlai.F for populating XLAI array 09 Apr 2012 - R. Yantosca - Remove refs to CMN_VEL_mod.F and XYLAI array; these are now obsolete 17 Apr 2012 - R. Yantosca - Now rename "map" object to "mapping" to avoid name confusion w/ an F90 intrinsic function 13 Dec 2012 - R. Yantosca - Add am_I_Root, State_Met, RC arguments 13 Dec 2012 - R. Yantosca - XLAI, XLAI2 are now carried in State_Met instead of in obsolete Headers/CMN_DEP_mod.F 23 Jun 2014 - R. Yantosca - Now accept Input_Opt via the arg list 09 Oct 2014 - C. Keller - Removed GC_LAI_PM, GC_LAI_CM, GC_LAI_NM and MODIS_LAI_PM. 08 Jul 2015 - E. Lundgren - Now compute LAI and CHLR data. Abstracted compute code to new routine Compute_MODIS

6.2.4 compute_modis

INTEGER,

Subroutine COMPUTE_MODIS computes either the daily MODIS leaf area indices or the daily chlorophyll for GEOS-Chem directly from the native grid resolution $(0.25 \times 0.25 \text{ or } 0.5 \times 0.5)$. The XLAI array (used in the legacy soil NOx and dry deposition routines) are populated accordingly. The XYLAI array is now obsolete and has been replaced by XLAI.

INTERFACE:

```
SUBROUTINE Compute_Modis( am_I_Root, ComputeLAI, & Input_Opt, State_Met, doy, & mm, mapping, wasModisRead, RC)
```

USES:

USE ErrCode_Mod

USE Input_Opt_Mod, ONLY : OptInput USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

```
LOGICAL,
                INTENT(IN) :: am_I_Root
                                            ! Are we on the root CPU?
LOGICAL,
                INTENT(IN) :: ComputeLAI
TYPE(OptInput), INTENT(IN) :: Input_Opt
                                            ! Input Options object
                                            ! Day of year
INTEGER,
                INTENT(IN)
                           :: doy
                                             ! Month for LAI data
INTEGER.
                INTENT(IN) :: mm
                            :: mapping(:,:) ! "fine" -> "coarse" grid map
TYPE(MapWeight), POINTER
LOGICAL,
                INTENT(IN) :: wasModisRead ! Was LAI data just read in?
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REMARKS:

Uses same algorithm as RDISOLAI in the existing lai_mod.F.

REVISION HISTORY:

```
07 Jul 2015 - E. Lundgren - Initial version, contains old Compute_Modis_Lai code plus modifications to compute CHLR
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
```

6.2.5 find_lai_month

Function FIND_LAI_MONTH returns the corresponding LAI month and year for the current calendar date. Note that the LAI data starts at mid-month.

INTERFACE:

```
SUBROUTINE Find_Lai_Month( doy, month, year, mm, yyyy )
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: doy ! Current day of year
INTEGER, INTENT(IN) :: month ! Current month
INTEGER, INTENT(IN) :: year ! Current year
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: mm     ! Output month for LAI data
INTEGER, INTENT(OUT) :: yyyy     ! Output year for LAI data
```

```
05 Jan 1994 - Y. H. Wang, G.M. Gardner, D. Jacob - Initial version
```

- (1) Updated comments, cosmetic changes (bmy, 4/4/03)
- (2) Add the current simulation year as input & the current LAI as output. This is necessary for reading in MODIS LAI (mpb,2009).
- 08 Dec 2009 R. Yantosca Added ProTeX headers
- 03 Apr 2012 R. Yantosca Renamed to FIND_LAI_MONTH; made PUBLIC

6.2.6 RoundOff

Rounds a number X to N decimal places of precision.

INTERFACE:

```
FUNCTION RoundOff( X, N ) RESULT( Y )
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: X ! Number to be rounded INTEGER, INTENT(IN) :: N ! Number of decimal places to keep
```

RETURN VALUE:

```
REAL(fp) :: Y ! Number rounded to N decimal places
```

REMARKS:

The algorithm to round ${\tt X}$ to ${\tt N}$ decimal places is as follows:

- (1) Multiply X by 10**(N+1)
- (2) If X < 0, then add -5 to X; otherwise add 5 to X
- (3) Take the integer part of X
- (4) Divide X by 10**(N+1)
- (5) Truncate X to N decimal places: INT(X * 10**N) / 10**N

Rounding algorithm from: Hultquist, P.F, "Numerical Methods for Engineers and Computer Scientists", Benjamin/Cummings, Menlo Park CA, 1988, p. 20.

Truncation algorithm from: http://en.wikipedia.org/wiki/Truncation

The two algorithms have been merged together for efficiency.

REVISION HISTORY:

```
06 Apr 2012 - R. Yantosca - Initial version
09 Apr 2012 - R. Yantosca - Changed all variables & arguments to REAL(fp)
```

6.2.7 init_modis

Subroutine INIT_MODIS_LAI initializes and allocates all module variables.

INTERFACE:

```
SUBROUTINE Init_Modis_Lai( am_I_Root, Input_Opt, RC )
```

USES:

```
USE ErrCode_Mod
USE Input_Opt_Mod, ONLY : OptInput
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REVISION HISTORY:

```
03 Apr 2012 - R. Yantosca - Initial version
03 Feb 2014 - M. Sulprizio- Force last year of MODIS data to 2008. There is a large difference in the 2009 file that still needs to be investigated (skim, 1/29/14)
23 Jun 2014 - R. Yantosca - Now accept am_I_Root, Input_Opt, RC
08 Jul 2015 - E. Lundgren - New end years to match files from M. Johnson
```

6.2.8 cleanup_modis_lai

Subroutine CLEANUP_MODIS_LAI deallocates all previously-allocated module variables.

INTERFACE:

```
SUBROUTINE Cleanup_Modis_Lai
```

REVISION HISTORY:

```
03 Apr 2012 - R. Yantosca - Initial version
```

6.3 Fortran: Module Interface olson_landmap_mod.F90

Module OLSON_LANDMAP_MOD reads the Olson land map and computes the IREG, ILAND, and IUSE arrays. This module was written to facilitate Grid-Independent GEOS-Chem development while still keeping backwards compatibility with existing legacy code. It replaces the old routine rdland.F.

INTERFACE:

```
MODULE Olson_LandMap_Mod
```

USES:

```
USE CMN_SIZE_MOD ! Size parameters

USE ERROR_MOD ! Error checking routines

USE GC_GRID_MOD ! Horizontal grid definition

USE MAPPING_MOD ! Mapping weights & areas

USE PhysConstants ! Physical constants

USE PRECISION_MOD ! For GEOS-Chem Precision (fp)
```

IMPLICIT NONE

PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: Init_Olson_Landmap
PUBLIC :: Compute_Olson_Landmap
PUBLIC :: Cleanup_Olson_LandMap

REMARKS:

The Olson land types are as follows:

______ 25 Deciduous 50 Desert 1 Urban 26 Deciduous 51 Desert 27 Conifer 2 Shrub 52 Steppe 3 ---28 Dwarf forest 53 Tundra 29 Trop. broadleaf 4 ---54 rainforest 5 ---30 Agricultural 55 mixed wood/open 31 Agricultural 56 mixed wood/open 6 Trop. evergreen 7 ---32 Dec. woodland 57 mixed wood/open 8 Desert 33 Trop. rainforest 58 mixed wood/open 9 ---34 ---59 mixed wood/open 10 ---35 ---60 conifers 11 ---36 Rice paddies 61 conifers 12 ---37 agric 62 conifers 13 ---38 agric 63 Wooded tundra 14 ---39 agric. 64 Moor 40 shrub/grass 15 ---65 coastal 16 Scrub 41 shrub/grass 66 coastal 42 shrub/grass 17 Ice 67 coastal 18 ---43 shrub/grass 68 coastal 19 ---44 shrub/grass 69 desert 45 wetland 70 ice 20 Conifer 21 Conifer 46 scrub 71 salt flats 47 scrub 72 wetland 22 Conifer 23 Conifer/Deciduous 48 scrub 73 water 24 Deciduous/Conifer 49 scrub

Arrays computed by olson_landmap_mod.F90

```
(1) IREG (in CMN_DEP_mod.F): # of Olson land types per G-C grid box
(2) ILAND (in CMN_DEP_mod.F): List of all Olson land types in G-C grid box
(3) IUSE (in CMN_DEP_mod.F): Coverage of each Olson type in G-C grid box
(4) IJREG (in CMN_VEL_mod.F): %%%% OBSOLETE: NOW REPLACED BY IREG %%%%%
(5) IJLAND (in CMN_VEL_mod.F): %%%% OBSOLETE: NOW REPLACED BY ILAND %%%%%
(6) IJUSE (in CMN_VEL_mod.F): %%%%% OBSOLETE: NOW REPLACED BY IUSE %%%%%
(7) FRCLND (in CMN_DEP_mod.F): Fraction of G-C grid box that is not water
```

NOTES:

(1) IREG, ILAND, IUSE are used by the soil NOx emissions routines

- (2) IJREG, IJLAND, IJUSE are used by the drydep routines (legacy code)
- (3) FRCLND is used by various GEOS-Chem routines

BUG IN THE OLD "rdland.F" FOR 2 X 2.5 DEGREE RESOLUTION

This module ("olson_landmap_mod.F") replaces the old routine "rdland.F", which previously read in the Olson landtype data from the ASCII format file named "vegtype.global". There used to be a different "vegtype.global" file for each different horizontal grid resolution.

The "vegtype.global" stored the following quantities, such that values for a single grid box were saved on a single line:

```
I, J, IREG(I,J), ILAND(I,J,K), IUSE(I,J,K) (where K=1, IREG(I,J))
```

Routine "rdland.F" reads these quantities from "vegtype.global" assuming there were 20 integer characters on a single line (i.e. using Fortran FORMAT '(20i4)'). However, ~ 12 lines of the 2 x 2.5 "vegtype.global" file contained more than 20 integer values. This caused "rdland.F", to read in the values from these lines improperly, which in turn caused the IREG, ILAND, IUSE, IJREG, IJLAND, IJUSE, and FRCLND arrays to be improperly initialized for the grid boxes corresponding to these lines in the "vegtype.global" file.

Bob Yantosca has validated that "olson_landmap_mod.F" returns results 100% identical to the "vegtype.global" file. Therefore, if you want to compare the output of model simulations using "olson_landmap_mod.F" the output of simulations using "rdland.F", you will see a slight difference in the MCL lifetime and tracer concentrations.

If you need to run a GEOS-Chem simulation with an older version of the code using "rdland.F", then this bug may be corrected by changing the line of code:

```
101 FORMAT(2014)
```

to:

```
#if defined( GRID2x25 )
101 FORMAT(25I4)
#else
100 FORMAT(20I4)
#endif
```

This is more or less a moot point, as "olson_landmap_mod.F" will be installed into GEOS-Chem v9-01-03 and higher versions.

NOTE FOR 0.5 x 0.666 grids

As of 21 Mar 2012, the IUSE values computed by "olson_landmap_mod.F90" may slightly differ from those specified in the "vegtype.global" files for 0.5×0.666 nested grids. We attribute this to roundoff error caused by the the longitude spacing being an irrational number (0.6666666...). We are still investigating.

REVISION HISTORY:

```
13 Mar 2012 - R. Yantosca - Initial version
19 Mar 2012 - R. Yantosca - Minor last-minute bug fixes
21 Mar 2012 - R. Yantosca - Now use REAL*4 for computations
22 Mar 2012 - R. Yantosca - Now read surface area from the file
22 Mar 2012 - R. Yantosca - Now make lon, lat, OLSON, A_CM2 allocatable
22 Mar 2012 - R. Yantosca - Now define I_OLSON, J_OLSON, N_OLSON, D_LON,
                            and D_LAT in routine Init_Olson_LandMap
27 Mar 2012 - R. Yantosca - Now reference USE_OLSON_2001 from logical_mod.F
02 Apr 2012 - R. Yantosca - Now reference mapping_mod.F90
02 Apr 2012 - R. Yantosca - Moved routine GET_MAP_WT to mapping_mod.F90
02 Apr 2012 - R. Yantosca - Now Save mapping info for later use
09 Apr 2012 - R. Yantosca - Removed IJREG, IJUSE, IJLAND; these are now
                            replaced by IREG, IUSE, ILAND arrays
09 Apr 2012 - R. Yantosca - Removed reference to CMN_VEL_mod.F
20 Mar 2014 - R. Yantosca - Speed up Olson computation by skipping boxes
24 Jun 2014 - R. Yantosca - Remove references to logical_mod.F
17 Nov 2014 - M. Yannetti - Added PRECISION_MOD
29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90
```

6.3.1 compute_olson_landmap

Subroutine COMPUTE_OLSON_LANDMAP computes the GEOS-Chem arrays IREG, ILAND, IUSE (and corresponding 1-D arrays IJREG, IJLAND, IJUSE) on-the-fly from the Olson Land map file. This routine, which is intended to facilitate the Grid-Independent GEOS-Chem, replaces the old rdland.F, which read from pre-computed "vegtype.global" files.

INTERFACE:

USES:

```
SUBROUTINE Compute_Olson_LandMap( am_I_Root, mapping, State_Met )
```

USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

INPUT/OUTPUT PARAMETERS:

```
TYPE(MapWeight), POINTER :: mapping(:,:) ! "fine" -> "coarse" mapping
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

REMARKS:

This routine supplies arrays that are required for legacy code routines:

- (1) IREG, ILAND, IUSE are used by the Soil NOx routines
- (2) IJREG, IJLAND, IJUSE are used by the dry deposition routines

REVISION HISTORY:

```
13 Mar 2012 - R. Yantosca - Initial version
19 Mar 2012 - R. Yantosca - Reorder ILAND, IUSE, IJLAND, IJUSE to be
                            consistent w/ the leaf area indices
19 Mar 2012 - R. Yantosca - Compute the FRCLND array (from CMN_DEP_mod.F)
21 Mar 2012 - R. Yantosca - Now use REAL*4 for computation, to reduce
                            roundoff errors at high-resolution
22 Mar 2012 - R. Yantosca - Now get surface area directly from variable
                            A_CM2 (read from disk) instead of computing it
02 Apr 2012 - R. Yantosca - Now pass MAP (mapping weight object) via the
                            arg list, to save the mapping info for later
09 Apr 2012 - R. Yantosca - Remove IJLOOP variable
09 Apr 2012 - R. Yantosca - Now do not compute IJREG, IJLAND, IJUSE; these
                            are replaced by IREG, ILAND, IUSE arrays
17 Apr 2012 - R. Yantosca - Rename "map" object to "mapping" to avoid name
                            confusion with an F90 intrinsic function
                          - Replaced all met field arrays with State_Met
09 Nov 2012 - M. Payer
                            derived type object
29 Nov 2012 - R. Yantosca - Added am_I_Root argument
12 Dec 2012 - R. Yantosca - Now get IREG, ILAND, IUSE from State_Met
20 Mar 2014 - R. Yantosca - Add shunts in lat & lon to reduce wall time
```

6.3.2 init_olson_landmap

Subroutine INIT_OLSON_LANDMAP reads Olson land map information from disk (in netCDF format).

INTERFACE:

```
SUBROUTINE Init_Olson_LandMap( am_I_Root, Input_Opt, RC )
```

USES:

```
USE ErrCode_Mod

USE Input_Opt_Mod, ONLY: OptInput

USE m_netcdf_io_open

USE m_netcdf_io_read

USE m_netcdf_io_readattr
```

```
USE m_netcdf_io_close

IMPLICIT NONE
```

include "netcdf.inc"

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

OUTPUT PARAMETERS:

REMARKS:

Assumes that you have:

- (1) A netCDF library (either v3 or v4) installed on your system
- (2) The NcdfUtilities package (from Bob Yantosca) source code

REVISION HISTORY:

```
13 Mar 2012 - R. Yantosca - Initial version

22 Mar 2012 - R. Yantosca - Also read in surface areas [m2] from file

27 Mar 2012 - R. Yantosca - Now read the "units" attribute of each variable

27 Mar 2012 - R. Yantosca - Now echo file I/O status info to stdout

27 Mar 2012 - R. Yantosca - Now can read Olson 1992 or Olson 2001 land map

29 Nov 2012 - R. Yantosca - Add am_I_Root to the argument list

26 Feb 2013 - M. Long - Now pass DATA_DIR_1x1 via the argument list

24 Jun 2014 - R. Yantosca - Now accept Input_Opt, RC via the arg list
```

6.3.3 cleanup_olson_landmap

Subroutine CLEANUP_OLSON_LANDMAP deallocates all allocated global module variables.

05 Mar 2015 - R. Yantosca - Now read data w/r/t ExtData/CHEM_INPUTS

INTERFACE:

```
SUBROUTINE Cleanup_Olson_LandMap( am_I_Root )
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
```

```
22 Mar 2012 - R. Yantosca - Initial version
29 Nov 2012 - R. Yantosca - Add am_I_Root as an argument
```

6.4 Fortran: Module Interface mapping_mod.F90

Module MAPPING_MOD contains a derived-type object to compute and save the mapping weight (i.e. fraction of each "fine" grid box that fits into the "coarse" grid box") and areal mapping (i.e. the area of each "fine" grid box contained within a "coarse" grid box).

INTERFACE:

```
MODULE Mapping_Mod
```

USES:

```
USE CMN_SIZE_MOD ! Size parameters
USE ERROR_MOD ! Error handling routines
USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

IMPLICIT NONE
PRIVATE
```

PUBLIC DATA MEMBERS:

```
PUBLIC :: MapWeight
TYPE MapWeight
   INTEGER
                                    ! # of "fine" boxes per "coarse" box
                  :: count
   INTEGER, POINTER :: II(:)
                                    ! Longitude indices,
                                                                  grid
                                                         "fine"
                                    ! Latitude indices,
   INTEGER, POINTER :: JJ(:)
                                                         "fine"
                                                                  grid
   INTEGER, POINTER :: olson(:)
                                    ! Olson land type,
                                                         "fine"
                                                                  grid
   INTEGER, POINTER :: ordOlson(:) ! Ordering of Olson land types
   REAL*4, POINTER :: area(:)
                                    ! Surface areas,
                                                         "fine"
                                                                  grid
   REAL*4
                                   ! Total surface area, "coarse" grid
                   :: sumarea
END TYPE MapWeight
```

PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: Init_Mapping
PUBLIC :: Get_Map_Wt
PUBLIC :: Cleanup_Mapping
```

REMARKS:

The mapping weights and areal mapping are initialized when the Olson land map is read from disk (in olson_landmap_mod.F90). They are used again when the MODIS leaf area index data is prepared for input into GEOS-Chem's (legacy) dry deposition module.

Also, we do not define the mapping weight object within this module. This allows you to create more than one mapping weight object for different native grids (e.g. 0.5×0.5 and 0.25×0.25 , etc.)

```
03 Apr 2012 - R. Yantosca - Initial version
05 Apr 2012 - R. Yantosca - Comment out mapwt field of MapWeight type,
leave this for future expansion
17 Apr 2012 - R. Yantosca - Rename pointer object "map" to "mapping,
to remove confusion w/ F90 intrinsic
17 Nov 2014 - M. Yannetti - Added PRECISION_MOD
```

6.4.1 init_mapping

Subroutine INIT_MAPPING allocates and initializes a derived-type object containing grid mapping information.

INTERFACE:

```
SUBROUTINE Init_Mapping( am_I_Root, Input_Opt, I_FINE, J_FINE, & I_COARSE, J_COARSE, mapping, RC )
```

USES:

```
USE ErrCode_Mod
USE Input_Opt_Mod, ONLY : OptInput
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INTEGER, INTENT(IN) :: I_FINE ! # of lons on the "fine" grid

INTEGER, INTENT(IN) :: J_FINE ! # of lats on the, "fine" grid

INTEGER, INTENT(IN) :: I_COARSE ! # of lons on the "coarse" grid

INTEGER, INTENT(IN) :: J_COARSE ! # of lats on the "coarse" grid
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(MapWeight), POINTER, INTENT(INOUT) :: mapping(:,:) !"fine" -> "coarse"
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

```
03 Apr 2012 - R. Yantosca - Initial version

10 Apr 2012 - R. Yantosca - Now add a different # to FINE_PER_COARSE
depending on which Olson map we are using

17 Apr 2012 - R. Yantosca - Rename to "map" to "mapping" to avoid confusion
with a F90 intrinsic function

17 Apr 2012 - R. Yantosca - Add error check for mapping object

18 Apr 2012 - R. Yantosca - Improve error check for sub-fields of mapping
object so as not to interfere w/ parallel loop

23 Jun 2014 - R. Yantosca - Now accept am_I_Root, Input_Opt, RC
```

6.4.2 get_map_wt

Subroutine GET_MAP_Wt returns the "mapping weight", that is, the fraction that each "fine" grid box fits into each "coarse" grid box.

INTERFACE:

```
SUBROUTINE Get_Map_Wt( xedge_w, xedge_e, xedgeC_w, xedgeC_e, & yedge_s, yedge_n, yedgeC_s, yedgeC_n, & mapWt )
```

INPUT PARAMETERS:

```
REAL*4, INTENT(IN) :: xedge_w, xedge_e ! Lon edges, fine grid
REAL*4, INTENT(IN) :: xedgeC_w, xedgeC_e ! Lon edges, coarse grid
REAL*4, INTENT(IN) :: yedge_s, yedge_n ! Lat edges, fine grid
REAL*4, INTENT(IN) :: yedgeC_s, yedgeC_n ! Lat edges, coarse grid
REAL*4, INTENT(OUT) :: mapWt ! Mapping weight
```

REMARKS:

Follows the algorithm from GAMAP routine ctm_getweight.pro

REVISION HISTORY:

```
30 Jan 2012 - R. Yantosca - Initial version
21 Mar 2012 - R. Yantosca - Typo: set x0verLap to zero if it is out of the range of 0-1. (We had set y0verLap=0 before)
21 Mar 2012 - R. Yantosca - Now use REAL*4 for computations to avoid roundoff errors at hi-res grids
03 Apr 2012 - R. Yantosca - Moved from "olson_landmap_mod.F90" to here; renamed "Get_Mapping"
```

6.4.3 cleanup_mapping

Subroutine CLEANUP_MAPPING deallocates memory from a derived-type object containing mapping information.

INTERFACE:

```
SUBROUTINE Cleanup_Mapping( mapping )
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(MapWeight), POINTER, INTENT(INOUT) :: mapping(:,:)
```

```
03 Mar 2012 - R. Yantosca - Initial version
17 Apr 2012 - R. Yantosca - Rename to "map" to "mapping to avoid name confusion with a F90 intrinsic function
```

6.5 Fortran: Module Interface get_ndep_mod.F

Module GET_NDEP_MOD contains routines for computing the accumulated nitrogen dry and wet deposition between emission time steps. These variables are needed for soil NOx emission calculations.

This module is basically a simple wrapper module to save out the nitrogen dry and wet deposition rates and pass them to HEMCO for soil NOx emission calculation (via hcoi_gc_main_mod.F90).

IMPORTANT: Routine RESET_DEP_N resets the deposition arrays to zero. It is called in hcoi_gc_main_mod.F90 after the emission calculations.

INTERFACE:

```
MODULE GET_NDEP_MOD
```

USES:

```
USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

IMPLICIT NONE
PRIVATE
```

PUBLIC DATA MEMBERS:

```
! Soil NOx deposited N arrays

REAL(fp), PUBLIC, POINTER :: DRY_TOTN (:,:) => NULL() ! Drydep'd N

REAL(fp), PUBLIC, POINTER :: WET_TOTN (:,:) => NULL() ! Wetdep'd N
```

PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: SOIL_DRYDEP
PUBLIC :: SOIL_WETDEP
PUBLIC :: RESET_DEP_N
PUBLIC :: Init_Get_Ndep
PUBLIC :: Cleanup_Get_Ndep
```

```
23 Oct 2012 - M. Payer - Added ProTeX headers
25 Jul 2014 - R. Yantosca - Moved module variables DEP_RESERVOIR, DRY_TOTN, and WET_TOTN here from Headers/commsoil_mod.F90
25 Jul 2014 - R. Yantosca - Add routine INIT_GET_NDEP
25 Jul 2014 - R. Yantosca - Add routine CLEANUP_GET_NDEP
09 Oct 2014 - C. Keller - Removed obsolete routines DEP_RESERVOIR, GET_DEP_N, SOURCE_DRYN, and SOURCE_WETN. These are now handled in hcox_soilnox_mod.F90.
13 Nov 2014 - M. Yannetti - Added PRECISION_MOD
16 Jun 2016 - C. Miller - Now define species ID flags with Ind_
17 Jun 2016 - R. Yantosca - Add species ID flags as module variables
```

6.5.1 soil_drydep

Subroutine SOIL_DRYDEP holds dry deposited species [molec/cm2/s]. This is called from dry_dep_mod.F.

INTERFACE:

```
SUBROUTINE SOIL_DRYDEP( I, J, L, NN, TDRYFX )
```

USES:

```
USE State_Chm_Mod, only : Ind_
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I     ! I
INTEGER, INTENT(IN) :: J     ! J
INTEGER, INTENT(IN) :: L     ! Level
```

INTEGER, INTENT(IN) :: NN ! Dry Dep Tracer #

REAL(fp), INTENT(IN) :: TDRYFX ! Dry dep flux [molec/cm2/s]

REVISION HISTORY:

```
23 Oct 2012 - M. Payer - Added ProTeX headers
14 Mar 2013 - M. Payer - Replace NOx with NO2 as part of removal of NOx-Ox partitioning
16 Jun 2016 - C. Miller - Now use
```

6.5.2 soil_wetdep

Subroutine SOIL_WETDEP holds wet deposited species [molec/cm2/s]. This is called from wetscav_mod.F.

INTERFACE:

```
SUBROUTINE SOIL_WETDEP( I, J, L, NN, TWETFX )
```

USES:

```
USE State_Chm_Mod, Only : Ind_
```

INPUT PARAMETERS:

REAL(fp), INTENT(IN) :: TWETFX ! Wet dep flux [kg/s]

```
23 Oct 2012 - M. Payer - Added ProTeX headers
```

6.5.3 reset_dep_N

Subroutine RESET_DEP_N resets the dry and wet deposition arrays and variables so that they can be refilled.

INTERFACE:

```
SUBROUTINE RESET_DEP_N()
```

REVISION HISTORY:

```
03 Apr 2014 - C. Keller - Initial version
```

6.5.4 Init_Get_Ndep

Routine INIT_GET_NDEP allocates all module arrays.

INTERFACE:

```
SUBROUTINE Init_Get_Ndep( am_I_Root, RC )
```

USES:

```
USE CMN_SIZE_Mod
USE ErrCode_Mod
USE State_Chm_Mod, ONLY : Ind_
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC     ! Success or failure
```

REMARKS:

We now allocate the DEP_RESERVOIR, DRY_TOTN, and WET_TOTN arrays within get_ndep_mod.F. These were formerly contained in Headers/commsoil_mod.F90, which was rendered mostly obsolete by HEMCO.

```
25 Jul 2014 - R. Yantosca - Initial version
09 Oct 2014 - C. Keller - Removed obsolete variable DEP_RESERVOIR
```

6.5.5 cleanup_commsoil

Subroutine CLEANUP_COMMSOIL deallocates all module arrays.

INTERFACE:

```
SUBROUTINE Cleanup_Get_NDep(am_I_Root, RC)
```

USES:

USE ErrCode_Mod

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
```

OUTPUT PARAMETERS:

REVISION HISTORY:

```
25 Jul 2014 - R. Yantosca - Initial version
09 Oct 2014 - C. Keller - Removed obsolete variable DEP_RESERVOIR
```

7 Emisions and chemistry modules

These modules contain routines to (1) call HEMCO to compute emissions rates and (2) feed them into the FlexChem/KPP chemstry solver.

7.1 Fortran: Module Interface emissions_mod.F90

Module emissions_mod.F90 is a wrapper module to interface GEOS-Chem and HEMCO. It basically just calls the GEOS-Chem - HEMCO interface routines. For some specialty sims, a few additional steps are required that are also executed here.

INTERFACE:

MODULE EMISSIONS_MOD

USES:

IMPLICIT NONE PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: EMISSIONS_INIT
PUBLIC :: EMISSIONS_RUN
PUBLIC :: EMISSIONS_FINAL

```
27 Aug 2014 - C. Keller - Initial version.
20 Jun 2016 - R. Yantosca - Declare species ID flags as module variables
```

7.1.1 emissions_init

Subroutine EMISSIONS_INIT calls the HEMCO - GEOS-Chem interface initialization routines.

INTERFACE:

```
SUBROUTINE EMISSIONS_INIT( am_I_Root, Input_Opt, State_Met, State_Chm, & RC, HcoConfig)
```

USES:

```
USE ERROR_MOD, ONLY : ERROR_STOP
USE HCOI_GC_MAIN_MOD, ONLY : HCOI_GC_INIT
USE HCO_TYPES_MOD, ONLY : ConfigObj
USE Input_Opt_Mod, ONLY : OptInput
USE State_Met_Mod, ONLY : MetState
USE State_Chm_Mod, ONLY : ChmState
USE State_Chm_Mod, ONLY : Ind_
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root ! root CPU?

TYPE(MetState), INTENT(IN ) :: State_Met ! Met state

TYPE(ChmState), INTENT(IN ) :: State_Chm ! Chemistry state
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input opts
TYPE(ConfigObj), POINTER, OPTIONAL :: HcoConfig ! HEMCO config object
INTEGER, INTENT(INOUT) :: RC ! Failure or success
```

REVISION HISTORY:

```
27 Aug 2014 - C. Keller - Initial version
16 Jun 2016 - J. Sheng - Added tracer index retriever
20 Jun 2016 - R. Yantosca - Now define species IDs only in the INIT phase
```

7.1.2 emissions_run

Subroutine EMISSIONS_RUN calls the HEMCO - GEOS-Chem interface run routines.

INTERFACE:

```
SUBROUTINE EMISSIONS_RUN( am_I_Root, Input_Opt, State_Met, & State_Chm, EmisTime, Phase, RC)
```

USES:

```
USE BROMOCARB_MOD,
                           ONLY : SET_BRO
    USE BROMOCARB_MOD,
                           ONLY : SET_CH3BR
    USE CARBON_MOD,
                           ONLY : EMISSCARBON
    USE CO2_MOD,
                           ONLY: EMISSCO2
    USE ErrCode_Mod
    USE ERROR_MOD,
                           ONLY : GC_Error
    USE GLOBAL_CH4_MOD,
                           ONLY: EMISSCH4
    USE HCOI_GC_MAIN_MOD,
                           ONLY : HCOI_GC_RUN
    USE Input_Opt_Mod,
                           ONLY : OptInput
    USE State_Met_Mod,
                           ONLY : MetState
    USE State_Chm_Mod,
                           ONLY : ChmState
#if defined ( TOMAS )
    USE CARBON_MOD,
                         ONLY : EMISSCARBONTOMAS ! jkodros
    USE SULFATE_MOD,
                           ONLY : EMISSSULFATETOMAS !jkodros
#endif
    ! Use old mercury code for now (ckeller, 09/23/2014)
    USE MERCURY_MOD,
                      ONLY : EMISSMERCURY
    ! For UCX, use Seb's routines for now
#if defined( UCX )
    USE UCX_MOD,
                      ONLY : EMISS_BASIC
#endif
INPUT PARAMETERS:
    LOGICAL,
                    INTENT(IN ) :: am_I_Root ! root CPU?
                    INTENT(IN
                                ) :: EmisTime ! Emissions in this time step
    LOGICAL,
    INTEGER,
                    INTENT(IN ) :: Phase ! Run phase
INPUT/OUTPUT PARAMETERS:
                    INTENT(INOUT) :: State_Met ! Met state
    TYPE(MetState),
    TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry state
                   INTENT(INOUT) :: Input_Opt ! Input opts
    TYPE(OptInput),
    INTEGER,
                     INTENT(INOUT) :: RC    ! Failure or success
```

REVISION HISTORY:

27 Aug 2014 - C. Keller - Initial version
13 Nov 2014 - C. Keller - Added EMISSCARBON (for SESQ and POA)
21 Nov 2014 - C. Keller - Added EMISSVOC to prevent VOC build-up above tropopause

22 Sep 2016 - R. Yantosca - Don't call EMISSCARBON unless we are doing

a fullchem or aerosol simulation

7.1.3 emissions_final

Subroutine EMISSIONS_FINAL calls the HEMCO - GEOS-Chem interface finalization routines.

INTERFACE:

```
SUBROUTINE EMISSIONS_FINAL( am_I_Root, ERROR )
```

USES:

```
USE HCOI_GC_MAIN_MOD, ONLY : HCOI_GC_FINAL
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root ! root CPU?
```

LOGICAL, INTENT(IN) :: ERROR ! Cleanup after crash?

REVISION HISTORY:

```
27 Aug 2014 - C. Keller - Initial version
```

7.2 Fortran: Module Interface chemgrid_mod.F

Module CHEMGRID_MOD contains routines and variables for reading and returning vertical layer limits.

INTERFACE:

MODULE CHEMGRID_MOD

USES:

```
USE CMN_SIZE_MOD, ONLY : LLSTRAT
```

USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

IMPLICIT NONE

PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: CLEANUP_CHEMGRID
PUBLIC :: CHECK_VAR_TROP
PUBLIC :: DIAG_TROPOPAUSE

PUBLIC :: GET_MIN_CHEMGRID_LEVEL
PUBLIC :: GET_MAX_CHEMGRID_LEVEL

PUBLIC :: GET_MIN_TPAUSE_LEVEL
PUBLIC :: GET_MAX_TPAUSE_LEVEL

PUBLIC :: GET_TPAUSE_LEVEL

PUBLIC :: GET_CHEMGRID_LEVEL

PUBLIC :: INIT_CHEMGRID
PUBLIC :: ITS_IN_THE_TROP
PUBLIC :: ITS_IN_THE_STRAT

PUBLIC :: ITS_IN_THE_MESO

```
PUBLIC :: ITS_IN_THE_STRATMESO

PUBLIC :: ITS_IN_THE_CHEMGRID

PUBLIC :: ITS_IN_THE_NOCHEMGRID

PUBLIC :: READ_TROPOPAUSE
```

PUBLIC DATA MEMBERS:

```
! Scalars

INTEGER, PUBLIC :: LMIN  ! Minimum level where chemistry happens

INTEGER, PUBLIC :: LMAX  ! Maximum levle where chemistry happens
```

REVISION HISTORY:

```
22 Aug 2005 - R. Yantosca - Initial version
```

- (1) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (2) Simplify counting of tropospheric boxes (bmy, 11/1/05)
- (3) Added case of variable tropopause.

The definition of the tropopause boxes is different in the two cases. They are part of the troposphere in the case of a variable troposphere. LMAX, LMIN are the min and max extent of the troposphere in that case. (bdf, phs, 1/19/07)

- (4) Bug fix: set NCS=NCSURBAN for safety's sake (bmy, 4/25/07)
- (5) Updated comments (bmy, 9/18/07)
- (6) Bug fix: make ITS_IN_THE_STRAT more robust. (phs, 11/14/08)
- 09 Sep 2010 R. Yantosca Added ProTeX headers
- 24 Mar 2013 S. D. Eastham Adapted from tropopause_mod.F. Can now identify atmospheric layers, chemistry grids and aerosol grids independently of one another
- 20 Feb 2014 M. Sulprizio Removed "define.h", this is now obsolete 21 Feb 2014 M. Sulprizio Now make INIT_CHEMGRID a public function
- 06 Nov 2014 M. Yannetti Added PRECISION_MOD

7.2.1 check_var_trop

Subroutine CHECK_VAR_TROP checks that the entire variable troposphere is included in the 1..LLTROP range, and set the LMIN and LMAX to current min and max tropopause.

INTERFACE:

```
SUBROUTINE CHECK_VAR_TROP( State_Met )
```

USES:

```
USE CMN_SIZE_MOD
```

USE ERROR_MOD, ONLY : GEOS_CHEM_STOP

USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

```
TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

REVISION HISTORY:

```
24 Aug 2006 - P. Le Sager - Initial version
```

- (1) LLTROP is set at the first level entirely above 20 km (phs, 9/29/06)
- (2) Fix LPAUSE for CH4 chemistry (phs, 1/19/07)
- 09 Sep 2010 R. Yantosca Added ProTeX headers
- 21 Feb 2014 M. Sulprizio- Now pass State_Met object via the arg list

7.2.2 read_tropopause

Subroutine READ_TROPOPAUSE reads in the annual mean tropopause.

INTERFACE:

```
SUBROUTINE READ_TROPOPAUSE( am_I_Root, Input_Opt, RC )
```

USES:

```
USE BPCH2_MOD, ONLY : GET_NAME_EXT, GET_RES_EXT
```

USE CMN_SIZE_MOD

USE ErrCode_Mod

USE ERROR_MOD, ONLY : GEOS_CHEM_STOP

USE m_netcdf_io_open

USE m_netcdf_io_read

USE m_netcdf_io_readattr

USE m_netcdf_io_close

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

REVISION HISTORY:

```
13 Dec 1999 - Q. Li, R. Yantosca - Initial version
```

(1) Call READ_BPCH2 to read in the annual mean tropopause data which is stored in binary punch file format. (bmy, 12/13/99)

- (2) Now also read integer flags for ND27 diagnostic -- these determine how to sum fluxes from boxes adjacent to the annual mean tropoause. (qli, bmy, 1/7/00)
- (3) Cosmetic changes (bmy, 3/17/00)
- (4) Reference F90 module "bpch2_mod" which contains routine "read_bpch2" for reading data from binary punch files (bmy, 6/28/00)
- (5) Call TRANSFER_2D from "transfer_mod.f" to cast data from REAL*4 to INTEGER and also to resize to (IIPAR, JJPAR). ARRAY needs to be of size (IIPAR, JJPAR). Also updated comments and made cosmetic changes. Removed obsolete variables.(bmy, 9/26/01)
- (6) Removed obsolete code from 9/01 (bmy, 10/26/01)
- (7) Now read annual mean tropopause files from the ann_mean_trop_200202/ subdirectory of DATA_DIR (bmy, 1/24/02)
- (8) Eliminated obsolete code from 1/02 (bmy, 2/27/02)
- (9) Now write file name to stdout (bmy, 4/3/02)
- (10) Now reference GEOS_CHEM_STOP from "error_mod.f", which frees all allocated memory before stopping the run. (bmy, 10/15/02)
- (11) Now call READ_BPCH2 with QUIET=.TRUE. to suppress printing of extra info to stdout. Also updated FORMAT strings. (bmy, 3/14/03)
- (12) Now references DATA_DIR from "directory_mod.f" (bmy, 7/20/04)
- (13) Now bundled into "tropopause_mod.f' (bmy, 2/10/05)
- (14) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (15) Simplify counting of # of tropospheric boxes (bmy, 11/1/05)
- 09 Sep 2010 R. Yantosca Added ProTeX headers
- 21 Feb 2014 M. Sulprizio- Remove call to INIT_TROPOPAUSE, this is now done in the init stage
- 20 Jun 2014 R. Yantosca Now accept am_I_Root, Input_Opt, RC
- 06 Nov 2014 R. Yantosca Replace TRANSFER_2D with direct casts
- 17 Dec 2014 R. Yantosca Leave time/date variables as 8-byte
- 05 Mar 2015 R. Yantosca Add Input_Opt%RES_DIR to data path
- 06 Mar 2015 R. Yantosca Now read ann mean trop from netCDF

7.2.3 get_max_tpause_level

Function GET_MAX_TPAUSE_LEVEL returns GEOS-Chem level at the highest extent of the annual mean tropopause.

INTERFACE:

FUNCTION GET_MAX_TPAUSE_LEVEL() RESULT(L_MAX)

RETURN VALUE:

INTEGER :: L_MAX ! Maximum tropopause level

- 10 Feb 2005 R. Yantosca Initial version
- 09 Sep 2010 R. Yantosca Added ProTeX headers

7.2.4 get_min_tpause_level

Function GET_MIN_TPAUSE_LEVEL returns GEOS-Chem level at the lowest extent of the annual mean tropopause.

INTERFACE:

```
FUNCTION GET_MIN_TPAUSE_LEVEL() RESULT( L_MIN )
```

RETURN VALUE:

```
INTEGER :: L_MIN   ! Minimum tropopause level
```

REVISION HISTORY:

```
10 Feb 2005 - R. Yantosca - Initial version
09 Sep 2010 - R. Yantosca - Added ProTeX headers
```

7.2.5 get_min_chemgrid_level

Function GET_MIN_CHEMGRID_LEVEL returns GEOS-Chem level at the lowest extent of the chemistry grid

INTERFACE:

```
FUNCTION GET_MIN_CHEMGRID_LEVEL() RESULT( L_MIN )
```

USES:

RETURN VALUE:

```
INTEGER :: L_MIN  ! Minimum chemistry grid level
```

REVISION HISTORY:

```
10 Feb 2005 - R. Yantosca - Initial version
09 Sep 2010 - R. Yantosca - Added ProTeX headers
25 Mar 2013 - S. D. Eastham - Adapted from GET\_MIN\_TPAUSE\_LEVEL
```

7.2.6 get_max_chemgrid_level

Function GET_MAX_CHEMGRID_LEVEL returns GEOS-Chem level at the highest extent of the chemistry grid.

INTERFACE:

```
FUNCTION GET_MAX_CHEMGRID_LEVEL() RESULT( L_MAX )
```

USES:

RETURN VALUE:

```
INTEGER :: L_MAX    ! Maximum chemistry grid level
```

REVISION HISTORY:

```
10 Feb 2005 - R. Yantosca - Initial version
09 Sep 2010 - R. Yantosca - Added ProTeX headers
28 Aug 2013 - S. D. Eastham - Adapted from GET\_MAX\_TPAUSE\_LEVEL
```

7.2.7 get_chemgrid_level

Function GET_CHEMGRID_LEVEL returns the chemistry grid limit L_CHEM at surface location (I,J). Therefore, grid box (I,J,L_CHEM) is partially within the chemistry grid and partially outside of it. The grid box below this, (I,J,L_CHEM-1), is the last fully legitimate chemistry grid box in the column.

INTERFACE:

```
FUNCTION GET_CHEMGRID_LEVEL( I, J, State_Met ) RESULT( L_CHEM )
```

USES:

```
USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

RETURN VALUE:

```
INTEGER :: L_CHEM ! Chemgrid limit at (I,J)
```

REVISION HISTORY:

```
25 Mar 2013 - S. D. Eastham - Initial version
21 Feb 2014 - M. Sulprizio - Now pass State_Met object via the arg list
```

7.2.8 get_tpause_level

Function GET_TPAUSE_LEVEL returns the tropopause level L_TP at surface location (I,J). Therefore, grid box (I,J,L_TP) is partially in the troposphere and partially in the stratosphere. The grid box below this, (I,J,L_TP-1), is the last totally tropospheric box in the column.

INTERFACE:

FUNCTION GET_TPAUSE_LEVEL(I, J, State_Met) RESULT(L_TP)

USES:

USE ERROR_MOD, ONLY : GEOS_CHEM_STOP

USE CMN_SIZE_MOD ! Size parameters

INPUT PARAMETERS:

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

RETURN VALUE:

INTEGER :: L_TP ! Tropopause level at (I,J)

REVISION HISTORY:

22 Aug 2005 - R. Yantosca - Initial version

09 Sep 2010 - R. Yantosca - Added ProTeX headers

10 Sep 2010 - R. Yantosca - Update comments, remove obsolete documentation

21 Feb 2014 - M. Sulprizio- Now pass State_Met object via the arg list

26 Feb 2015 - E. Lundgren - Replace GET_PEDGE with State_Met%PEDGE.

Remove dependency on pressure_mod.

7.2.9 its_in_the_trop

Function ITS_IN_THE_TROP returns TRUE if grid box (I,J,L) lies within the troposphere, or FALSE otherwise.

INTERFACE:

FUNCTION ITS_IN_THE_TROP(I, J, L, State_Met) RESULT (IS_TROP)

USES:

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: I ! Longitude index
INTEGER, INTENT(IN) :: J ! Latitude index
INTEGER, INTENT(IN) :: L ! Level index

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

RETURN VALUE:

LOGICAL :: IS_TROP ! =T if we are in the troposphere

REMARKS:

REVISION HISTORY:

```
10 Feb 2005 - P. Le Sager - Initial version
(1 ) Modified for variable tropopause (phs, 9/14/06)
09 Sep 2010 - R. Yantosca - Added ProTeX headers
21 Feb 2014 - M. Sulprizio- Now pass State_Met object via the arg list
26 Feb 2015 - E. Lundgren - Replace GET_PEDGE with State_Met%PEDGE.
```

Remove dependency on pressure_mod.

7.2.10 its_in_the_stratmeso

Function ITS_IN_THE_STRATMESO returns TRUE if grid box (I,J,L) lies without the troposphere, or FALSE otherwise.

INTERFACE:

```
FUNCTION ITS_IN_THE_STRATMESO( I, J, L, State_Met )
& RESULT( IS_SMESO )
```

USES:

USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I     ! Longitude index
INTEGER, INTENT(IN) :: J     ! Latitude index
INTEGER, INTENT(IN) :: L     ! Level index
```

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

RETURN VALUE:

LOGICAL :: IS_SMESO ! =F if we are in the trop

- 10 Feb 2005 P. Le Sager Initial version
- (1) Modified for variable tropopause (phs, 9/14/06)
- (2) Now return the opposite value of ITS_IN_THE_TROP. This should help to avoid numerical issues. (phs, 11/14/08)
- 09 Sep 2010 R. Yantosca Added ProTeX headers
- 25 Mar 2013 S. D. Eastham Adapted from ITS_IN_THE_STRAT
- 21 Feb 2014 M. Sulprizio Now pass State_Met object via the arg list

7.2.11 its_in_the_strat

Function ITS_IN_THE_STRAT returns TRUE if grid box (I,J,L) lies within the stratosphere, or FALSE otherwise.

INTERFACE:

```
FUNCTION ITS_IN_THE_STRAT( I, J, L, State_Met ) RESULT( IS_STRAT )
```

USES:

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I ! Longitude index
INTEGER, INTENT(IN) :: J ! Latitude index
INTEGER, INTENT(IN) :: L ! Level index
```

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

RETURN VALUE:

```
LOGICAL :: IS_STRAT ! =T if we are in the stratosphere
```

REVISION HISTORY:

```
10 Feb 2005 - P. Le Sager - Initial version
```

- (1) Modified for variable tropopause (phs, 9/14/06)
- (2) Now return the opposite value of ITS_IN_THE_TROP. This should help to avoid numerical issues. (phs, 11/14/08)
- 09 Sep 2010 R. Yantosca Added ProTeX headers
- 24 Mar 2013 S. D. Eastham Now distinguish between strat and mesosphere
- 21 Feb 2014 M. Sulprizio Now pass State_Met object via the arg list

Function ITS_IN_THE_MESO returns TRUE if grid box (I,J,L) lies within the mesosphere, or FALSE otherwise.

INTERFACE:

```
FUNCTION ITS_IN_THE_MESO( I, J, L ) RESULT( IS_MESO )
```

INPUT PARAMETERS:

7.2.12 its_in_the_meso

RETURN VALUE:

LOGICAL :: IS_MESO ! =T if we are in the mesosphere

REVISION HISTORY:

```
10 Feb 2005 - P. Le Sager - Initial version
(1 ) Modified for variable tropopause (phs, 9/14/06)
(2 ) Now return the opposite value of ITS_IN_THE_TROP. This should help to avoid numerical issues. (phs, 11/14/08)
09 Sep 2010 - R. Yantosca - Added ProTeX headers
24 Mar 2013 - S. D. Eastham - Now distinguish between strat and mesosphere
```

7.2.13 its_in_the_chemgrid

Function ITS_IN_THE_CHEMGRID returns TRUE if grid box (I,J,L) lies within the chemistry grid, or FALSE otherwise.

INTERFACE:

```
FUNCTION ITS_IN_THE_CHEMGRID( I, J, L, State_Met ) & RESULT( IS_CHEM )
```

USES:

```
USE State_Met_Mod, ONLY : MetState
USE CMN_SIZE_MOD, Only : LLCHEM
```

INPUT PARAMETERS:

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

RETURN VALUE:

```
LOGICAL :: IS_CHEM ! =T if we are in the chem grid
```

REVISION HISTORY:

```
24 Mar 2013 - S. D. Eastham - Initial version
21 Feb 2014 - M. Sulprizio - Now pass State_Met object via the arg list
```

7.2.14 its_in_the_nochemgrid

Function ITS_IN_THE_NOCHEMGRID returns TRUE if grid box (I,J,L) lies outside the chemistry grid, or FALSE otherwise.

INTERFACE:

```
FUNCTION ITS_IN_THE_NOCHEMGRID( I, J, L, State_Met ) & RESULT( IS_NOCHEM )
```

USES:

USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: I ! Longitude index
INTEGER, INTENT(IN) :: J ! Latitude index
INTEGER, INTENT(IN) :: L ! Level index

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

RETURN VALUE:

LOGICAL :: IS_NOCHEM ! =F if we are in the chem grid

REVISION HISTORY:

```
24 Mar 2013 - S. D. Eastham - Initial version
21 Feb 2014 - M. Sulprizio - Now pass State_Met object via the arg list
```

-

7.2.15 diag_tropopause

Subroutine DIAG_TROPOPAUSE archives the ND55 tropopause diagnostic.

INTERFACE:

```
SUBROUTINE DIAG_TROPOPAUSE( am_I_Root, Input_Opt, State_Met, RC )
```

USES:

```
USE CMN_SIZE_MOD ! Size parameters
USE CMN_DIAG_MOD ! Diagnostic switches
```

#if defined(BPCH_DIAG)

USE DIAG_MOD, ONLY : AD55

#endif

USE ErrCode_Mod

USE Input_Opt_Mod, ONLY : OptInput
USE State_Met_Mod, ONLY : MetState

#if defined(NC_DIAG)

USE HCO_INTERFACE_MOD, ONLY : HcoState
USE Error_Mod, ONLY : Error_Stop
USE HCO_Diagn_Mod, ONLY : Diagn_Update

USE HCO_Error_Mod

#endif

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input options object
```

INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC ! Success or failure

REMARKS:

For GEOS-4, GEOS-5, 'MERRA', we use the tropopause pressure from the met field archive to determine if we are in the tropopause or not. Therefore, the 3rd slot of AD55 should be archived with the tropopause pressure from the met fields.

For other met fields, we have to estimate the tropopause pressure from the tropopause level. Archive the pressure at the midpoint of the level in which the tropopause occurs. NOTE: this may result in lower minimum tropopause pressure than reality.

- 30 Nov 1999 H. Liu, R. Yantosca Initial version
- (1) Make sure the DO-loops go in the order L-J-I, wherever possible.
- (2) Now archive ND55 diagnostic here rather than in DIAG1.F. Also, use an allocatable array (AD55) to archive tropopause heights.
- (3) HTPAUSE is now a local variable, since it is only used here.
- (4) Make LTPAUSE a local variable, since LPAUSE is used to store the annual mean tropopause. (bmy, 4/17/00)
- (5) Replace PW(I,J) with P(I,J). Also updated comments. (bmy, 10/3/01)
- (6) Removed obsolete code from 9/01 and 10/01 (bmy, 10/24/01)
- (7) Added polar tropopause for GEOS-3 in #if defined(GEOS_3) block (bmy, 5/20/02)
- (8) Replaced all instances of IM with IIPAR and JM with JJPAR, in order to prevent namespace confusion for the new TPCORE (bmy, 6/25/02)
- (9) Now use GET_PCENTER from "pressure_mod.f" to compute the pressure at the midpoint of box (I,J,L). Also deleted obsolete, commented-out code. (dsa, bdf, bmy, 8/21/02)
- (10) Now reference BXHEIGHT and T from "dao_mod.f". Also reference routine ERROR_STOP from "error_mod.f" (bmy, 10/15/02)
- (11) Now uses routine GET_YMID from "grid_mod.f" to compute grid box latitude. (bmy, 2/3/03)
- (12) Add proper polar tropopause level for GEOS-4 (bmy, 6/18/03)
- (13) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (14) Get tropopause level from TROPOPAUSE_MOD.F routines (phs, 10/17/06)
- 10 Sep 2010 R. Yantosca Added ProTeX headers
- 10 Sep 2010 R. Yantosca For GEOS-4, GEOS-5, MERRA met fields, take the the tropopause pressure directly from the met fields rather than computing it here.
- 10 Sep 2010 R. Yantosca Remove reference to LPAUSE, it's obsolete
- 10 Sep 2010 R. Yantosca Reorganize #if blocks for clarity
- 10 Sep 2010 R. Yantosca Renamed to DIAG_TROPOPAUSE and bundled into tropopause_mod.f
- 21 Feb 2014 M. Sulprizio- Now pass State_Met object via the arg list

```
26 Feb 2015 - E. Lundgren - Replace GET_PEDGE and GET_PCENTER with

State_Met%PEDGE and State_Met%PMID.

Remove dependency on pressure_mod.

21 Jan 2016 - E. Lundgren - Update diagnostic for netcdf output using HEMCO

29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
```

7.2.16 init_chemgrid

Subroutine INIT_CHEMGRID allocates and zeroes module arrays.

INTERFACE:

```
SUBROUTINE INIT_CHEMGRID( am_I_Root, Input_Opt, RC )
```

USES:

```
USE CMN_SIZE_MOD
USE ErrCode_Mod
```

USE ERROR_MOD, ONLY : ALLOC_ERR
USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REVISION HISTORY:

```
10 Feb 2005 - R. Yantosca - Initial version
```

09 Sep 2010 - R. Yantosca - Added ProTeX headers

29 Mar 2013 - R. Yantosca - Now made public so we can shadow LVARTROP

7.2.17 cleanup_chemgrid

Subroutine CLEANUP_CHEMGRID deallocates module arrays.

INTERFACE:

SUBROUTINE CLEANUP_CHEMGRID

```
10 Feb 2005 - R. Yantosca - Initial version
09 Sep 2010 - R. Yantosca - Added ProTeX headers
```

7.3 Fortran: Module Interface chemistry_mod.F

Module CHEMISTRY_MOD is used to call the proper chemistry subroutine for the various GEOS-Chem simulations.

INTERFACE:

MODULE CHEMISTRY_MOD

USES:

```
USE PRECISION_MOD ! For GEOS-Chem Precision (fp)
USE GEOS_TIMERS_MOD ! For GEOS-Chem timers (optional)

IMPLICIT NONE
```

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: INIT_CHEMISTRY
PUBLIC :: DO_CHEMISTRY
PUBLIC :: RECOMPUTE_OD

PRIVATE :: CHEM_PASSIVE_TRACER

REVISION HISTORY:

PRIVATE

- (1) Bug fix in DO_CHEMISTRY (bnd, bmy, 4/14/03)
- (2) Now references DEBUG_MSG from "error_mod.f" (bmy, 8/7/03)
- (3) Now references "tagged_ox_mod.f"(bmy, 8/18/03)
- (4) Now references "Kr85_mod.f" (jsw, bmy, 8/20/03)
- (5) Bug fix: Now also call OPTDEPTH for GEOS-4 (bmy, 1/27/04)
- (6) Now references "carbon_mod.f" and "dust_mod.f" (rjp, tdf, bmy, 4/5/04)
- (7) Now references "seasalt_mod.f" (rjp, bec, bmy, 4/20/04)
- (8) Now references "logical_mod.f", "tracer_mod.f", "diag20_mod.f", and "diag65_mod.f", and "aerosol_mod." (bmy, 7/20/04)
- (9) Now references "mercury_mod.f" (bmy, 12/7/04)
- (10) Updated for SO4s, NITs chemistry (bec, bmy, 4/13/05)
- (11) Now call CHEM_HCN_CH3CN from "hcn_ch3cn_mod.f". Also remove all references to the obsolete CO-OH param simulation. (xyp, bmy, 6/24/05)
- (12) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (13) Now call MAKE_RH from "main.f" (bmy, 3/16/06)
- (14) Updated for SOA from isoprene (dkh, bmy, 6/1/06)
- (15) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (16) For now, replace use RPMARES instead of ISORROPIA. (bmy, 4/2/08)
- (17) Added KPP chemistry driver subroutine (phs,ks,dhk, 09/15/09)
- (18) Added public member function recompute_OD (skim, 02/03/11)
- 17 Dec 2009 R. Yantosca Added ProTeX headers
- 28 Jan 2010 C. Carouge, R. Yantosca Modified for ISORROPIA II
- 08 Aug 2012 R. Yantosca Now align IF statements better
- 10 Aug 2012 R. Yantosca Cosmetic changes
- 25 Mar 2013 M. Payer Now pass State_Chm to several routines

```
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete

19 May 2014 - C. Keller - Added INIT_CHEMISTRY

15 Dec 2014 - M. Yannetti - KPP code is commented out unless compiling KPP

08 Jan 2015 - M. Sulprizio- Now restrict KPP to REAL*8 to allow for KPP code
to compile properly

13 Aug 2015 - E. Lundgren - Tracer units are now kg/kg and converted to
kg within DO_CHEMISTRY

03 Nov 2016 - C. Keller - Added wrapper routine for passive tracers.
```

7.3.1 do_chemistry

Subroutine DO_CHEMISTRY is the driver routine which calls the appropriate chemistry subroutine for the various GEOS-Chem simulations.

INTERFACE:

```
SUBROUTINE DO_CHEMISTRY( am_I_Root, Input_Opt, & State_Chm, State_Met, RC )
```

USES:

```
USE AEROSOL_MOD,
                        ONLY : AEROSOL_CONC
USE AEROSOL_MOD,
                        ONLY: RDAER
USE AEROSOL_MOD,
                        ONLY : SOILDUST
USE C2H6_MOD,
                        ONLY: CHEMC2H6
USE CARBON_MOD,
                        ONLY: CHEMCARBON
USE CMN_DIAG_MOD
USE CMN_SIZE_MOD
USE DUST_MOD,
                        ONLY: CHEMDUST
USE DUST_MOD,
                        ONLY : RDUST_ONLINE
USE ErrCode_Mod
USE ERROR_MOD
                        ONLY : Do_FlexChem
USE FlexChem_Mod,
USE GLOBAL_CH4_MOD,
                        ONLY: CHEMCH4
                        ONLY : OptInput
USE Input_Opt_Mod,
USE ISOROPIAII_MOD,
                        ONLY : DO_ISOROPIAII
                        ONLY: CHEMMERCURY
USE MERCURY_MOD,
USE POPS_MOD,
                        ONLY: CHEMPOPS
USE RnPbBe_MOD,
                        ONLY: CHEMRnPbBe
                        ONLY : DO_RPMARES
USE RPMARES_MOD,
USE SEASALT_MOD,
                        ONLY: CHEMSEASALT
USE SULFATE_MOD,
                        ONLY: CHEMSULFATE
USE State_Chm_Mod,
                        ONLY : ChmState
USE State_Chm_Mod,
                        ONLY : Ind_
USE State_Met_Mod,
                        ONLY : MetState
USE STRAT_CHEM_MOD,
                        ONLY : DO_STRAT_CHEM
USE TAGGED_CO_MOD,
                        ONLY : CHEM_TAGGED_CO
USE TAGGED_03_MOD,
                       ONLY: CHEM_TAGGED_03
```

USE TIME_MOD, ONLY : GET_ELAPSED_MIN USE TIME_MOD, ONLY : GET_TS_CHEM

#if defined(USE_TEND)

USE TENDENCIES_MOD

#endif

USE UnitConv_Mod

#if defined (UCX)

USE UCX_MOD, ONLY : CALC_STRAT_AER ! (SDE 04/20/13)

USE UCX_MOD, ONLY : READ_PSC_FILE
USE UCX_MOD, ONLY : WRITE_STATE_PSC

#endif

#if defined(TOMAS)

USE TOMAS_MOD, ONLY: DO_TOMAS !(win, 7/14/09)

#endif

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INPUT/OUTPUT PARAMETERS:

TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REMARKS:

- (1) Now reference DELP, T from "dao_mod.f" since we need to pass this to OPTDEPTH for GEOS-1 or GEOS-STRAT met fields (bnd, bmy, 4/14/03)
- (2) Now references DEBUG_MSG from "error_mod.f" (bmy, 8/7/03)
- (3) Removed call to CHEMO3, it's obsolete. Now calls CHEM_TAGGED_OX !
 from "tagged_ox_mod.f" when NSRCX==6. Now calls Kr85 chemistry if
 NSRCX == 12 (jsw, bmy, 8/20/03)
- (4) Bug fix: added GEOS-4 to the #if block in the call to OPTDEPTH. (bmy, 1/27/04)
- (5) Now calls CHEMCARBON and CHEMDUST to do carbon aerosol & dust aerosol chemistry (rjp, tdf, bmy, 4/2/04)
- (6) Now calls CHEMSEASALT to do seasalt aerosol chemistry (rjp, bec, bmy, 4/20/04)
- (7) Now references "logical_mod.f" & "tracer_mod.f". Now references AEROSOL_CONC, AEROSOL_RURALBOX, and RDAER from "aerosol_mod.f". Now includes "CMN_DIAG" and "comode.h". Also call READER, READCHEM, and INPHOT to initialize the FAST-J arrays so that we can save out!

- AOD's to the ND21 diagnostic for offline runs. (bmy, 7/20/04)
- (8) Now call routine CHEMMERCURY from "mercury_mod.f" for an offline HgO/Hg2/HgP simulation. (eck, bmy, 12/7/04)
- (9) Now do not call DO_RPMARES if we are doing an offline aerosol run with crystalline sulfur & aqueous tracers (cas, bmy, 1/7/05)
- (10) Now use ISOROPIA for aer thermodyn equilibrium if we have seasalt tracers defined, or RPMARES if not. Now call CHEMSEASALT before CHEMSULFATE. Now do aerosol thermodynamic equilibrium before aerosol chemistry for offline aerosol runs. Now also reference CLDF from "dao_mod.f" (bec, bmy, 4/20/05)
- (11) Now modified for GCAP met fields. Now call CHEM_HCN_CH3CN from "hcn_ch3cn_mod.f". Also remove allreferences to the obsolete CO-OH param simulation. (xyp, bmy, 6/23/05)
- (12) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (13) Now call MAKE_RH from "main.f" (bmy, 3/16/06)
- (14) Removed ISOP_PRIOR as a local variable (dkh, bmy, 6/1/06)
- (15) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (16) Now use DRYFLXH2HD and CHEM_H2_HD for H2/HD sim (lyj, phs, 9/18/07)
- (17) Bug fix: now hardwired to use RPMARES since ISORROPIA can return very unphysical values at low RH. Wait for ISORROPIA II. (bmy, 4/2/08)
- (18) The dry deposition diagnostic (ND44) is done in vdiff_mod if using non-local PBL (lin, ccc, 5/29/09)
- (19) Now calls CHEMPOPS from "pops_mod.f" for an offline POPs simulation (eck, 9/20/10)
- 17 Dec 2009 R. Yantosca Added ProTeX headers
- 25 Jan 2010 R. Yantosca Now call DO_TOMAS for TOMAS microphysics
- 28 Jan 2010 C. Carouge, R. Yantosca Modified for ISORROPIA II
- 19 Mar 2012 R. Yantosca Add C-preprocessor switch to shut off ISORROPIA to facilitate debugging
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument, and pass this down to lower-level chem routines for GIGC
- 08 Aug 2012 R. Yantosca Now align IF statements better
- 10 Aug 2012 R. Yantosca Cosmetic changes
- 18 Oct 2012 R. Yantosca Rename GC_MET argument to State_Met
- 18 Oct 2012 R. Yantosca Rename CHEM_STATE argument to State_Chem
- 19 Oct 2012 R. Yantosca Now reference gigc_state_chm_mod.F90
- 19 Oct 2012 R. Yantosca Now reference gigc_state_met_mod.F90
- 25 Oct 2012 R. Yantosca Add comments for GIGC #ifdefs
- 25 Oct 2012 R. Yantosca Add the RC output argument for the GIGC
- 08 Nov 2012 R. Yantosca Now pass Input_Opt argument for the GIGC and use fields of Input_Opt to replace logicals
- 15 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 26 Nov 2012 R. Yantosca Now pass Input_Opt, State_Chm, RC to routine DO_STRAT_CHEM (in GeosCore/strat_chem_mod.F90)
- 11 Dec 2012 R. Yantosca Remove NI, NJ, NL, NCNST arguments; these are now obtained either from CMN_SIZE_mod.F or from the Input_Opt object

```
05 Mar 2013 - R. Yantosca - Now pass am_I_Root, Input_Opt, RC to DRYFLX
25 Mar 2013 - H. Amos
                         - merged C. Friedman's PAH code into v9-01-03
28 Mar 2013 - S.D. Eastham- Updated to use FAST_JX_MOD
31 May 2013 - R. Yantosca - Now pass Input_Opt, State_Chm to DO_TOMAS
19 May 2014 - C. Keller - Removed call for acetone ocean sink - now done
                            in HEMCO.
06 Nov 2014 - M. Yannetti - Added PRECISION_MOD
08 May 2015 - C. Keller - Added WRITE_STATE_PSC.
18 May 2015 - R. Yantosca - Remove DIAG_STATE_PSC, that is not used anymore
15 Jun 2015 - R. Yantosca - Removed calls to DRYFLXRnPbBe, that's obsolete
04 Sep 2015 - C. Keller
                          - Added passive tracer call.
17 Mar 2016 - M. Sulprizio- Remove call to OPTDEPTH. The optical depth fields
                            are now saved into State_Met%OPTD in the routines
                            that read the met fields from disk.
16 May 2016 - M. Sulprizio- Remove call to AEROSOL_RURALBOX. The FlexChem
                            implementation has rendered the routine obsolete.
16 Jun 2016 - C. Miller
                         - Now use Ind_ function to define species ID's
17 Jun 2016 - R. Yantosca - Now define species ID's only on first call
17 Jun 2016 - R. Yantosca - Now reset first-time flag at end of routine
30 Jun 2016 - R. Yantosca - Remove instances of STT.
19 Jul 2016 - R. Yantosca - Now bracket DO_TEND calls with #ifdef USE_TEND
10 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code
11 Aug 2016 - R. Yantosca - Clean up calls to error subroutines
```

7.3.2 recompute_od

Subroutine RECOMPUTE_OD will update the optical depth values before accumulating or writing the diagnostics.

INTERFACE:

```
SUBROUTINE RECOMPUTE_OD( am_I_Root, Input_Opt,
& State_Met, State_Chm, RC )
```

USES:

```
! References to F90 modules
USE AEROSOL_MOD,
                        ONLY : AEROSOL_CONC
USE AEROSOL_MOD,
                        ONLY: RDAER
USE AEROSOL_MOD,
                        ONLY: SOILDUST
USE DUST_MOD,
                       ONLY : RDUST_ONLINE
USE DUST_MOD,
                        ONLY : RDUST_OFFLINE
USE ErrCode_Mod
USE ERROR_MOD,
                        ONLY : DEBUG_MSG
                        ONLY : OptInput
USE Input_Opt_Mod,
USE State_Chm_Mod,
                       ONLY : ChmState
USE State_Met_Mod,
                       ONLY : MetState
USE TIME_MOD,
                       ONLY : GET_MONTH
```

USE TIME_MOD, ONLY : GET_YEAR

INPUT PARAMETERS:

:: am_I_Root ! Is this the root CPU? LOGICAL, INTENT(IN) TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

```
03 Fev 2011 - Adapted from chemdr.f by skim
30 Jul 2012 - R. Yantosca - Now accept am_I_Root as an argument when
                           running with the traditional driver main.F
13 Nov 2012 - R. Yantosca - Now pass Input_Opt and RC arguments for GIGC
15 Nov 2012 - M. Payer - Now pass all met fields via State_Met
25 Mar 2013 - R. Yantosca - Now accept am_I_Root, Input_Opt, State_Chm, RC
12 Aug 2015 - E. Lundgren - Input tracer units are now [kg/kg] and
                            are converted to [kg] for recomputing OD
```

7.3.3 chem_passive_tracer

Subroutine RUN_PASSIVE_TRACER performs loss chemistry on all passive tracers.

INTERFACE:

```
SUBROUTINE CHEM_PASSIVE_TRACER ( am_I_Root, Input_Opt,
                                 State_Met, State_Chm, RC )
```

USES:

```
USE ErrCode_Mod
USE ERROR_MOD,
                      ONLY : GC_Error
USE Input_Opt_Mod,
                     ONLY : OptInput
USE State_Chm_Mod,
                      ONLY : ChmState
USE State_Met_Mod,
                       ONLY : MetState
USE State_Chm_Mod,
                       ONLY : ind_
USE PASSIVE_TRACER_MOD, ONLY : PASSIVE_TRACER_GETRATE
```

USE PASSIVE_TRACER_MOD, ONLY : NPASSIVE, PASSIVE_NAME

USE TIME_MOD, ONLY : GET_TS_CHEM

INPUT PARAMETERS:

```
INTENT(IN ) :: am_I_Root ! root CPU?
LOGICAL.
                           ) :: Input_Opt ! Input options object
TYPE(OptInput),
              INTENT(IN
TYPE(MetState), INTENT(IN ) :: State_Met ! Meteorology state object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(IN ) :: State_Chm ! Chemistry state object
INTEGER, INTENT(INOUT) :: RC ! Failure or success
!REMARKS
```

REVISION HISTORY:

```
04 Sep 2015 - C. Keller - Initial version
03 Nov 2016 - C. Keller - Moved to chemistry_mod
```

7.3.4 init_chemistry

Subroutine INIT_CHEMISTRY initializes chemistry variables.

INTERFACE:

```
SUBROUTINE INIT_CHEMISTRY( am_I_Root, Input_Opt, State_Chm, RC )
```

ONLY : LLTROP

USES:

```
USE ErrCode_Mod

USE FAST_JX_MOD, ONLY : INIT_FJX

USE FlexChem_Mod, ONLY : Init_FlexChem

USE Input_Opt_Mod, ONLY : OptInput

USE State_Chm_Mod, ONLY : ChmState
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?
```

INPUT/OUTPUT PARAMETERS:

USE CMN_SIZE_MOD,

```
TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input Options object
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
INTEGER, INTENT(INOUT) :: RC ! Success or failure?
```

REVISION HISTORY:

```
19 May 2014 - C. Keller - Initial version (stripped from do_chemistry and chemdr.F)
20 Jun 2014 - R. Yantosca - Now pass Input_Opt to INIT_FJX
23 Jun 2016 - R. Yantosca - Remove call to SETTRACE, it's obsolete
```

7.4 Fortran: Module Interface fast_jx_mod.F

Module FAST_JX_MOD contains routines and variables for calculating photolysis rates using the Fast-JX scheme (Prather et al). Current implementation is version 7.0a.

INTERFACE:

MODULE FAST_JX_MOD

USES:

USE CMN_FJX_MOD

USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

IMPLICIT NONE

PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: EXITC PUBLIC :: PHOTO_JX PUBLIC :: INIT_FJX PUBLIC :: FAST_JX PUBLIC :: PHOTRATE_ADJ

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: SOLAR_JX PRIVATE :: OPMIE PRIVATE :: MIESCT PRIVATE :: LEGNDO PRIVATE :: BLKSLV PRIVATE :: GEN_ID PRIVATE :: JRATET PRIVATE :: X_INTERP PRIVATE :: SPHERE2 PRIVATE :: EXTRAL PRIVATE :: RD_PROF_NC PRIVATE :: RD_XXX PRIVATE :: RD_AOD PRIVATE :: RD_MIE PRIVATE :: RD_JS_JX

REVISION HISTORY:

PRIVATE :: SET_AER

27 Mar 2013 - S. D. Eastham - Initial version (based on original GEOS-Chem files and instructions from J. Mao)

28 Mar 2013 - S. D. Eastham - Upgraded to Fast-JX v7.0

20 Feb 2014 - M. Sulprizio - Removed "define.h", this is now obsolete

13 Nov 2014 - M. Yannetti - Added PRECISION_MOD

29 Mar 2016 - R. Yantosca - Add flags for rxns adjusted by PHOTRATE_ADJ 27 Jun 2016 - M. Sulprizio - Remove FJXFUNC and JV_INDEX routines. We now obtain the photolysis rates directly from the

ZPJ array.

29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90

7.4.1 fast_jx

Subroutine FAST_JX loops over longitude and latitude, and calls PHOTO_JX to compute J-Values for each column at every chemistry time-step.

INTERFACE:

```
SUBROUTINE FAST_JX( WLAOD, am_I_Root, Input_Opt, State_Met,
& State_Chm, RC )
```

USES:

```
USE CHEMGRID_MOD,
                       ONLY : GET_CHEMGRID_LEVEL
USE CMN_SIZE_MOD,
                       ONLY: IIPAR, JJPAR, LLPAR
USE CMN_SIZE_MOD,
                       ONLY : NDUST
USE ErrCode_Mod
USE ERROR_MOD,
                      ONLY : ERROR_STOP, ALLOC_ERR
USE ERROR_MOD,
                      ONLY : DEBUG_MSG
                     ONLY : GET_YMID
USE GC_GRID_MOD,
USE Input_Opt_Mod, ONLY: OptInput
USE State_Chm_Mod,
                       ONLY : ChmState
                       ONLY : Ind_
USE State_Chm_Mod,
USE State_Met_Mod,
                       ONLY : MetState
USE TIME_MOD,
                       ONLY: GET_MONTH, GET_DAY, GET_DAY_OF_YEAR
USE TIME_MOD,
                       ONLY : GET_TAU,
                                         GET_YEAR
USE TOMS_MOD,
                       ONLY : GET_OVERHEAD_O3
IMPLICIT NONE
```

Uncomment the appropriate #define statement to denote which of the available cloud overlap options that you wish to use.

```
! Linear overlap
#define USE_LINEAR_OVERLAP 1
```

Approximate random overlap (balance between accuracy & speed) #define USE_APPROX_RANDOM_OVERLAP 1

```
! Maximum random cloud overlap (most computationally intensive)
#define USE_MAXIMUM_RANDOM_OVERLAP 1
```

INPUT PARAMETERS:

```
! How was AOD calculated? (1: 550 nm, 0: 999 nm)
INTEGER, INTENT(IN) :: WLAOD
! Is this the root CPU?
LOGICAL, INTENT(IN) :: am_I_Root
```

! Input options

TYPE(OptInput), INTENT(IN) :: Input_Opt

! Meteorology State object

TYPE(MetState), INTENT(IN) :: State_Met

! Chemistry State object

TYPE(ChmState), INTENT(IN) :: State_Chm

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC

REMARKS:

Parameter to choose cloud overlap algorithm:

(1) OVERLAP (INTEGER) : 1 - Linear Approximation (used up to v7-04-12)

2 - Approximate Random Overlap (default)

3 - Maximum Random Overlap (computation intensive)

- 01 Apr 1998 P. Murti, R. Martin, R. Yantosca Initial version
- (1) Call this routine EACH chemistry time-step, before solver.
- (2) This routine must know IMAX, JMAX, LMAX.
- (3) Now use new !\$OMP compiler directives for parallelization (bmy, 5/2/00)
- (4) Now reference "cmn_fj.h" and "jv_cmn.h" for the aerosol optical depths (bmy, 10/2/00)
- (5) Add OPTDUST as a local variable -- make OPTDUST private for the parallel DO-loop, since it stores 1 column of aerosol optical depth for each dust type (bmy, rvm, 10/2/00)
- (6) For now, LPAR in "cmn_fj.h" = LGLOB in "CMN_SIZE". Therefore we assume that we are always doing global runs. (bmy, 10/2/00)
- (7) Removed obsolete code from 10/2/00 (bmy, 12/21/00)
- (8) Replace {IJL}GLOB w/ IIPAR, JJPAR, LLPAR everywhere. Also YLMID(NLAT) needs to be referenced by YLMID(NLAT+JO). (bmy, 9/26/01)
- (9) Remove obsolete code from 9/01. Updated comments. (bmy, 10/24/01)
- (10) Add OPTAER as a local variable, make it private for the parallel DO loop, since it stores 1 column of aerosol optical depths for each aerosol type. Pass OPTAER to PHOTOJ via the argument list. Declare OPTAER as PRIVATE for the parallel DO-loop. (rvm, bmy, 2/27/02)
- (11) Now reference GET_PEDGE from "pressure_mod.f", which returns the correct "floating" pressure. (dsa, bdf, bmy, 8/20/02)
- (12) Now reference T from "dao_mod.f" (bmy, 9/23/02)
- (13) Now uses routine GET_YMID from "grid_mod.f" to compute grid box latitude. Now make IDAY, MONTH local variables. Now use function GET_DAY_OF_YEAR from "time_mod.f". Bug fix: now IDAY (as passed to photoj.f) is day of year rather than cumulative days since Jan 1,

1985. (bmy, 2/11/03)

- (14) Now reference routine GET_YEAR from "time_mod.f". Added LASTMONTH as a SAVEd variable. Now call READ_TOMSO3 from "toms_mod.f" at the beginning of a new month (or the first timestep) to read TOMS O3 columns which will be used by "set_prof.f". Now also reference routine GET_DAY from "time_mod.f". Rename IDAY to DAY_OF_YR. Pass day of month to PHOTOJ. Updated comments, cosmetic changes. (bmy, 7/17/03)
- (15) Bug fix: PRES needs to be the true surface pressure for GEOS-4, but PS-PTOP for all prior GEOS models. (bmy, 2/6/04)
- (16) Now account for cloud overlap (Maximum-Random Overlap and Random Overlap) in each column (hyl, phs, bmy, 9/18/07)
- (17) Now initialize the PJ array here, instead of two layers below in "set_prof.f". Now no longer pass PRES to "photoj.f". (bmy, 11/29/07)
- (18) Now switch to approx. random overlap option (hyl, phs, bmy, 10/7/08)
- (19) Now can handle GEOS-5 reprocessed met data with OPTDEPTH being in-cloud optical depths. (bmy, hyl, 10/24/08)
- (10) Remove references to IN_CLOUD_OD (bmy, 10/15/09)
- 13 Aug 2010 R. Yantosca Added ProTeX headers
- 13 Aug 2010 R. Yantosca Treat MERRA in the same way as GEOS-5
- 08 Feb 2012 R. Yantosca Treat GEOS-5.7.x in the same way as MERRA
- 01 Mar 2012 R. Yantosca Now use GET_YMID(I,J,L) from grid_mod.F90
- 06 Mar 2012 R. Yantosca Now call GET_OVERHEAD_03 to get the total overhead 03 column for FAST-J
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 10 Aug 2012 R. Yantosca Replace IPAR, JPAR, LPAR w/ IIPAR, JJPAR, LLPAR
- 27 Mar 2013 S.D. Eastham- Rolled in FAST_JX_MOD
- 21 Feb 2014 M. Sulprizio- Replaced all met field arrays with State_Met derived type object
- 28 Feb 2014 M. Sulprizio- Now obtain O3_CTM directly from CSPEC
- 05 Mar 2014 R. Yantosca Cosmetic changes
- 06 Nov 2014 R. Yantosca Now use State_Met%CLDF(I,J,L)
- 06 Nov 2014 R. Yantosca Now use State_Met%OPTD(I,J,L)
- 26 Feb 2015 E. Lundgren Replace GET_PEDGE with State_Met%PEDGE.

 Remove dependency on pressure_mod and
 redundant PEDGE pre-preprocessor block if
 EXTERNAL_GRID.
- 09 Apr 2015 R. Yantosca Bug fixes: Add missing vars to !\$OMP+PRIVATE clause and error check for JLOOP > 0
- 11 Aug 2015 R. Yantosca MERRA2 behaves the same way as for GEOS-FP
- 21 Dec 2015 M. Sulprizio- Replace CSPEC with State_Chm%Species
- 17 Jun 2016 R. Yantosca Now define id_03 with the Ind_ function

7.4.2 blkslv

Subroutine BLKSLV solves the block tri-diagonal system

INTERFACE:

```
SUBROUTINE BLKSLV
```

& (FJ,POMEGA,FZ,ZTAU,ZFLUX,RFL,PM,PMO,FJTOP,FJBOT,ND)

USES:

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: ND
REAL(fp), INTENT(IN) :: POMEGA(M2_,N_,W_),FZ(N_,W_),ZTAU(N_,W_),
& PM(M_,M2_),PMO(M2_),
& RFL(W_),ZFLUX(W_)
```

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT) :: FJ(N_,W_),FJTOP(W_),FJBOT(W_)
```

REMARKS:

```
The block tri-diagonal system:

A(I)*X(I-1) + B(I)*X(I) + C(I)*X(I+1) = H(I)
```

REVISION HISTORY:

```
27 Mar 2013 - S. D. Eastham - Copied from GEOS-Chem v9-01-03
```

7.4.3 gen_id

Subroutine GEN generates coefficient matrices for the block tri-diagonal system described in BLKSLV.

INTERFACE:

```
SUBROUTINE GEN_ID(POMEGA,FZ,ZTAU,ZFLUX,RFL,PM,PMO ,B,CC,AA,A,H,C, ND)
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: ND
REAL(fp), INTENT(IN) :: POMEGA(M2_,N_),PM(M_,M2_),PMO(M2_)
REAL(fp), INTENT(IN) :: ZFLUX,RFL
REAL(fp), INTENT(IN),DIMENSION(N_) :: FZ,ZTAU
```

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT), DIMENSION(M_,M_,N_) :: B,AA,CC REAL(fp), INTENT(OUT), DIMENSION(M_,N_) :: A,C,H
```

```
28 Mar 2013 - S. D. Eastham - Copied from Fast-JX v7.0
```

7.4.4 jratet

Subroutine JRATET calculates temperature-dependent J-rates.

INTERFACE:

```
SUBROUTINE JRATET(PPJ,TTJ,FFF,VALJL,LCTM,LCHEM,NJXU)
```

USES:

INPUT PARAMETERS:

```
integer, intent(in) :: LCTM,LCHEM,NJXU
real(fp), intent(in) :: PPJ(JXL1_+1),TTJ(JXL1_+1)
real(fp), intent(inout) :: FFF(W_,LCTM)
!OUTPUT VARIABLES:
real(fp), intent(out), dimension(LCTM,NJXU) :: VALJL
```

REMARKS:

REVISION HISTORY:

```
28 Mar 2013 - S. D. Eastham - Copied from Fast-JX v7.0
02 Apr 2013 - S. D. Eastham - Now only assign J-rates on levels within the chemistry grid.
```

$7.4.5 x_{interp}$

Subroutine X_INTERP is an up-to-three-point linear interp. function for cross-sections.

INTERFACE:

```
SUBROUTINE X_INTERP (TINT, XINT, T1, X1, T2, X2, T3, X3, L123)
```

USES:

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: TINT,T1,T2,T3, X1,X2,X3
INTEGER, INTENT(IN) :: L123
!OUTPUT VARIABLES:
    REAL(fp), INTENT(OUT) :: XINT
```

REMARKS:

```
28 Mar 2013 - S. D. Eastham - Copied from Fast-JX v7.0
```

7.4.6 sphere2

Subroutine SPHERE2 is an AMF2.

INTERFACE:

SUBROUTINE SPHERE2 (UO, ZHL, AMF2, L1U, LJX1U)

USES:

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: L1U, LJX1U
REAL(fp), INTENT(IN) :: U0,ZHL(L1U+1)

!OUTPUT VARIABLES:

REAL(fp), INTENT(OUT) :: AMF2(2*LJX1U+1,2*LJX1U+1)

REMARKS:

Quoting from the original:

New v6.2: does AirMassFactors for mid-layer, needed for SZA ~ 90
This new AMF2 does each of the half-layers of the CTM separately,
whereas the original, based on the pratmo code did the whole layers
and thus calculated the ray-path to the CTM layre edges, NOT the middle.
Since fast-JX is meant to calculate the intensity at the mid-layer, the
solar beam at low sun (interpolated between layer edges) was incorrect.
This new model does make some approximations of the geometry of the layers:
the CTM layer is split evenly in mass (good) and in height (approx).

Calculation of spherical geometry; derive tangent heights, slant path lengths and air mass factor for each layer. Not called when SZA > 98 degrees. Beyond 90 degrees, include treatment of emergent beam (where tangent height is below altitude J-value desired at).

```
Inputs:
```

U0 cos(solar zenith angle)

RAD radius of Earth mean sea level (cm)

ZHL(L) height (cm) of the bottom edge of CTM level L

ZZHT scale height (cm) used above top of CTM (ZHL(L_+1))

L1U dimension of CTM = levels +1 (L+1 = above-CTM level)

Outputs:

 $\label{eq:amf2} \begin{tabular}{ll} AMF2(I,J) = air mass factor for CTM level I for sunlight reaching J \\ (these are calculated for both layer middle and layer edge) \\ \end{tabular}$

```
28 Mar 2013 - S. D. Eastham - Copied from Fast-JX v7.0
04 Dec 2014 - R. Yantosca - Now use SQRT instead of DSQRT
```

7.4.7 extral

Subroutine EXTRAL adds sub-layers to thick cloud/aerosol layers using log-spacing for sub-layers of increasing thickness ATAU.

INTERFACE:

SUBROUTINE EXTRAL (DTAUX, L1X, L2X, NX, JXTRA)

USES:

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: L1X,L2X !index of cloud/aerosol
integer, intent(in) :: NX !Mie scattering array size
real(fp), intent(in) :: DTAUX(L1X) !cloud+3aerosol OD in each layer
!OUTPUT VARIABLES:
integer, intent(out):: JXTRA(L2X+1) !number of sub-layers to be added
```

REMARKS:

```
DTAUX(L=1:L1X) = Optical Depth in layer L (generally 600 nm OD)
   This can be just cloud or cloud+aerosol, it is used only to set
   the number in levels to insert in each layer L
   Set for log-spacing of tau levels, increasing top-down.
```

N.B. the TTAU, etc calculated here are NOT used elsewhere

The log-spacing parameters have been tested for convergence and chosen to be within 0.5% for ranges OD=1-500, rflect=0-100%, mu0=0.1-1.0 use of ATAU = 1.18 and min = 0.01, gives at most +135 pts for OD=100 ATAU = 1.12 now recommended for more -accurate heating rates (not J's)

REVISION HISTORY:

```
28 Mar 2013 - S. D. Eastham - Copied from Fast-JX v7.0
```

7.4.8 exitc

Subroutine EXITC forces an error in GEOS-Chem and quits.

INTERFACE:

```
SUBROUTINE EXITC (T_EXIT)
```

USES:

```
USE ERROR_MOD, ONLY : ERROR_STOP
```

INPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(IN) :: T_EXIT
!OUTPUT VARIABLES:
```

REMARKS:

REVISION HISTORY:

```
28 Mar 2013 - S. D. Eastham - Copied from Fast-JX v7.0
```

7.4.9 int_fjx

Subroutine INIT_FJX initializes Fast-JX variables.

INTERFACE:

```
SUBROUTINE INIT_FJX( am_I_Root, Input_Opt, RC )
```

USES:

```
USE CMN_DIAG_MOD, ONLY : ND64
```

USE ErrCode_Mod

USE Input_Opt_Mod, ONLY : OptInput
USE inquireMod, ONLY : findFreeLUN

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

OUTPUT PARAMETERS:

REVISION HISTORY:

```
28 Mar 2013 - S. D. Eastham - Copied from Fast-JX v7.0 05 Mar 2014 - R. Yantosca - Use correct filenames for use w/ ESMF
```

$7.4.10 \text{ rd}_{-xxx}$

Subroutine RD_XXX reads in wavelength bins, solar fluxes, Rayleigh and temperature-dependent cross-sections.

INTERFACE:

SUBROUTINE RD_XXX (NUN, NAMFIL, am_I_Root)

USES:

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NUN
CHARACTER(*), INTENT(IN) :: NAMFIL
LOGICAL, INTENT(IN) :: am_I_Root
!OUTPUT VARIABLES:
```

REMARKS:

```
NEW v-6.8 now allow 1 to 3 sets of X-sects for T or P
    LQQ = 1, 2, or 3 to determine interpolation with T or P
    IF the temperatures TQQQ are <0, then use as pressure interp (hPa)
    NB - the temperatures and pressures must be increasing
NEW v-6.4 changed to collapse wavelengths & x-sections to Trop-only:
    WX_ = 18 should match the JX_spec.dat wavelengths
    W_ = 12 (Trop-only) or 18 (std) is set in (CMN_FJX.F).
if W_=12 then drop strat wavels, and drop x-sects (e.g. N2O, ...)
    W_ = 8, reverts to quick fix: fast-J (12-18) plus bin (5) scaled</pre>
```

NAMFIL Name of spectral data file (FJX_spec.dat) >> j2 for fast-J2 NUN Channel number for reading data file Number of species to calculate J-values for NJX NWWW Number of wavelength bins, from 1:NWWW Boundaries of wavelength bins WBIN WL Centres of wavelength bins - 'effective wavelength' FL Solar flux incident on top of atmosphere (cm-2.s-1) Rayleigh parameters (effective cross-section) (cm2) QRAYL Q02 02 cross-sections Q03 03 cross-sections Q1D 03 => 0(1D) quantum yield Temperature for supplied cross sections TQQ Supplied cross sections in each wavelength bin (cm2) QQQ

REVISION HISTORY:

```
28 Mar 2013 - S. D. Eastham - Copied from Fast-JX v7.0 09 May 2014 - S. D. Eastham - Fixed bug when using <18 wavelengths
```

7.4.11 rd_mie

Subroutine RD_MIE retrieves aerosol scattering data for FJX.

INTERFACE:

```
SUBROUTINE RD_MIE(NUN,NAMFIL,am_I_Root, Input_Opt )
```

USES:

USE FILE_MOD, ONLY : IOERROR
USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: NUN
CHARACTER(*), INTENT(IN) :: NAMFIL
LOGICAL, INTENT(IN) :: am_I_Root

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

!OUTPUT VARIABLES:

REMARKS:

NAMFIL Name of scattering data file (e.g., FJX_scat.dat)

NUN Channel number for reading data file

NAA Number of categories for scattering phase functions

QAA Aerosol scattering phase functions

WAA 5 Wavelengths for the supplied phase functions

PAA Phase function: first 8 terms of expansion

RAA Effective radius associated with aerosol type

SAA Single scattering albedo

REVISION HISTORY:

```
28 Mar 2013 - S. D. Eastham - Adapted from GEOS-Chem v9-1-3
25 Jun 2015 - M. Sulprizio - Add brown carbon optical properties from M. Hammer
```

$7.4.12 \quad rd_aod$

Subroutine RD_AOD reads aerosol phase functions that are used to scale diagnostic output to an arbitrary wavelengh. This facilitates comparing with satellite observations.

INTERFACE:

```
SUBROUTINE RD_AOD( NJ1, am_I_Root, Input_Opt )
```

USES:

USE FILE_MOD, ONLY : IOERROR USE Input_Opt_Mod, ONLY : OptInput

IMPLICIT NONE

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NJ1   ! Unit # of file to open
TYPE(OptInput), INTENT(IN) :: Input_Opt   ! Input Options object
LOGICAL, INTENT(IN) :: am_I_Root   ! Is this the root CPU?
```

INPUT/OUTPUT PARAMETERS:

REMARKS:

The .dat files for each species contain the optical properties at multiple wavelengths to be used in the online calculation of the aerosol optical depth diagnostics.

These properties have been calculated using the same size and optical properties as the FJX_spec.dat file used for the FAST-J photolysis calculations (which is now redundant for aerosols, the values in the .dat files here are now used). The file currently contains 11 wavelengths for Fast-J and other commonly used wavelengths for satellite and AERONET retrievals. 30 wavelengths follow that map onto RRTMG wavebands for radiative flux calculations (not used if RRTMG is off). A complete set of optical properties from 250-2000 nm for aerosols is available at:

ftp://ftp.as.harvard.edu/geos-chem/data/aerosol_optics/hi_spectral_res

- -- Colette L. Heald, 05/10/10)
- -- David A. Ridley, 05/10/13 (update for new optics files)

REVISION HISTORY:

```
10 May 2010 - C. Heald
                         - Initial version
06 Aug 2010 - C. Carouge
                           - Add an error check when opening the file
01 Aug 2012 - R. Yantosca - Now restore NJ1 to INTENT(IN) status
31 Mar 2013 - S. D. Eastham - Added to Fast-JX v7.0 implementation
30 Mar 2015 - M. Sulprizio - Removed NAMFIL argument. Now specify filenames
                              for aerosol LUT files in this routine.
                            - Append '.rc' to species files in ESMF mode.
02 Apr 2015 - C. Keller
12 May 2015 - R. Yantosca
                            - Bug fix: For PGI compiler, you need to have
                              exactly as many elements in the DATA statement
                             as there are elements in the SPECFIL array.
25 Jun 2015 - M. Sulprizio - Add brown carbon optical properties from
                             M. Hammer
                            - Removed ".rc" file specifier. Not necessary.
04 Aug 2015 - M. Long
```

7.4.13 calc_aod

Subroutine CALC_AOD works out the closest tie points in the optics LUT wavelengths and the coefficients required to calculate the angstrom exponent for interpolating optics to the

requested wavelength. If the wavelength requested matches a standard wavelength in the LUT then we skip the interpolation (DAR 09/2013)

INTERFACE:

```
SUBROUTINE CALC_AOD( am_I_Root )
```

USES:

```
USE CMN_FJX_MOD, ONLY: NWVAA, NWVAAO, WVAA

USE CMN_FJX_MOD, ONLY: WVSELECT, IWVSELECT, NWVSELECT

USE CMN_FJX_MOD, ONLY: IRTWVSELECT

USE CMN_FJX_MOD, ONLY: ACOEF_WV, BCOEF_WV, CCOEF_WV

USE CMN_FJX_MOD, ONLY: ACOEF_RTWV, BCOEF_RTWV, CCOEF_RTWV

USE CMN_FJX_MOD, ONLY: NWVREQUIRED, IWVREQUIRED

USE CMN_FJX_MOD, ONLY: NRTWVREQUIRED, IRTWVREQUIRED

#if defined( RRTMG )

USE PARRRTM, ONLY: NBNDLW

#endif
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?
```

REMARKS:

Now the user is able to select any 3 wavelengths for optics output in the input.geos file we need to be able to interpolate to those wavelengths based on what is available in the optics look-up table.

The standard lookup table currently has values for 11 common wavelengths followed by 30 that are required by RRTMG. Only those required to interpolate to user requested wavelengths are selected from the standard wavelengths. RRTMG wavelengths are not used in the interpolation for AOD output (DAR 10/2013)

UPDATE: because the RT optics output doesnt have access to the standard wavelengths we now calculate two sets of values: one for the ND21 and diag3 outputs that use the standard wavelengths and one for ND72 that interpolates the optics from RRTMG wavelengths. Perhaps a switch needs adding to switch off the RT optics output (and interpolation) if this ends up costing too much and is not used, but it is ideal to have an optics output that matches exactly what RRTMG uses to calculate the fluxes

```
18 Jun 2013 - D. Ridley - Initial version
15 Dec 2014 - M. Sulprizio- Added ProTeX headers
02 Apr 2015 - C. Keller - Added am_I_Root argument
```

$7.4.14 \quad rd_js_jx$

Subroutine RD_JS_JX reads in 'FJX_j2j.dat', which defines the mapping of Fast-JX J's (TITLEJX(1:NJX)) onto the CTM reactions. Reaction number JJ, named T_REACT, uses Fast-JX's T_FJX (including scaling factor F_FJX).

INTERFACE:

```
SUBROUTINE RD_JS_JX(NUNIT, NAMFIL, TITLEJX, NJXX, am_I_Root)
```

USES:

```
USE CHARPAK_MOD, ONLY : CSTRIP
USE ERROR_MOD, ONLY : ERROR_STOP
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NUNIT
INTEGER, INTENT(IN) :: NJXX
CHARACTER(LEN=*), INTENT(IN) :: NAMFIL
CHARACTER(LEN=6), INTENT(IN), DIMENSION(NJXX) :: TITLEJX
LOGICAL, INTENT(IN) :: am_I_Root
```

REMARKS:

Now flag special reactions that are to be adjusted for FlexChem later.

REVISION HISTORY:

```
28 Mar 2013 - S. D. Eastham - Copied from Fast-JX v7.0
31 Mar 2013 - S. D. Eastham - Modified to track number of branches
29 Mar 2016 - R. Yantosca - Now flag rxn numbers for use in PHOTRATE_ADJ
27 Jun 2016 - M. Sulprizio - Add RXN_NO2 flag for PARANOX
```

7.4.15 solar_jx

Subroutine SOLAR_JX handles solar zenith angles.

INTERFACE:

```
SUBROUTINE SOLAR_JX(NDAY, COSSZA, SZA, SOLFX)
```

USES:

```
USE PhysConstants, ONLY : PI
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: COSSZA
INTEGER, INTENT(IN) :: NDAY
!OUTPUT VARIABLES:
```

REAL(fp), INTENT(OUT) :: SZA, SOLFX

REMARKS:

```
NDAY = integer day of the year (used for solar lat and declin)

SZA = solar zenith angle in degrees

COSSZA = U0 = cos(SZA)

SOLFX = Solar function
```

REVISION HISTORY:

```
28 Mar 2013 - S. D. Eastham - Adapted from Fast-JX v7.0 06 Jan 2016 - E. Lundgren - Use global PI rather than local definition
```

7.4.16 photo_jx

Subroutine PHOTO_JX is the core subroutine of Fast-JX. calc J's for a single column atmosphere (aka Indep Colm Atmos or ICA) needs P, T, O3, clds, aersls; adds top-of-atmos layer from climatology needs day-fo-year for sun distance, SZA (not lat or long)

INTERFACE:

```
SUBROUTINE PHOTO_JX( UO,
                                       REFLB,
                                                   P_COL,
&
                       T_COL,
                                       03_COL,
                                                   O3_TOMS,
                       AOD999,
                                       ODAER_COL, ODMDUST_COL,
&
                       ODCLOUD_COL_IN, ILON,
                                                   ILAT,
&
&
                       YLAT,
                                       DAY_OF_YR, MONTH,
                                       am_I_Root, Input_Opt )
&
                       DAY,
```

USES:

```
USE CMN_DIAG_MOD, ONLY: LD22, LD64, ND22, ND64
USE DIAG_MOD, ONLY: AD22, AD64, LTJV
USE Input_Opt_Mod, ONLY: OptInput
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN)
                                                  :: ILON, ILAT
INTEGER, INTENT(IN)
                                                  :: DAY_OF_YR
INTEGER, INTENT(IN)
                                                  :: MONTH, DAY
REAL(fp), INTENT(IN)
                                                  :: YLAT
REAL(fp), INTENT(IN)
                                                  :: UO, REFLB
REAL(fp), INTENT(IN), DIMENSION(L1_+1)
                                                  :: P_COL
REAL(fp), INTENT(IN),DIMENSION(L1_)
                                                  :: T_COL
REAL(fp), INTENT(IN), DIMENSION(L1_)
                                                 :: 03_COL
REAL(fp), INTENT(IN)
                                                 :: 03_TOMS
REAL(fp), INTENT(IN), DIMENSION(L_,A_)
REAL(fp), INTENT(IN), DIMENSION(L_,NDUST)
                                                 :: ODAER_COL
                                                 :: ODMDUST_COL
REAL(fp), INTENT(IN), DIMENSION(L_)
                                                 :: ODCLOUD_COL_IN
```

```
LOGICAL, INTENT(IN) :: AOD999
LOGICAL, INTENT(IN) :: am_I_Root
TYPE(OptInput), INTENT(IN) :: Input_Opt
```

REMARKS:

REVISION HISTORY:

```
28 Mar 2013 - S. D. Eastham - Copied from Fast-JX v7.0 05 Mar 2014 - R. Yantosca - Now only save ND64 with LD64 specified levels
```

7.4.17 opmie

Subroutine OPMIE is a core Fast-JX scattering subroutine, specifically for Mie scattering.

INTERFACE:

```
SUBROUTINE OPMIE (DTAUX, POMEGAX, UO, RFL, AMF2, JXTRA, & FJACT, FJTOP, FJBOT, FSBOT, FJFLX, FLXD, FLXDO, LU)
```

USES:

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: DTAUX(JXL1_,W_),POMEGAX(8,JXL1_,W_)
REAL(fp), INTENT(IN) :: AMF2(2*JXL1_+1,2*JXL1_+1)
REAL(fp), INTENT(IN) :: U0,RFL(W_)
INTEGER, INTENT(IN) :: JXTRA(JXL2_+1), LU
!OUTPUT VARIABLES:
REAL(fp), INTENT(OUT) :: FJACT(JXL_,W_),FJTOP(W_)
REAL(fp), INTENT(OUT) :: FJBOT(W_),FSBOT(W_)
REAL(fp), INTENT(OUT) :: FJFLX(JXL_,W_),FLXD(JXL1_,W_),FLXDO(W_)
```

REMARKS:

REVISION HISTORY:

```
28 Mar 2013 - S. D. Eastham - Copied from Fast-JX v7.0
```

7.4.18 miesct

Subroutine MIESCT is an adaptation of the Prather radiative transfer code (mjp, 10/95).

INTERFACE:

SUBROUTINE MIESCT(FJ,FJT,FJB, POMEGA,FZ,ZTAU,ZFLUX,RFL,UO,ND)

USES:

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: ND
REAL(fp), INTENT(IN) :: POMEGA(M2_,N_,W_),FZ(N_,W_),ZTAU(N_,W_)
& ,RFL(W_),UO,ZFLUX(W_)
!OUTPUT VARIABLES:
REAL(fp), INTENT(OUT) :: FJ(N_,W_),FJT(W_),FJB(W_)
```

REMARKS:

```
Prather, 1974, Astrophys. J. 192, 787-792.

Solution of inhomogeneous Rayleigh scattering atmosphere.
(original Rayleigh w/ polarization)

Cochran and Trafton, 1978, Ap.J., 219, 756-762.

Raman scattering in the atmospheres of the major planets.
(first use of anisotropic code)

Jacob, Gottlieb and Prather, 1989, J.Geophys.Res., 94, 12975-13002.
Chemistry of a polluted cloudy boundary layer,
(documentation of extension to anisotropic scattering)
```

takes atmospheric structure and source terms from std J-code ALSO limited to 4 Gauss points, only calculates mean field! (M=1)

REVISION HISTORY:

```
28 Mar 2013 - S. D. Eastham - Copied from Fast-JX v7.0
```

7.4.19 legnd0

Subroutine LEGND0 calculates ordinary Legendre functions of X (real) from $P[0] = PL(1) = 1, P[1] = X, \dots, P[N-1] = PL(N)$

INTERFACE:

```
SUBROUTINE LEGNDO (X,PL,N)
```

USES:

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: N
    REAL(fp), INTENT(IN) :: X
!OUTPUT VARIABLES:
    REAL(fp), INTENT(OUT) :: PL(N)
```

REMARKS:

REVISION HISTORY:

```
28 Mar 2013 - S. D. Eastham - Copied from Fast-JX v7.0
```

7.4.20 set_prof

Subroutine SET_PROF sets vertical profiles for a given latitude and longitude.

INTERFACE:

```
SUBROUTINE SET_PROF (YLAT,
                              MONTH, DAY,
                                               T_CTM, P_CTM,
                     CLDOD,
                              DSTOD, AEROD,
                                               03_CTM, 03_TOMS,
&
                              T_CLIM, O3_CLIM, Z_CLIM, AIR_CLIM,
&
                     AERCOL,
&
                     Input_Opt )
```

USES:

```
USE Input_Opt_Mod,
                      ONLY : OptInput
                      ONLY: AIRMW, AVO, gO, BOLTZ
USE PhysConstants,
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN)
                             :: YLAT
                                                  ! Latitude (degrees)
   INTEGER, INTENT(IN)
                             :: MONTH
                                                  ! Month
                                                  ! Day *of month*
   INTEGER, INTENT(IN)
                             :: DAY
   REAL(fp), INTENT(IN)
                           :: T_CTM(L1_)
                                                  ! CTM temperatures (K)
   REAL(fp), INTENT(IN)
                            :: 03_TOMS
                                                  ! O3 column (DU)
   REAL(fp), INTENT(IN)
                           :: P_CTM(L1_+1)
                             :: P_CTM(L1_+1)
:: CLDOD(L_)
                                                  ! CTM edge pressures (hPa)
   REAL(fp), INTENT(INOUT)
                                                  ! Cloud optical depth
                             :: DSTOD(L_,NDUST)
   REAL(fp), INTENT(IN)
                                                  ! Mineral dust OD
   REAL(fp), INTENT(IN)
                             :: AEROD(L_,A_)
                                                  ! Aerosol OD
   REAL(fp), INTENT(IN) :: O3_CTM(L1_)
                                                  ! CTM ozone (molec/cm3)
   TYPE(OptInput), INTENT(IN) :: Input_Opt
                                                  ! Input options
!OUTPUT VARIABLES:
                             :: AERCOL(A_,L1_)
   REAL(fp), INTENT(OUT)
                                                  ! Aerosol column
                             :: T_CLIM(L1_)
:: Z_CLIM(L1_+1)
   REAL(fp), INTENT(OUT)
                                                  ! Clim. temperatures (K)
   REAL(fp), INTENT(OUT)
                                                  ! Edge altitudes (cm)
                             :: AIR_CLIM(L1_)
   REAL(fp), INTENT(OUT)
                                                  ! 03 column depth (#/cm2)
   REAL(fp), INTENT(OUT)
                                                  ! 03 column depth (#/cm2)
```

REMARKS:

```
30 Mar 2013 - S. D. Eastham - Adapted from J. Mao code
05 Jan 2016 - E. Lundgren - Use global physical parameters
```

7.4.21 set_aer

Subroutine SET_AER fills out the array MIEDX. Each entry connects a GEOS-Chem aerosol to its Fast-JX counterpart: MIEDX(Fast-JX index) = (GC index)

INTERFACE:

```
SUBROUTINE SET_AER(am_I_Root)
```

USES:

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root !OUTPUT VARIABLES:
```

REMARKS:

REVISION HISTORY:

```
31 Mar 2013 - S. D. Eastham - Adapted from J. Mao FJX v6.2 implementation
```

7.4.22 rd_prof_nc

Subroutine RAD_PROF_NC reads in the reference climatology from a NetCDF file rather than an ASCII .dat.

INTERFACE:

```
SUBROUTINE RD_PROF_NC( am_I_Root, Input_Opt, RC )
```

USES:

```
! Modules for netCDF read
USE m_netcdf_io_open
USE m_netcdf_io_read
USE m_netcdf_io_readattr
USE m_netcdf_io_close
USE ErrCode_Mod
USE Input_Opt_Mod, ONLY : OptInput
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REMARKS:

This file was automatically generated by the Perl scripts in the NcdfUtilities package (which ships w/ GEOS-Chem) and was subsequently hand-edited.

REVISION HISTORY:

7.4.23 photrate_adj

Subroutine PHOTRATE_ADJ adjusts certain photolysis rates for chemistry.

INTERFACE:

```
SUBROUTINE PHOTRATE_ADJ( am_I_root, I, J, & L, AD, TEMP, & C_H2O, FRAC, RC )
```

USES:

```
USE CMN_DIAG_MOD, ONLY : LD22, ND22
USE DIAG_MOD, ONLY : AD22, LTJV
USE ErrCode_Mod
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INTEGER, INTENT(IN) :: I, J, L ! Grid box indices (lon, lat, lev)

REAL(fp), INTENT(IN) :: AD ! Air number density [molec/m3] ??

REAL(fp), INTENT(IN) :: TEMP ! Temperature [K]

REAL(fp), INTENT(IN) :: C_H2O ! H2O conc [molec/cm3]

REAL(fp), INTENT(IN) :: FRAC ! Result of SO4_PHOTFRAC,

! called from flex_chemdr.F
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure
```

REMARKS:

%%%% NOTE: WE SHOULD UPDATE THE COMMENTS TO MAKE SURE THAT WE DO %%%% %%%% NOT KEEP ANY CONFLICTING OR INCORRECT INFORMATION (bmy, 3/28/16) %%%%

REVISION HISTORY:

```
10 Mar 2016 - M. Sulprizio- Added ProTeX header
18 Apr 2016 - R. Yantosca - Remove Input_Opt, State_Met, State_Chm args
and pass air density & temperature instead
18 Apr 2016 - R. Yantosca - Also prevent div-by-zero conditions
```

7.5 Fortran: Module Interface uvalbedo_mod.F90

Module UVALBEDO_MOD contains variables and routines for reading the UV Albedo data. This data is required by the FAST-JX photolysis module. UV albedo data will now be obtained from the HEMCO data structure.

INTERFACE:

MODULE UValbedo_Mod

USES:

```
USE Precision_Mod   ! For GEOS-Chem Precision (fp)
```

IMPLICIT NONE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: Get_UValbedo

REMARKS:

References:

```
Herman, J.R and Celarier, E.A., "Earth surface reflectivity climatology at 340-380 nm from TOMS data", __J. Geophys. Res__, Vol. 102, D23, pp. 28003-28011, Dec 20, 1997.
```

```
06 Jan 2015 - R. Yantosca - Initial version
19 Apr 2002 - R. Yantosca - Initial version
```

- (1) Now read uvalbedo file directly from DATA_DIR/uvalbedo_200111 subdirectory. (bmy, 4/2/02)
- (2) Now divide module header into MODULE PRIVATE, MODULE VARIABLES, and MODULE ROUTINES sections. (bmy, 5/28/02)
- (3) Now references "error_mod.f" (bmy, 10/15/02)
- (4) Minor modification in READ_UVALBEDO (bmy, 3/14/03)
- (5) Now references "directory_mod.f" (bmy, 7/20/04)
- (6) Bug fix for GCAP grid in READ_UVALBEDO (bmy, 8/16/05)
- (7) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 24 Nov 2014 M. Yannetti Added PRECISION_MOD
- 17 Dec 2014 R. Yantosca Leave time/date variables as 8-byte
- 12 Jan 2015 R. Yantosca Remove CLEANUP_UVALBEDO routine
- 04 Mar 2015 R. Yantosca UV albedo data now comes via HEMCO

7.5.1 get_uvalbedo

Copies the UV Albedo data from the HEMCO data structure into the State_Met derived type object.

INTERFACE:

```
SUBROUTINE Get_UValbedo( am_I_root, Input_Opt, State_Met, RC )
```

USES:

```
USE ErrCode_Mod

USE Error_Mod, ONLY : Error_Stop

USE HCO_INTERFACE_MOD, ONLY : HcoState

USE HCO_EmisList_Mod, ONLY : HCO_GetPtr

USE Input_Opt_Mod, ONLY : OptInput

USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REVISION HISTORY:

```
06 Jan 2015 - R. Yantosca - Initial version
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
```

7.5.2 set_prof_o3

Subroutine SET_PROF_O3 sets up atmospheric profiles required by RRTMG in the stratosphere using a doubled version of the level scheme used in the CTM. First pressure and z* altitude are defined, then O3 and T are taken from the supplied climatology and integrated to the CTM levels (may be overwritten with values directly from the CTM, if desired). This is a stripped down version of SET_PROF; it does O3 only.

INTERFACE:

```
SUBROUTINE SET_PROF_03( YLAT, MONTH, DAY, T_CTM, & P_CTM, 03_CTM, 03_TOMS, T_CLIM, & 03_CLIM, Z_CLIM, AIR_CLIM, Input_Opt )
```

USES:

```
USE CMN_FJX_MOD
USE Input_Opt_Mod, ONLY : OptInput
```

USE PhysConstants ! Physical constants

USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

IMPLICIT NONE

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN)
                              :: YLAT
                                                    ! Latitude (degrees)
   INTEGER, INTENT(IN)
                              :: MONTH
                                                    ! Month
   INTEGER, INTENT(IN)
                              :: DAY
                                                    ! Day *of month*
   REAL(fp), INTENT(IN)
                              :: T_CTM(L1_)
                                                    ! CTM temperatures (K)
   REAL(fp), INTENT(IN)
                              :: 03_TOMS
                                                    ! O3 column (DU)
   REAL(fp), INTENT(IN)
                              :: P_CTM(L1_+1)
                                                    ! CTM edge pressures (hPa)
   REAL(fp), INTENT(IN)
                              :: 03_CTM(L1_)
                                                    ! CTM ozone (molec/cm3)
   TYPE(OptInput), INTENT(IN) :: Input_Opt
                                                    ! Input options
!OUTPUT VARIABLES:
   REAL(fp), INTENT(OUT)
                              :: T_CLIM(L1_)
                                                    ! Clim. temperatures (K)
   REAL(fp), INTENT(OUT)
                              :: Z_CLIM(L1_+1)
                                                    ! Edge altitudes (cm)
   REAL(fp), INTENT(OUT)
                              :: 03_CLIM(L1_)
                                                    ! 03 column depth (#/cm2)
                                                    ! 03 column depth (#/cm2)
   REAL(fp), INTENT(OUT)
                              :: AIR_CLIM(L1_)
```

AUTHOR:

Oliver Wild & Michael Prather

REMARKS:

- 01 Jun 1996 M. Prather & O. Wild Initial version
- (1) Since we parallelize over columns, T, ODCOL, OPTDUST, and OPTAER are 1-D vectors. In the original code from Oliver Wild, these were 3-D arrays. Also P and SA are just scalars since we just pass one surface location at a time w/in the parallel loop. (bmy, 9/13/99)
- (2) Mineral dust profiles are also constructed (rvm, 06/04/00)
- (3) Other aerosol profiles are also constructed (rvm, bmy, 2/27/02)
- (4) Added NLON, NLAT, DAY to the arg list. Now weight the O3 column by the observed monthly mean EP-TOMS data. Also updated comments and added standard GEOS-CHEM documentation header. (mje, bmy, 7/13/03)
- (5) We don't need to initialize the PJ array with ETAA and ETAB anymore. PJ is now defined in "fast_j.f". Updated comments. (bmy, 10/30/07)
- (6) Modified to use GEOS-5 03 columns when TOMS/SBUV data don't exist, i.e. after 2008. (ccc, 7/13/09)
- 08 Dec 2009 R. Yantosca Added ProTeX headers
- 15 Dec 2014 M. Sulprizio- Modified for Fast-JX. Now consistent with

```
subroutine SET_PROF in fast_jx_mod.F.

20 Mar 2015 - M. Sulprizio- Modified for flexible precision

05 Jan 2016 - E. Lundgren - Use global physical parameters
```

7.6 Fortran: Module Interface toms_mod.F

Module TOMS_MOD contains variables and routines for reading the TOMS/SBUV O3 column data from disk (for use w/ the FAST-J photolysis routines).

INTERFACE:

MODULE TOMS_MOD

PRIVATE

USES:

```
USE CMN_SIZE_MOD ! Size parameters
USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

IMPLICIT NONE
```

PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: INIT_TOMS
PUBLIC :: READ_TOMS
```

PUBLIC :: COMPUTE_OVERHEAD_O3
PUBLIC :: GET_OVERHEAD_O3
PUBLIC :: CLEANUP_TOMS

PUBLIC DATA MEMBERS:

```
! First & last years for which TOMS/SBUV data is is available ! (update these as new data is added to the archive)
INTEGER, PUBLIC, PARAMETER :: FIRST_TOMS_YEAR = 1979
INTEGER, PUBLIC, PARAMETER :: LAST_TOMS_YEAR = 2010
```

REMARKS:

References:

```
Version 8 Merged Ozone Data Sets
Total Ozone Revision 05
DATA THROUGH: MAR 2009
```

LAST MODIFIED: 01 MAY 2009

http://acdb-ext.gsfc.nasa.gov/Data_services/merged/index.html

TOMS/SBUV MERGED TOTAL OZONE DATA, Version 8, Revision 5.

Resolution: 5 x 10 deg.

- * Includes reprocessed N16 and N17 SBUV/2 data using latest calibration.
- * OMI data updated from Collection 2 to Collection 3.
- * New offsets derived based on revised data sets.
- * 1970-1972 N4 BUV data added with no adjustments. User may wish to apply offset based on Comparisons between BUV and Dobson Measurements.

```
Responsible NASA official:
Dr. Richard Stolarski (Richard.S.Stolarski@nasa.gov)
Stacey Frith (Stacey.M.Frith@nasa.gov)
```

REVISION HISTORY:

```
14 Jul 2003 - R. Yantosca - Initial version
```

- (1) Now references "directory_mod.f" (bmy, 7/20/04)
- (2) Now can read files for GEOS or GCAP grids (bmy, 8/16/05)
- (3) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (4) Now always use 2002 TOMS 03 data for GCAP (swu, bmy, 10/3/06)
- (5) Now reads from TOMS_200701 directory, w/ updated data (bmy, 2/1/07)
- (6) Now don't replace any tokens in the DATA_DIR variable (bmy, 12/5/07)
- (7) Latest year of TOMS data is now 2007 (bmy, 1/14/09)
- 01 Dec 2010 R. Yantosca Added ProTeX headers
- 06 Mar 2012 R. Yantosca Added function GET_TOTAL_03
- 06 Mar 2012 R. Yantosca Added parameters FIRST_TOMS_YEAR, LAST_TOMS_YEAR
- 06 Mar 2012 R. Yantosca Updated comments
- 06 Mar 2012 R. Yantosca Now make TOMS, DTOMS1, DTOMS2 arrays PRIVATE
- 06 Mar 2012 R. Yantosca Add TO3_DAILY as a PRIVATE module array
- 25 Jun 2012 S. Kim Now reads from TOMS_201203 directory, w/ updated data
- 03 Jul 2012 R. Yantosca Restrict reading from TOMS_201203 directory to GEOS-5.7.2 met data for the time being.
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 21 Nov 2014 M. Yannetti Added PRECISION_MOD
- 16 Mar 2015 R. Yantosca Retire bpch input; now read TOMS via HEMCO
- 03 Nov 2016 B. Henderson- Added fix for weird 03 in GEOS-5 simulations

7.6.1 read_toms

Subroutine READ_TOMS reads in TOMS O3 column data from a binary punch file for the given grid, month and year.

INTERFACE:

```
SUBROUTINE READ_TOMS( am_I_Root, Input_Opt, RC )
```

USES:

```
USE ErrCode_Mod
```

USE Error_Mod, ONLY : Error_Stop

USE HCO_Interface_Mod, ONLY : HcoState
USE HCO_EmisList_Mod, ONLY : HCO_GetPtr
USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

TOMS/SBUV MERGED TOTAL OZONE DATA, Version 8, Revision 5.

Resolution: $5 \times 10 \text{ deg.}$

Methodology

FAST-J comes with its own default 03 column climatology (from McPeters 1992 & Nagatani 1991), which is stored in the input file "jv_atms.dat". These "FAST-J default" 03 columns are used in the computation of the actinic flux and other optical quantities for the FAST-J photolysis.

The TOMS/SBUV 03 columns and 1/2-monthly 03 trends (contained in the TOMS_200906 directory) are read into GEOS-Chem by routine READ_TOMS in "toms_mod.f". Missing values (i.e. locations where there are no data) in the TOMS/SBUV 03 columns are defined by the flag -999.

After being read from disk in routine READ_TOMS, the TOMS/SBUV 03 data are then passed to the FAST-J routine "set_prof.F". In "set_prof.F", a test is done to make sure that the TOMS/SBUV 03 columns and 1/2-monthly trends do not have any missing values for (lat,lon) location for the given month. If so, then the TOMS/SBUV 03 column data is interpolated to the current day and is used to weight the "FAST-J default" 03 column. This essentially "forces" the "FAST-J default" 03 column values to better match the observations, as defined by TOMS/SBUV.

If there are no TOMS/SBUV 03 columns (and 1/2-monthly trends) at a (lat, lon) location for given month, then FAST-J will revert to its own "default" climatology for that location and month. Therefore, the TOMS 03 can be thought of as an "overlay" data -- it is only used if it exists.

Note that there are no TOMS/SBUV 03 columns at the higher latitudes. At these latitudes, the code will revert to using the "FAST-J default" 03 columns.

As of March 2012, we have TOMS/SBUV data for 1979 thru 2008. We will update to the latest TOMS/SBUV data set shortly.

This methodology was originally adopted by Mat Evans.

```
#####
            NOTE: BINARY PUNCH INPUT IS BEING PHASED OUT. THIS DATA
                                                                     #####
   #####
            WILL EVENTUALLY BE READ IN FROM netCDF FILES VIA HEMCO!
                                                                     #####
               -- Bob Yantosca (05 Mar 2015)
   #####
                                                                     #####
   REVISION HISTORY:
   10 Dec 2002 - M. Evans - Initial version
   (1) Bundled into "toms_mod.f" (bmy, 7/14/03)
   (2) Now references DATA_DIR from "directory_mod.f" (bmy, 7/20/04)
    (3) Now can read files for GEOS or GCAP grids (bmy, 8/16/05)
    (4) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
    (5) Now always use 2002 TOMS 03 data for GCAP (swu, bmy, 10/3/06)
    (6) Now reads from TOMS_200701 directory, w/ updated data. Also always
         use 1979 data prior to 1979 or 2005 data after 2005. (bmy, 2/12/07)
    (7) Bug fix: don't include DATA_DIR in filename, just in case someone's
         file path has replaceable tokens (e.g. hh, mm, MM etc.) (bmy, 12/5/07)
    (8) Latest year of TOMS data is now 2007 (bmy, 1/14/09)
    (9) Updated TOMS data in TOMS_200906. Latest year is 2008. (ccc, 6/15/09)
   08 Dec 2009 - R. Yantosca - Added ProTeX headers
   03 Jul 2012 - R. Yantosca - Restrict reading from TOMS_201203 directory
                              to GEOS-5.7.2 met data for the time being.
   13 Dec 2013 - M. Sulprizio- Now pass USE_03_FROM_MET logical flag so that
                              we bypass reading TOMS 03 data when using TO3
                              from the met fields.
   05 Mar 2014 - M. Sulprizio- Now regrid TOMS 03 from the files on GEOS 1x1
                              grid (J. Lin)
```

- 20 Jun 2014 R. Yantosca Now accept am_I_Root, Input_Opt, RC
- 23 Jun 2014 R. Yantosca Now use Input_Opt%DATA_DIR_1x1
- 06 Nov 2014 R. Yantosca Replace TRANSFER_2D with direct casts
- 17 Dec 2014 R. Yantosca Leave time/date variables as 8-byte
- 05 Mar 2015 R. Yantosca Now read data w/r/t ExtData/CHEM_INPUTS

7.6.2 compute_overhead_o3

Subroutine COMPUTE_OVERHEAD_O3 returns the resultant total overhead O3 column for the FAST-J photolysis. This will be one of two options:

- 1. Default: TOMS/SBUV overhead O3 columns. These will be used be the FAST-J routine set_prof.F to overwrite the existing FAST-J climatology (cf McPeters & Nagatani 1992). Missing data (i.e. for months & locations where TOMS/SBUV data does not exist) is denoted by the value -999; FAST-J will skip over these points.
- 2. Overhead O3 columns taken directly from the met fields. These will be returned if the flag USE_O3_FROM_MET is set to TRUE.

INTERFACE:

```
SUBROUTINE COMPUTE_OVERHEAD_O3( am_I_Root, DAY, & USE_O3_FROM_MET, TO3)
```

INPUT PARAMETERS:

```
! Root CPU?
```

LOGICAL, INTENT(IN) :: am_I_Root

! Day of month

INTEGER, INTENT(IN) :: DAY

! Switch to denote if we should use the default TO3

! directly from the met fields

LOGICAL, INTENT(IN) :: USE_03_FROM_MET

! TO3 from the met fields [Dobsons]

REAL(fp), INTENT(IN) :: TO3(IIPAR, JJPAR)

REMARKS:

Reference for the TOMS/SBUV merged 03 columns:

1985 - 2005 are taken from:

http://code916.gsfc.nasa.gov/Data_services/merged/index.html

TOMS/SBUV MERGED TOTAL OZONE DATA, Version 8, Revision 3. Resolution: $5 \times 10 \text{ deg}$.

Contact person for the merged data product: Stacey Hollandsworth Frith (smh@hyperion.gsfc.nasa.gov)

2006 and 2007 are taken from:

http://code916.gsfc.nasa.gov/Data_services/merged/index.html

Version 8 Merged Ozone Data Sets

Revision 04

DATA THROUGH: SEP 2008 LAST MODIFIED: 20 OCT 2008

Methodology (bmy, 2/12/07)

FAST-J comes with its own default 03 column climatology (from McPeters 1992 & Nagatani 1991), which is stored in the input file "jv_atms.dat". These "FAST-J default" 03 columns are used in the computation of the actinic flux and other optical quantities for the FAST-J photolysis.

The TOMS/SBUV 03 columns and 1/2-monthly 03 trends (contained in the TOMS_200701 directory) are read into GEOS-Chem by routine READ_TOMS in "toms_mod.f". Missing values (i.e. locations where there are no data) in the TOMS/SBUV 03 columns are defined by the flag -999.

After being read from disk in routine READ_TOMS, the TOMS/SBUV 03 data are then passed to the FAST-J routine "set_prof.f". In "set_prof.f", a test is done to make sure that the TOMS/SBUV 03 columns and 1/2-monthly trends do not have any missing values for (lat,lon) location for the given month. If so, then the TOMS/SBUV 03 column data is interpolated to the current day and is used to weight the "FAST-J default" 03 column. This essentially "forces" the "FAST-J default" 03 column values to better match the observations, as defined by TOMS/SBUV.

If there are no TOMS/SBUV 03 columns (and 1/2-monthly trends) at a (lat,lon) location for given month, then FAST-J will revert to its own "default" climatology for that location and month. Therefore, the TOMS 03 can be thought of as an "overlay" data -- it is only used if it exists.

Note that there are no TOMS/SBUV 03 columns at the higher latitudes. At these latitudes, the code will revert to using the "FAST-J default" 03 columns.

As of February 2007, we have TOMS/SBUV data for 1979 thru 2005. 2006 TOMS/SBUV data is incomplete as of this writing. For years 2006 and onward, we use 2005 TOMS 03 columns.

This methodology was originally adopted by Mat Evans. Symeon Koumoutsaris was responsible for creating the downloading and processing the TOMS 03 data files from 1979 thru 2005 in the TOMS_200701 directory.

REVISION HISTORY:

06 Mar 2012 - R. Yantosca - Initial version, pulled code out from the FAST-J routine SET_PROF; based on the GEOS-Chem column code routine

22 Oct 2014 - C. Keller - Added am_I_Root parameter.

7.6.3 get_overhead_o3

Function GET_OVERHEAD_O3 returns the total overhead O3 column [DU] (which is taken either from TOMS/SBUV or directly from the met fields) at a given surface grid box location (I,J).

INTERFACE:

FUNCTION GET_OVERHEAD_O3(I, J) RESULT(OVERHEAD_O3)

INPUT PARAMETERS:

RETURN VALUE:

REAL(fp) :: OVERHEAD_O3 ! Total overhead O3 column [DU]

REVISION HISTORY:

06 Mar 2012 - R. Yantosca - Initial version

7.6.4 init_toms

Subroutine INIT_TOMS allocates and zeroes all module arrays.

INTERFACE:

```
SUBROUTINE INIT_TOMS( am_I_Root, Input_Opt, RC )
```

USES:

USE CMN_SIZE_MOD
USE ErrCode_Mod

USE ERROR_MOD, ONLY : ALLOC_ERR
USE ERROR_MOD, ONLY : ERROR_STOP
USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! root CPU?
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input opts

INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Failure or success

REVISION HISTORY:

14 Jul 2003 - R. Yantosca - Initial version

01 Dec 2010 - R. Yantosca - Added ProTeX headers

06 Mar 2012 - R. Yantosca - Now allocate TO3_DAILY

16 Mar 2015 - R. Yantosca - TOMS, DTOMS1, DTOMS2 are now pointers

16 Mar 2015 - R. Yantosca - Add Input_Opt, RC arguments for std interface

03 Nov 2016 - B. Henderson- Add extra fields to fix OH issue for GEOS-5

7.6.5 cleanup_toms

Subroutine CLEANUP_TOMS deallocates all module arrays.

INTERFACE:

SUBROUTINE CLEANUP_TOMS

REVISION HISTORY:

```
14 Jul 2003 - R. Yantosca - Initial version
01 Dec 2010 - R. Yantosca - Added ProTeX headers
06 Mar 2012 - R. Yantosca - Now deallocate TO3_DAILY
03 Nov 2016 - R. Yantosca - Deallocate and nullify extra fields
```

7.7 Fortran: Module Interface flexchem_mod.F90

Module FlexChem_Mod contines arrays and routines for the FlexChem chemical solver.

INTERFACE:

```
MODULE FlexChem_Mod
```

USES:

```
USE Precision_Mod ! For GEOS-Chem Precision (fp)

IMPLICIT NONE

PRIVATE
```

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: Do_FlexChem

PUBLIC :: Init_FlexChem

PUBLIC :: Cleanup_FlexChem

```
14 Dec 2015 - M.S. Long - Initial version
15 Jun 2016 - M. Sulprizio- Remove STTTOCSPEC mapping array. Species and tracers have a 1:1 mapping currently so mapping is not required
18 Jul 2016 - M. Sulprizio- Remove FAMILIES_KLUDGE routine. Family tracers have been eliminated.
24 Aug 2016 - M. Sulprizio- Rename from flexchem_setup_mod.F90 to flexchem_mod.F90
29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90
```

7.7.1 do_flexchem

Subroutine Do_FlexChem is the driver subroutine for full chemistry with KPP.

INTERFACE:

```
SUBROUTINE Do_FlexChem( am_I_Root, Input_Opt, State_Met, State_Chm, RC )
USES:
      USE AEROSOL_MOD,
                                      ONLY : SOILDUST, AEROSOL_CONC, RDAER
      USE CHEMGRID_MOD,
                                       ONLY : ITS_IN_THE_CHEMGRID
      USE CMN_FJX_MOD
                                 ONLY: IIPAR, JJPAR, LLPAR
ONLY: AD65
ONLY: DO_DIAG_OH
ONLY: DIAG2O, POx, LOx
ONLY: RDUST_ONLINE, RDUST_OFFLINE
      USE CMN_SIZE_MOD,
      USE DIAG_MOD,
      USE DIAG_OH_MOD,
      USE DIAG20_MOD,
      USE DUST_MOD,
      USE ErrCode_Mod
      USE ERROR_MOD
      USE FAST_JX_MOD,
                                      ONLY : PHOTRATE_ADJ, FAST_JX
      USE FUTURE_EMISSIONS_MOD, ONLY : GET_FUTURE_YEAR
      USE GCKPP_HetRates, ONLY : SET_HET
USE GCKPP_Monitor, ONLY : SPC_NAMES, FAM_NAMES
      USE GCKPP_Parameters
      USE GCKPP_Integrator, ONLY : INTEGRATE, NHnew
      USE GCKPP_Function
      USE GCKPP_Model
      USE GCKPP_Global
      USE GCKPP_Rates, ONLY : UPDATE_RCONST, RCONST
USE GCKPP_Initialize, ONLY : Init_KPP => Initialize
USE GC_GRID_MOD, ONLY : GET_YMID
USE Input_Opt_Mod, ONLY : OptInput
      USE PhysConstants,
                                      ONLY : AVO
      USE PRESSURE_MOD
      USE Species_Mod,
                                    ONLY : Species
                                      ONLY : ChmState
      USE State_Chm_Mod,
      USE State_Chm_Mod,
                                      ONLY : Ind_
                                   ONLY : Ind_
ONLY : MetState
ONLY : GET_TS_CHEM
ONLY : GET_MONTH
ONLY : GET_YEAR
      USE State_Met_Mod,
      USE TIME_MOD,
      USE TIME_MOD,
      USE TIME_MOD,
                                      ONLY : GET_YEAR
      USE UnitConv_Mod
 #if defined( UCX )
                                ONLY : CALC_STRAT_AER
ONLY : SO4_PHOTFRAC
ONLY : UCX_NOX
ONLY : UCX_H2SO4PHOT
      USE UCX_MOD,
      USE UCX_MOD,
      USE UCX_MOD,
      USE UCX_MOD,
 #endif
        defined( TOMAS )
 #if
```

USE TOMAS_MOD, ONLY : H2SO4_RATE

#endif

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INPUT/OUTPUT PARAMETERS:

TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

- 14 Dec 2015 M.S. Long Initial version

 18 Dec 2015 M. Sulprizio- Add calls to OHSAVE and DO_DIAG_OH

 22 Dec 2015 M. Sulprizio- Set NUMDEN to State_Met%AIRNUMDEN for conversions between v/v and molec/cm3

 28 Mar 2016 R. Yantosca Added several fixes for OpenMP parallelization

 30 Mar 2016 R. Yantosca Bug fix, now make sure to copy C back into State_Chm%Species. Also block out temp diags.

 16 May 2016 M. Sulprizio- Remove call to RURALBOX. The implemementation of FlexChem has rendered the routine obsolete.

 31 May 2016 E. Lundgren Use species database MW instead of XNUMOL

 06 Jun 2016 M. Sulprizio- Replace NTSPEC with State_Chm%nSpecies and NAMEGAS with SpcInfo%Name from species database
 - 14 Jun 2016 M. Sulprizio- Replace loops over N_TRACERS with loops over State_Chm%nSpecies and add checks for Is_Advected and Is_Kpp to avoid introducing numerical noise by applying unit conversions to non-KPP species
 - 16 Jun 2016 M. Sulprizio- Now define IDTCH4 locally
 - 20 Jun 2016 R. Yantosca Renamed IDTCH4 to id_CH4 for consistency
 - 18 Jul 2016 M. Sulprizio- Remove calls to FAMILIES_KLUDGE. Family tracers have been eliminated. Also simplify code to copy to/from STT so that unit conversions to/from molec/cm3 are done in the same step as the copy.
 - 02 Aug 2016 M. Sulprizio- Connect production and loss rates from KPP to ND65 diagnostic
 - 16 Aug 2016 E. Lundgren Remove all references to tracers, including STT and Input_Opt%N_TRACERS, and use routines in unitconv_mod.F for species kg <-> molec/cm3
 - 24 Aug 2016 M. Sulprizio- Replace CSPECTOKPP with State_Chm%Map_KppSpc
 - 24 Aug 2016 M. Sulprizio- Move this subroutine to flexchem_mod.F90 and rename from FLEX_CHEMDR to Do_FlexChem
 - 22 Sep 2016 R. Yantosca Add extra debug printout after FAST_JX
 - 14 Nov 2016 E. Lundgren Move UCX calls to after spc conversion to kg

7.7.2 init_flexchem

Subroutine Init_FlexChem is used to allocate arrays for the KPP solver.

INTERFACE:

```
SUBROUTINE Init_FlexChem( am_I_Root, Input_Opt, RC)
```

USES:

USE CMN_SIZE_MOD
USE ErrCode_Mod

USE gckpp_Global, ONLY : NREACT
USE gckpp_Monitor, ONLY : EQN_NAMES
USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

14 Dec 2015 - M.S. Long - Initial version 22 Dec 2015 - M. Sulprizio- Use State_Met%AIRNUMDEN to convert initial species concentrations from v/v to molec/cm3 29 Jan 2016 - M. Sulprizio- Add calls to Register_Tracer and Register_Species to populate Tracer_Name, Tracer_Id, Species_Name, and Species_ID fields in State_Chm 06 Jun 2016 - M. Sulprizio- Replace NTSPEC with State_Chm%nSpecies and NAMEGAS with SpcInfo%Name from species database 06 Jun 2016 - M. Sulprizio- Replace Get_Indx with Spc_GetIndx to use the fast-species lookup from the species database 06 Jun 2016 - M. Sulprizio- Remove calls to Register_Tracer and Register_Species; these routines were made obsolete by the species database 14 Jun 2016 - M. Sulprizio- Replace Spc_GetIndx with Ind_ (M. Long) 25 Jul 2016 - E. Lundgren - Add check that species was not in restart file prior to v/v -> molec/cm3 conversion 02 Aug 2016 - E. Lundgren - Move unit conversion of species background values to restart_mod 24 Aug 2016 - M. Sulprizio- Remove CSPECTOKPP array. State_Chm%Map_KppSpc is now used instead. 20 Sep 2016 - R. Yantosca - Use fixed integer with in WRITE statement

7.7.3 cleanup_flexchem

Subroutine Cleanup_FlexChem deallocate module variables.

INTERFACE:

```
SUBROUTINE Cleanup_FlexChem()
```

REVISION HISTORY:

```
24 Aug 2016 - M. Sulprizio- Initial version
```

7.8 Fortran: Module Interface gckpp_HetRates

FlexChem module for heterogeneous chemistry, via KPP.

INTERFACE:

```
MODULE GCKPP_HETRATES
```

USES:

```
ONLY: NDUST
USE CMN_FJX_MOD,
USE CMN_FJX_MOD,
                        ONLY : NAER
USE CMN_SIZE_MOD,
                        ONLY : LLSTRAT
USE PHYSCONSTANTS,
                        ONLY : CONSVAP
                        ONLY : ERROR_STOP
USE ERROR_MOD,
USE ERROR_MOD,
                        ONLY : GEOS_CHEM_STOP
USE ERROR_MOD,
                        ONLY : IS_SAFE_DIV
USE gckpp_Precision
USE gckpp_Parameters
USE gckpp_Global,
                        ONLY : HET
USE State_Chm_Mod,
                        ONLY : ChmState
USE State_Chm_Mod,
                        ONLY : Ind_
USE State_Met_Mod,
                        ONLY : MetState
USE Input_Opt_Mod,
                        ONLY: OptInput
USE PhysConstants,
                        ONLY : AVO
USE Precision_Mod,
                        ONLY : fp
IMPLICIT NONE
```

PRIVATE

PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: SET_HET
```

PRIVATE MEMBER FUNCTIONS:

```
! These functions are used for all mechanisms
PRIVATE :: HETNO3
```

```
PRIVATE :: HETNO2
  PRIVATE :: HETHO2
  PRIVATE :: HETHBr
  PRIVATE :: HETN205
  PRIVATE :: HETBrN03
  PRIVATE :: HETHOBr
  PRIVATE :: HETHOBr_ice
  PRIVATE :: HETHBr_ice
  PRIVATE :: N205
  PRIVATE :: HO2
  PRIVATE :: CLD1K_BrN03
  PRIVATE :: FCRO2HO2
  PRIVATE :: FYHORO
  PRIVATE :: FYRNO3
  PRIVATE :: ARSL1K
#if defined( UCX )
  ! These functions are only used for UCX-based mechanisms
  PRIVATE :: HETClN03_PSC1
  PRIVATE :: HETC1N03_PSC2
  PRIVATE :: HETC1N03_PSC3
  PRIVATE :: HETBrN03_PSC
  PRIVATE :: HETHOCl_PSC1
  PRIVATE :: HETHOC1_PSC2
  PRIVATE :: HETHOBr_PSC
  PRIVATE :: HETN205_PSC
#endif
  !PRIVATE DATA MEMBERS:
  ! Scalars
  INTEGER :: NAERO
  LOGICAL :: NATSURFACE,
                            PSCBOX,
                                       STRATBOX
  REAL(fp) :: TEMPK,
                            RELHUM,
                                       SPC_SO4
  REAL(fp) :: SPC_NIT,
                            GAMMA_HO2, XTEMP,
                                                XDENA
  REAL(fp) :: CLD_BRNO3_RC, KI_HBR, KI_HOBr, QLIQ
  REAL(fp) :: QICE
  ! Arrays
  REAL(fp) :: SCF2(3)
  REAL(fp) :: XAREA(25)
  REAL(fp) :: XRADI(25)
  REAL(fp) :: KHETI_SLA(11)
 $OMP THREADPRIVATE( NAERO,
                                   NATSURFACE, PSCBOX,
                                                          STRATBOX )
 $OMP THREADPRIVATE( TEMPK,
                                   RELHUM,
                                                SPC_NIT,
                                                          SPC_SO4 )
                                                                   )
 $OMP THREADPRIVATE( GAMMA_HO2,
                                   XTEMP,
                                                XDENA
 $OMP THREADPRIVATE( CLD_BRNO3_RC, KI_HBR,
                                                                   )
                                                KI_HOBr,
                                                          QLIQ
 $OMP THREADPRIVATE( QICE,
                                   SCF2,
                                                XAREA,
                                                          XRADI
                                                                   )
                                                                   )
 $OMP THREADPRIVATE( KHETI_SLA
```

DEFINED PARAMETERS:

REAL(fp), PARAMETER :: PSCMINLIFE = 1.e-3_fp

REMARKS:

Need

- TOTAREA (previously used for archiving N2O5 hydrolysis in the planeflight diagnostic only)
- Air NUM. DENSITY
- TEMPERATURE
- Aerosol Surface Area
- Aerosol Type
- Gamma (XSTKCF; sticking factor)
- ARR
- Species num density (mcl cm-3)
- Continental PBL or no?
- In stratosphere or no?
- Reaction index (e.g. NK1HBr, NK2HBr)

According to S. Eastham, we should also include cloud and ice area explicitly, in addition to aerosol area

REVISION HISTORY:

```
14 Dec 2015 - M. Long - Initial version

29 Jan 2016 - M. Sulprizio- Update to include heterogeneous chemistry for UCX mechanism

29 Mar 2016 - R. Yantosca - NOTE: SPC_HBR and SPC_HOBR are defined for trop-only mechanisms

29 Mar 2016 - R. Yantosca - Added ProTeX headers

29 Mar 2016 - R. Yantosca - Moved all the UCX-based functions to the end of the module, for clarity

01 Apr 2016 - R. Yantosca - Remove many global variables that can be declared locally from the THREADPRIVATES

06 Jun 2016 - M. Sulprizio- Replace Get_Indx with Spc_GetIndx to use the fast-species lookup from the species database

14 Jun 2016 - M. Sulprizio- Replace Spc_GetIndx with Ind_
```

7.8.1 Set_Het

Main heterogenous chemistry driver routine. Sets up the vector of heterogeneous chemistry rates for the KPP chemistry solver.

INTERFACE:

```
SUBROUTINE SET_HET( I, J, L, SC, SM, IO, SCF )
```

INPUT PARAMETERS:

```
INTEGER :: I, J, L ! Lon, lat, level indices
TYPE(MetState) :: SM ! Meteorology State object
TYPE(OptInput) :: IO ! Input Options object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState) :: SC ! Chemistry Sate object
```

REAL(fp) :: SCF(3) ! Coefficients (Need help documenting this)

REMARKS:

REVISION HISTORY:

```
06 Jan 2015 - R. Yantosca - Initial version
01 Apr 2016 - R. Yantosca - Define many variables locally that don't need to be in the THREADPRIVATE statements
01 Apr 2016 - R. Yantosca - Remove KII_KI; we now declare that locally
31 May 2016 - E. Lundgren - Replace IO%XNUMOL with emMW_g from species database (emitted species g/mol)
```

7.8.2 HetNO3

Set the heterogenous chemistry rate for NO3.

INTERFACE:

```
FUNCTION HETNO3( A, B ) RESULT( HET_NO3 )
```

INPUT PARAMETERS:

```
! Rate coefficients REAL(fp), INTENT(IN) :: A, B
```

RETURN VALUE:

```
REAL(fp) :: HET_NO3
```

REMARKS:

```
29 Mar 2016 - R. Yantosca - Added ProTeX header
01 Apr 2016 - R. Yantosca - Define N, XSTKCF, ADJUSTEDRATE locally
01 Apr 2016 - R. Yantosca - Replace KII_KI with DO_EDUCT local variable
```

7.8.3 HetNO2

Set the heterogenous chemistry rate for NO2.

INTERFACE:

```
FUNCTION HETNO2( A, B ) RESULT( HET_NO2 )
```

INPUT PARAMETERS:

```
! Rate coefficients REAL(fp), INTENT(IN) :: A, B
```

RETURN VALUE:

```
REAL(fp) :: HET_NO2
```

REMARKS:

REVISION HISTORY:

```
29 Mar 2016 - R. Yantosca - Added ProTeX header
01 Apr 2016 - R. Yantosca - Define N, XSTKCF, ADJUSTEDRATE locally
01 Apr 2016 - R. Yantosca - Replace KII_KI with DO_EDUCT local variable
```

7.8.4 HetHO2

Set the heterogenous chemistry rate for HO2.

INTERFACE:

```
FUNCTION HETHO2( A, B ) RESULT( HET_HO2 )
```

INPUT PARAMETERS:

```
! Rate coefficients REAL(fp), INTENT(IN) :: A, B
```

RETURN VALUE:

```
REAL(fp) :: HET_HO2
```

REMARKS:

```
29 Mar 2016 - R. Yantosca - Added ProTeX headers
01 Apr 2016 - R. Yantosca - Define N, XSTKCF, ADJUSTEDRATE locally
01 Apr 2016 - R. Yantosca - Replace KII_KI with DO_EDUCT local variable
```

7.8.5 HetHBr

Set the heterogeneous rate for HBr.

INTERFACE:

```
FUNCTION HETHBr( A, B ) RESULT( HET_HBr )
```

INPUT PARAMETERS:

```
! Rate coefficients REAL(fp), INTENT(IN) :: A, B
```

RETURN VALUE:

```
REAL(fp) :: HET_HBr
```

REMARKS:

REVISION HISTORY:

```
29 Mar 2016 - R. Yantosca - Added ProTeX headers
01 Apr 2016 - R. Yantosca - Define N, XSTKCF, ADJUSTEDRATE locally
01 Apr 2016 - R. Yantosca - Define local variable for educt adjustment
```

7.8.6 HetN2O5

Set heterogenous chemistry rate for N2O5.

INTERFACE:

```
FUNCTION HETN205( A, B ) RESULT( HET_N205 )
```

INPUT PARAMETERS:

```
! Rate coefficients REAL(fp), INTENT(IN) :: A, B
```

RETURN VALUE:

```
REAL(fp) :: HET_N205
```

REMARKS:

```
29 Mar 2016 - R. Yantosca - Added ProTeX header
01 Apr 2016 - R. Yantosca - Define N, XSTKCF, ADJUSTEDRATE locally
01 Apr 2016 - R. Yantosca - Replace KII_KI with DO_EDUCT local variable
```

7.8.7 HetBrNO3

Sets the heterogenous chemistry rate for BrNO3.

INTERFACE:

```
FUNCTION HETBrN03( A, B ) RESULT( HET_BrN03 )
```

INPUT PARAMETERS:

```
! Rate coefficients REAL(fp), INTENT(IN) :: A, B
```

RETURN VALUE:

```
REAL(fp) :: HET_BrN03
```

REMARKS:

REVISION HISTORY:

```
29 Mar 2016 - R. Yantosca - Added ProTeX header
01 Apr 2016 - R. Yantosca - Define N, XSTKCF, ADJUSTEDRATE locally
01 Apr 2016 - R. Yantosca - Replace KII_KI with DO_EDUCT local variable
```

7.8.8 HetHOBr

Sets the heterogenous chemistry rate for HOBr.

INTERFACE:

```
FUNCTION HETHOBr( A, B ) RESULT( HET_HOBr )
```

INPUT PARAMETERS:

```
! Rate coefficients REAL(fp), INTENT(IN) :: A, B
```

RETURN VALUE:

```
REAL(fp) :: HET_HOBr
```

REMARKS:

```
29 Mar 2016 - R. Yantosca - Added ProTeX header
01 Apr 2016 - R. Yantosca - Define N, XSTKCF, ADJUSTEDRATE locally
01 Apr 2016 - R. Yantosca - Replace KII_KI with DO_EDUCT local variable
```

7.8.9 HetHOBr_Ice

Sets the heterogenous chemistry rate for HOBr (on ice).

INTERFACE:

```
FUNCTION HETHOBr_ice( A, B ) RESULT( HET_HObr_ice )
```

INPUT PARAMETERS:

```
! Rate coefficients REAL(fp), INTENT(IN) :: A, B
```

RETURN VALUE:

```
REAL(fp) :: HET_HObr_ice
```

REMARKS:

REVISION HISTORY:

```
29 Mar 2016 - R. Yantosca - Added ProTeX header
```

7.8.10 HetBr_Ice

Sets the heterogenous chemistry rate for HBr (on ice).

INTERFACE:

```
FUNCTION HETHBr_ice( A, B ) RESULT( HET_HBr_ice )
```

INPUT PARAMETERS:

```
! Rate coefficients
REAL(fp), INTENT(IN) :: A, B
!RETURN VALUE
REAL(fp) :: HET_HBr_ice
```

REMARKS:

```
29 Mar 2016 - R. Yantosca - Added ProTeX header
```

7.8.11 N2O5

Internal function N2O5 computes the GAMMA sticking factor for N2O5 hydrolysis. (mje, bmy, 8/7/03)

INTERFACE:

```
FUNCTION N205( AEROTYPE, TEMP, RH ) RESULT( GAMMA )
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: AEROTYPE ! Denoting aerosol type (cf FAST_JX)
REAL(fp), INTENT(IN) :: TEMP ! Temperature [K]
REAL(fp), INTENT(IN) :: RH ! Relative humidity [1]
```

RETURN VALUE:

```
REAL(fp) :: GAMMA
```

REMARKS:

Taken from the old SMVGEAR function calcrate.F.

REVISION HISTORY:

```
29 Mar 2016 - R. Yantosca - Added ProTeX headers
```

7.8.12 HO2

Function HO2 computes the GAMMA reaction probability for HO2 loss in aerosols based on the recommendation of Thornton, Jaegle, and McNeill, "Assessing Known Pathways For HO2 Loss in Aqueous Atmospheric Aerosols: Regional and Global Impacts on Tropospheric Oxidants" J. Geophys. Res., doi:10.1029/2007JD009236, 2008

INTERFACE:

```
FUNCTION HO2( RADIUS, TEMP, DENAIR, & SQM, HO2DENS, AEROTYPE, & CONTINENTAL_PBL, Input_Opt ) & RESULT( GAMMA )
```

INTENT(IN) :: DENAIR

USES:

```
USE Input_Opt_Mod, ONLY : OptInput
```

INPUT PARAMETERS:

REAL(fp),

```
! Arguments

REAL(fp), INTENT(IN) :: RADIUS ! Aerosol radius [cm]

REAL(fp), INTENT(IN) :: TEMP ! Temperature [K]
```

! Air density [molec/cm3]

REAL(fp), INTENT(IN) :: HO2DENS ! HO2 density [molec/cm3] REAL(fp), INTENT(IN) :: SQM ! Square root of MW [g/mol] INTEGER, INTENT(IN) :: AEROTYPE ! Aerosol type (cf FAST-JX) INTENT(IN) :: CONTINENTAL_PBL ! Flag set to 1 if the box INTEGER, ! box is located in the ! continenal boundary ! layer, otherwise 0. ! Also check for ICE/SNOW ! (to disable this at ! high latitudes). TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

RETURN VALUE:

REAL(fp) :: GAMMA ! Reaction probability

REMARKS:

Taken from the old SMVGEAR routine calcrate.F. Gamma(HO2) is a function of aerosol type, radius, temperature.

eferences:

- (1) Jacob, D.J., Heterogeneous chemistry and tropospheric ozone, Atmos. Environ., 34, 2131-2159, 2000. [full text (pdf)]
- (2) J. Mao, Fan, S., Jacob, D. J., and Travis, K. R.: Radical loss in the atmosphere from Cu-Fe redox coupling in aerosols, Atmos. Chem. Phys., 13, 509-519, doi:10.5194/acp-13-509-2013, 2013.

REVISION HISTORY:

```
17 May 2013 - M. Payer - Add improved HO2 uptake (J. Mao)
22 May 2013 - M. Payer - Added option to read GAMMA_HO2 from input.geos. Recommended value is 0.2 based on Jacob et al (2000) and Mao et al. (2013).
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
29 Mar 2016 - R. Yantosca - Added ProTeX headers
```

7.8.13 Cld1k_BrNO3

Function CLD1K_BrNO3 calculates the rate constant for heterogeneous cycling of BrNO3 off of cloud particles.

INTERFACE:

```
FUNCTION CLD1K_BrN03( I, J, L, DENAIR, & QL, State_Met ) RESULT( cld1k )
```

USES:

```
USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I ! Longitude index
INTEGER, INTENT(IN) :: J ! Latitude index
INTEGER, INTENT(IN) :: L ! Altitude index
REAL(fp), INTENT(IN) :: DENAIR ! Density of air [#/cm3]
REAL(fp), INTENT(IN) :: QL ! Cloud water mixing ratio [kg/kg]
TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

RETURN VALUE:

```
REAL(fp) :: cld1k ! Rate constant for ! heterogeneous cycling ! of BrNO3 off of cloud ! particles
```

REMARKS:

The rate constant for heterogeneous cycling of BrNO3 off of cloud particles is calculated assuming:

```
1. A sticking coefficient of 0.3 [Yang et al. 2005]
2. uniform cloud droplet size for 2 types of clouds
- continental warm clouds: r = 6d-4 [cm]
- marine warm clouds: r = 10d-4 [cm]
* no distributions are assumed

** Calculation of a 1st order rate constent barrowed from the subroutine arsl1k.f. Below are comments from that code:

The 1st-order loss rate on wet aerosol (Dentener's Thesis, p. 14) is computed as:

ARSL1K [1/s] = area / [ radius/dfkg + 4./(stkcf * nu) ]
```

DFKG = Gas phase diffusion coeff [cm2/s] (order of 0.1)

= Mean molecular speed [cm/s] = sqrt(8R*TK/pi/M) for Maxwell

```
27 Feb 2011 - J. Parrella - Initial version
22 May 2012 - M. Payer - Added ProTeX headers
09 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met
derived type object
06 Nov 2014 - R. Yantosca - Now use State_Met%CLDF(I,J,L)
```

7.8.14 FcrO2HO2

!fgap, based on saunder 2003 k14

INTERFACE:

```
FUNCTION FCRO2HO2( XCARBN ) RESULT( FC_RO2HO2 )
```

INPUT PARAMETERS:

REAL(fp), INTENT(IN) :: XCARBN

RETURN VALUE:

REAL(fp) :: FC_RO2HO2

REVISION HISTORY:

24 Jul 2014 - R. Yantosca - Now inlined to calcrate.F

7.8.15 FyHORO

Overview

Function FYHORO returns returns the branching ratio between HOC2H4O oxidation and dissociation: (1) HOC2H4 –O2–; HO2 + GLYC (2) HOC2H4 ——; HO2 + 2CH2O

References

- 1. Orlando et al., 1998: Laboratory and theoretical study of the oxyradicals in the OH-and Cl-initiated oxidation of ethene, J. Phys. Chem. A, 102, 8116-8123.
- 2. Orlando et al., 2003: The atmospheric chemistry of alkoxy radicals, Chem. Rev., 103, 4657-4689.

INTERFACE:

```
FUNCTION FYHORO( ZDNUM, TT ) RESULT( FY_HORO )
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: ZDNUM ! Air density [molec/cm3] REAL(fp), INTENT(IN) :: TT ! Temperature [K ]
```

RETURN VALUE:

REAL(fp) :: FY_HORO

- (1) Branching ratio calculation (tmf, 2/6/05).
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 25 Jul 2014 R. Yantosca Now inlined into calcrate.F

7.8.16 FyrNO3

Function FYRNO3 returns organic nitrate yields YN = RKA/(RKA+RKB) from RO2+NO reactions as a function of the number N of carbon atoms.

INTERFACE:

```
FUNCTION FYRNO3 (XCARBN, ZDNUM, TT ) RESULT (FYR_NO3)
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: XCARBN ! Number of C atoms in RO2
REAL(fp), INTENT(IN) :: ZDNUM ! Air density [molec/cm3]
REAL(fp), INTENT(IN) :: TT ! Temperature [K ]
```

RETURN VALUE:

```
REAL(fp) :: FYR_NO3
```

REVISION HISTORY:

- (1) Original code from Larry Horowitz, Jinyou Liang, Gerry Gardner, and Daniel Jacob circa 1989/1990.
- (2) Updated following Atkinson 1990.
- (3) Change yield from Isoprene Nitrate (ISN2) from 0.44% to 12%, according to Sprengnether et al., 2002. (amf, bmy, 1/7/02)
- (4) Eliminate obsolete code from 1/02 (bmy, 2/27/02)
- (5) Updated comment description of XCARBN (bmy, 6/26/03)
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 25 Jul 2014 R. Yantosca Now inlined into calcrate.F

7.8.17 Arsl1k

Function ARSL1K calculates the 1st-order loss rate of species on wet aerosol surface.

INTERFACE:

```
FUNCTION ARSL1K( AREA, RADIUS, DENAIR, STKCF, STK, SQM ) & RESULT( ARS_L1K )
```

INPUT PARAMETERS:

```
! Surface area of wet aerosols/volume of air [cm2/cm3]
REAL(fp), INTENT(IN) :: AREA
! Radius of wet aerosol [cm], order of 0.01-10 um;
! Note that radius here is Rd, not Ro
REAL(fp), INTENT(IN) :: RADIUS
! Density of air [#/cm3]
```

```
REAL(fp), INTENT(IN) :: DENAIR

! Sticking coefficient [unitless], order of 0.1
REAL(fp), INTENT(IN) :: STKCF

! Square root of temperature [K]
REAL(fp), INTENT(IN) :: STK

! Square root of molecular weight [g/mole]
REAL(fp), INTENT(IN) :: SQM
```

RETURN VALUE:

REAL(fp) :: ARS_L1K

REMARKS:

The 1st-order loss rate on wet aerosol (Dentener's Thesis, p. 14) is computed as:

```
ARSL1K [1/s] = area / [ radius/dfkg + 4./(stkcf * xmms) ]
```

where XMMS = Mean molecular speed [cm/s] = sqrt(8R*TK/pi/M) for Maxwell DFKG = Gas phase diffusion coeff [cm2/s] (order of 0.1)

REVISION HISTORY:

```
01 Jul 1994 - lwh, jyl, gmg, djj - Initial version
```

04 Apr 2003 - R. Yantosca - Updated comments, cosmetic changes

07 Apr 2004 - R. Yantosca - Now return w/ default value if RADIUS is zero (i.e. is smaller than a very small number)

03 Dec 2009 - R. Yantosca - Prevent div-by-zero errors by returning the default value if any of the args are zero

03 Dec 2009 - R. Yantosca - Added ProTeX Header

20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete

$7.8.18 \quad HetN2O5_Psc$

Set heterogenous chemistry rate for N2O5(g) + HCl(l,s) in polar stratospheric clouds.

INTERFACE:

```
FUNCTION HETN205_PSC( A, B ) RESULT( HET_N205_PSC )
```

INPUT PARAMETERS:

```
! Rate coefficients REAL(fp), INTENT(IN) :: A, B
```

RETURN VALUE:

REAL(fp) :: HET_N2O5_PSC

REMARKS:

This routine is only activated for UCX-based mechanisms.

REVISION HISTORY:

- 29 Jan 2016 M. Sulprizio- Initial version, adapted from code previously in calcrate.F
- 29 Mar 2016 R. Yantosca Added ProTeX header
- 01 Apr 2016 R. Yantosca Define N, XSTKCF, ADJUSTEDRATE locally
- 01 Apr 2016 R. Yantosca Replace KII_KI with DO_EDUCT local variable
- 04 May 2016 M. Sulprizio- Add fixes for setting rate if not a STRATBOX

7.8.19 HetClNO3_Psc1

Set heterogenous chemistry rate for ClNO3(g) + H2O(l,s) in polar stratopsheric clouds.

INTERFACE:

```
FUNCTION HETClN03_PSC1( A, B ) RESULT( HET_ClN03_PSC1 )
```

INPUT PARAMETERS:

```
! Rate coefficients REAL(fp), INTENT(IN) :: A, B
```

RETURN VALUE:

REAL(fp) :: HET_ClNO3_PSC1

REMARKS:

This routine is only activated for UCX-based mechanisms.

REVISION HISTORY:

- 29 Jan 2016 M. Sulprizio- Initial version, adapted from code previously in calcrate.F
- 29 Mar 2016 R. Yantosca Added ProTeX header
- 01 Apr 2016 R. Yantosca Define N, XSTKCF, ADJUSTEDRATE locally
- 01 Apr 2016 R. Yantosca Replace KII_KI with DO_EDUCT local variable
- 04 May 2016 M. Sulprizio- Add fixes for setting rate if not a STRATBOX

7.8.20 HetClNO3_Psc2

Sets the heterogenous chemistry rate for ClNO3(g) + HCl(l,s) in polar stratospheric clouds.

INTERFACE:

FUNCTION HETC1N03_PSC2(A, B) RESULT(HET_C1N03_PSC2)

INPUT PARAMETERS:

! Rate coefficients

REAL(fp), INTENT(IN) :: A, B

RETURN VALUE:

REAL(fp) :: HET_ClNO3_PSC2

REMARKS:

This routine is only activated for UCX-based mechanisms.

REVISION HISTORY:

29 Jan 2016 - M. Sulprizio- Initial version, adapted from code previously in calcrate.F

29 Mar 2016 - R. Yantosca - Added ProTeX header

01 Apr 2016 - R. Yantosca - Define N, XSTKCF, ADJUSTEDRATE locally

01 Apr 2016 - R. Yantosca - Replace KII_KI with DO_EDUCT local variable

04 May 2016 - M. Sulprizio- Add fixes for setting rate if not a STRATBOX

7.8.21 HetClNO3_Psc3

Set heterogenous chemistry rate for ClNO3(g) + HBr(l,s) in polar stratospheric clouds.

INTERFACE:

FUNCTION HETC1NO3_PSC3(A, B) RESULT(HET_C1NO3_PSC3)

INPUT PARAMETERS:

! Rate coefficients

REAL(fp), INTENT(IN) :: A, B

RETURN VALUE:

REAL(fp) :: HET_ClN03_PSC3

REMARKS:

This routine is only activated for UCX-based mechanisms.

REVISION HISTORY:

29 Jan 2016 - M. Sulprizio- Initial version, adapted from code previously in calcrate.F

29 Mar 2016 - R. Yantosca - Added ProTeX header

01 Apr 2016 - R. Yantosca - Define N, XSTKCF, ADJUSTEDRATE locally

01 Apr 2016 - R. Yantosca - Replace KII_KI with DO_EDUCT local variable

04 May 2016 - M. Sulprizio- Add fixes for setting rate if not a STRATBOX

7.8.22 HetBrNo3_Psc

Set heterogenous chemistry rate for BrNO3(g) + HCl(l,s) in polar stratospheric clouds.

INTERFACE:

```
FUNCTION HETBrN03_PSC( A, B ) RESULT( HET_BrN03_PSC )
```

INPUT PARAMETERS:

```
! Rate coefficients REAL(fp), INTENT(IN) :: A, B
```

RETURN VALUE:

```
REAL(fp) :: HET_BrN03_PSC
```

REMARKS:

This routine is only activated for UCX-based mechanisms.

REVISION HISTORY:

```
29 Jan 2016 - M. Sulprizio- Initial version, adapted from code previously in calcrate.F
```

```
29 Mar 2016 - R. Yantosca - Added ProTeX header
```

- 01 Apr 2016 R. Yantosca Define N, XSTKCF, ADJUSTEDRATE locally
- 01 Apr 2016 R. Yantosca Replace KII_KI with DO_EDUCT local variable
- 04 May 2016 M. Sulprizio- Add fixes for setting rate if not a STRATBOX

7.8.23 HetHOCl_Psc1

Set heterogenous chemistry rate for HOCl(g) + HCl(l,s) in polar stratopsheric clouds.

INTERFACE:

```
FUNCTION HETHOCl_PSC1( A, B ) RESULT( HET_HOCl_PSC1 )
```

INPUT PARAMETERS:

```
! Rate coefficients REAL(fp), INTENT(IN) :: A, B
```

RETURN VALUE:

```
REAL(fp) :: HET_HOC1_PSC1
```

REMARKS:

This routine is only activated for UCX-based mechanisms.

```
29 Jan 2016 - M. Sulprizio- Initial version, adapted from code previously in calcrate.F
```

```
29 Mar 2016 - R. Yantosca - Added ProTeX header
```

- 01 Apr 2016 R. Yantosca Define N, XSTKCF, ADJUSTEDRATE locally
- 01 Apr 2016 R. Yantosca Replace KII_KI with DO_EDUCT local variable
- 04 May 2016 M. Sulprizio- Add fixes for setting rate if not a STRATBOX

7.8.24 HetHocl_Psc2

Set heterogenous chemistry rate for HOCl(g) + HBr(l,s) in polar stratospheric clouds.

INTERFACE:

```
FUNCTION HETHOC1_PSC2( A, B ) RESULT( HET_HOC1_PSC2 )
```

INPUT PARAMETERS:

```
! Rate coefficients
```

REAL(fp), INTENT(IN) :: A, B

RETURN VALUE:

REAL(fp) :: HET_HOC1_PSC2

REMARKS:

This routine is only activated for UCX-based mechanisms.

REVISION HISTORY:

```
29 Jan 2016 - M. Sulprizio- Initial version, adapted from code previously in calcrate.F
```

29 Mar 2016 - R. Yantosca - Added ProTeX header

01 Apr 2016 - R. Yantosca - Define N, XSTKCF, ADJUSTEDRATE locally

01 Apr 2016 - R. Yantosca - Replace KII_KI with DO_EDUCT local variable

04 May 2016 - M. Sulprizio- Add fixes for setting rate if not a STRATBOX

7.8.25 HetHOBr_Psc

Set heterogenous chemistry rate for HOBr(g) + HCl(l,s) in polar stratospheric clouds.

INTERFACE:

```
FUNCTION HETHOBr_PSC( A, B ) RESULT( HET_HOBr_PSC )
```

INPUT PARAMETERS:

```
! Rate coefficients
```

REAL(fp), INTENT(IN) :: A, B

RETURN VALUE:

REAL(fp) :: HET_HOBr_PSC

REMARKS:

This routine is only activated for UCX-based mechanisms.

REVISION HISTORY:

```
29 Jan 2016 - M. Sulprizio- Initial version, adapted from code previously in calcrate.F
```

29 Mar 2016 - R. Yantosca - Added ProTeX header

01 Apr 2016 - R. Yantosca - Define N, XSTKCF, ADJUSTEDRATE locally

01 Apr 2016 - R. Yantosca - Replace KII_KI with DO_EDUCT local variable

04 May 2016 - M. Sulprizio- Add fixes for setting rate if not a STRATBOX

7.8.26 Check_Nat

Subroutine CHECK_NAT determines whether the solid PSC is composed of ice or NAT (nitric acid trihydrate) (needed for heterogeneous chemistry), or indeed if there is any direct PSC calculation at all. This is important for determining whether to use the JPP or Kirner scheme for ice cloud radii.

INTERFACE:

```
SUBROUTINE CHECK_NAT( I, J, L, IS_NAT, IS_PSC, IS_STRAT, & Input_Opt, State_Met, State_Chm )
```

INPUT PARAMETERS:

```
! Grid indices
   INTEGER,
                   INTENT(IN) :: I,J,L
   TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input options
   TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
   TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object
!OUTPUT VARIABLES:
                                             ! Is surface NAT?
   LOGICAL,
                   INTENT(OUT) :: IS_NAT
   LOGICAL,
                   INTENT(OUT) :: IS_PSC
                                             ! Are there solid PSCs?
                   INTENT(OUT) :: IS_STRAT
                                             ! Are we in the strat?
   LOGICAL,
```

REMARKS:

This routine is only activated for UCX-based mechanisms

REVISION HISTORY:

```
17 Apr 2013 - S. D. Eastham - Initial version
21 Feb 2014 - M. Sulprizio - Now pass Input_Opt, State_Met, and State_Chm
objects via the arg list
08 Apr 2015 - R. Yantosca - Remove call to READ_PSC_FILE, this is
now done from DO_CHEMISTRY (chemistry_mod.F)
29 Jan 2016 - M. Sulprizio - Moved this routine from ucx_mod.F to
gckpp_HetRates.F90
```

7.9 Fortran: Module Interface ucx_mod.F

Module UCX_MOD contains routines and variables which are associated with the addition of full stratospheric chemistry to GEOS-Chem (based on the NASA GMI implementation, forming the Unified Chemistry eXtension (UCX).

INTERFACE:

MODULE UCX_MOD

USES:

```
USE CMN_SIZE_MOD
USE ERROR_MOD, ONLY : DEBUG_MSG
```

```
USE inquireMod,
                       ONLY : findFreeLUN
    USE PhysConstants ! Physical constants
    USE PRECISION_MOD ! For GEOS-Chem Precision (fp)
#if !defined(ESMF_)
     ! NcdfUtil modules for netCDF I/O
    USE m_netcdf_io_open
                                           ! netCDF open
    USE m_netcdf_io_get_dimlen
                                           ! netCDF dimension queries
    USE m_netcdf_io_read
                                          ! netCDF data reads
    USE m_netcdf_io_close
                                           ! netCDF close
#endif
     IMPLICIT NONE
#if !defined(ESMF_)
     include "netcdf.inc"
#endif
    PRIVATE
```

PUBLIC DATA MEMBERS:

```
CHARACTER(LEN=255), PUBLIC :: AVG_FILE_ROOT ! Directory for diurnal avg data
CHARACTER(LEN=255), PUBLIC :: NOON_FILE_ROOT ! Directory for noontime data
CHARACTER(LEN=255), PUBLIC :: MONTREAL_FILE_ROOT ! Root directoy for WHO data
                    PUBLIC :: T_STS ! Max temperature of STS formation (K)
                    PUBLIC :: T_NAT_SUPERCOOL ! NAT supercooling (K)
REAL(fp),
                    PUBLIC :: P_ICE_SUPERSAT ! Ice supersaturation (-)
REAL(fp),
                    PUBLIC :: NDENS_AER ! See below
                   PUBLIC :: CFCYEAR ! Year for CFC emissions
INTEGER,
```

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: SET_INITIAL_MIXRATIOS PUBLIC :: SET_H2O_TRAC PUBLIC :: SET_CLOCK_TRAC PUBLIC :: EMISS_BASIC PUBLIC :: SETTLE_STRAT_AER PUBLIC :: SO4_PHOTFRAC PUBLIC :: UCX_NOX PUBLIC :: UCX_H2SO4PHOT PUBLIC :: CALC_STRAT_AER PUBLIC :: GET_STRAT_OPT PUBLIC :: KG_STRAT_AER PUBLIC :: RHO_STRAT_AER

PUBLIC :: INIT_UCX PUBLIC :: DIAGINIT_UCX PUBLIC :: CLEANUP_UCX PUBLIC :: READ_PSC_FILE PUBLIC :: WRITE_STATE_PSC

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: APPLY_2DTRAC PRIVATE :: READ_SFC

PRIVATE :: SET_MONTREAL

PRIVATE :: SET_MONTREAL_NCDF
PRIVATE :: GET_MONTREAL_NCDF

PRIVATE :: MONTREAL_SCALEFAC

PRIVATE :: TERNARY

PRIVATE :: CARSLAW_DENSITY
PRIVATE :: CALC_H2SO4_GAS
PRIVATE :: CALC_SLA_GAMMA
PRIVATE :: MOLEC_SPEED
PRIVATE :: SFCMR_INIT
PRIVATE :: SFCMR_READ
PRIVATE :: SFCMR_GET
PRIVATE :: NOXCOEFF_INIT

PRIVATE :: GET_JJNOX

REVISION HISTORY:

26 Mar 2013 - S. D. Eastham - Initial version

04 Apr 2013 - S. D. Eastham - Rolled several routines into module

20 Feb 2014 - M. Sulprizio - Removed "define.h", this is now obsolete

24 Nov 2014 - M. Yannetti - Added PRECISION_MOD

05 Dec 2014 - C. Keller - Added SFCMR object for reading surface mixing

ratios to buffer (from ASCII file).

Now map NOx coefficients onto grids other than

4x5 or 2x25.

14 Jan 2014 - C. Keller - Now read and diagnose STATE_PSC through HEMCO.

08 Apr 2015 - R. Yantosca - Now make READ_PSC_FILE a PUBLIC routine

08 May 2015 - C. Keller - Added WRITE_STATE_PSC

05 Jan 2016 - E. Lundgren - Use global physical parameters AVO, PI, AIRMW,

RE, RSTARG, and ATM

28 Jan 2016 - M. Sulprizio - STATE_PSC and KHETI_SLA are now fields in

State_Chm instead of public arrays. These need to be added to the derived type object to be

accessed in gckpp_HetRates.F90.

28 Jan 2016 - M. Sulprizio - Move routine CHECK_NAT to gckpp_HetRates.F90

21 Jun 2016 - R. Yantosca - Now store species ID flags as module variables

23 Jun 2016 - R. Yantosca - Remove references to APM code; it is no longer

compatible with the FlexChem implementation

18 Jul 2016 - M. Sulprizio- Remove CFCX and HCFCX everywhere and replace with

their constituents. Family tracers have been

eliminated.

29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90

7.9.1 set_initial_mixratios

Subroutine SET_INITIAL_MIXRATIOS is a public interface. Concentrations of species are read from 2D estimates made using the AER 2D model.

INTERFACE:

```
SUBROUTINE SET_INITIAL_MIXRATIOS( am_I_Root, Input_Opt, State_Met,
& State_Chm )
```

USES:

```
USE ERROR_MOD, ONLY : ALLOC_ERR,ERROR_STOP
USE GC_GRID_MOD, ONLY : GET_YMID
USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState
USE TIME_MOD, ONLY : GET_MONTH
USE TIME_MOD, ONLY : GET_YEAR
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

REMARKS:

Concentrations of each of the following species are read from 2D estimates made using the AER 2D model:

(#) TRC	= Constituents	< Controlled by
(1) CH4	= CH4	< LSETCH4
(2) N2O	= N2O	< LSETN20
(3) OCS	= OCS	< LSETOCS
(4) SO4	= H2SO4	< LSETH2SO4
(5) CFC	= CFC-113/114/115	< LSETCFC
(6) HCFC	= HCFC-22/141b/142b	< LSETCFC
(7) CFC11	= CFC-11	< LSETCFC
(8) CFC12	= CFC-12	< LSETCFC
(9) H1202	= Halon 1202	< LSETCFC
(10) H1211	= Halon 1211	< LSETCFC
(11) H1301	= Halon 1301	< LSETCFC
(12) H2402	= Halon 2402	< LSETCFC
(13) Cl2	= C12	< LSETCL
(14) ClOx	= C1 + C10	< LSETCL
(15) CC14	= CC14	< LSETCL

(16)	CH3C1	= CH3Cl	< LSETCL
(17)	CH3CC13	= CH3CC13	< LSETCL
(18)	HC1	= HCl	< LSETCL
(19)	HOC1	= HOC1	< LSETCL
(20)	C1202	= C1202	< LSETCL
(21)	C1NO2	= C1NO2	< LSETCL
(22)	C10N02	= ClNO3	< LSETCL
(23)	OC10	= OC10	< LSETCL
(24)	C100	= C100	< LSETCL
(25)	BrCl	= BrCl	< (LSETCL LSETBR LSETBRSTRAT)
(26)	Br2	= Br2	< LSETBR LSETBRSTRAT
(27)	Br	= Br	< LSETBR LSETBRSTRAT
(28)	Br0	= BrO	< LSETBR LSETBRSTRAT
(29)	HOBr	= HOBr	< LSETBR LSETBRSTRAT
(30)	HBr	= HBr	< LSETBR LSETBRSTRAT
(31)	BrNO2	= BrNO2	< LSETBR LSETBRSTRAT
(32)	BrN03	= BrNO3	< LSETBR LSETBRSTRAT
(33)	CHBr3	= CHBr3	< LSETBR LSETBRSTRAT
(34)	CH2Br2	= CH2Br2	< LSETBR LSETBRSTRAT
(35)	CH3Br	= CH3Br	< LSETBR LSETBRSTRAT

REVISION HISTORY:

```
26 Mar 2013 - S. D. Eastham - Initial version
07 Feb 2014 - R. Yantosca - !$OMP DO loops now go in L-J-I order
21 Feb 2014 - M. Sulprizio - Now pass Input_Opt, State_Met, and State_Chm
                              objects via the arg list
18 Jun 2014 - S. D. Eastham - Now read data for individual NOx species
24 Nov 2014 - C. Keller
                            - Update for stratospheric NOy (as suggested by
                              Seb Eastham)
                            - Change tracer units from kg to kg/kg
16 Mar 2015 - E. Lundgren
16 Jun 2016 - S. D. Eastham - Remove references to tracerid_mod.F
21 Jun 2016 - R. Yantosca
                            - Now use module variables for species ID's
21 Jun 2016 - R. Yantosca
                            - Add error checks to make sure that each
                              species ID flag has a valid value before
                              calling APPLY_2DRATIO routine
22 Jun 2016 - M. Yannetti
                            - Replace TCVV with spc db MW and phys constant
                            - Replace tracer pointer with species pointer
07 Jul 2016 - E. Lundgren
```

7.9.2 montreal_scalefac

Function MONTREAL_SCALEFAC calculates a scaling factor for long-lived species between a future year and a reference year, based on WMO projections.

INTERFACE:

```
FUNCTION MONTREAL_SCALEFAC(MS_TRAC,MS_FUTRYR,
& MS_INITYR,MS_TARGMO) RESULT(SCALEFAC)
```

USES:

INPUT PARAMETERS:

```
CHARACTER(*),INTENT(IN) :: MS_TRAC
INTEGER,INTENT(IN) :: MS_FUTRYR ! Future year
INTEGER,INTENT(IN) :: MS_INITYR ! Future year
INTEGER,INTENT(IN) :: MS_TARGMO ! Target month
!OUTPUT VARIABLES:
REAL(fp) :: SCALEFAC ! Scaling factor
```

REMARKS:

(1) A remark

REVISION HISTORY:

```
28 Mar 2013 - S. D. Eastham - Initial version
```

7.9.3 ucx_nox

Subroutine UCX_NOX calculates NOx and N2O loss rates above the chemistry grid, based on estimates of j-rates from a 2D model and simple photochemical assumptiones.

INTERFACE:

```
SUBROUTINE UCX_NOX( Input_Opt, State_Met, State_Chm )
```

USES:

```
USE CHEMGRID_MOD,
                        ONLY : ITS_IN_THE_CHEMGRID
USE ERROR_MOD,
                        ONLY : ERROR_STOP
USE ERROR_MOD,
                        ONLY : DEBUG_MSG
USE GC_GRID_MOD,
                        ONLY : GET_YMID
USE Input_Opt_Mod,
                        ONLY : OptInput
USE State_Chm_Mod,
                        ONLY : ChmState
USE State_Met_Mod,
                        ONLY : MetState
USE TIME_MOD,
                        ONLY : GET_TS_CHEM
USE TIME_MOD,
                        ONLY : GET_DAY_OF_YEAR
USE TIME_MOD,
                        ONLY : GET_MONTH
USE TIME_MOD,
                        ONLY : ITS_A_LEAPYEAR
USE TIME_MOD,
                        ONLY : GET_HOUR
USE TIME_MOD,
                        ONLY : GET_LOCALTIME
USE TIME_MOD,
                        ONLY : GET_MINUTE
USE CHEMGRID_MOD,
                        ONLY : GET_CHEMGRID_LEVEL
USE CMN_FJX_MOD,
                        ONLY : ZPJ
USE FAST_JX_MOD,
                        ONLY: RXN_NO, RXN_NO2, RXN_NO3, RXN_N20
```

INPUT PARAMETERS:

```
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input options
TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

REVISION HISTORY:

```
16 Jul 2013 - S. D. Eastham - Initial version
14 Feb 2014 - R. Yantosca - Now pull computation of ZMID out of main
                             parallel DO loop. Switch loop order to L-J-I.
21 Feb 2014 - M. Sulprizio - Now pass Input_Opt, State_Met, and State_Chm
                             objects via the arg list
                           - Replace GET_PCENTER, which retrieves wet
24 Feb 2014 - E. Lundgren
                             air pressure, with State_Met%PMID_DRY.
                             Remove dependency on PRESSURE_MOD.
16 Jun 2016 - S. D. Eastham - Remove references to tracerid_mod.F
21 Jun 2016 - R. Yantosca
                           - Use the module variables for species ID flags
                           - Replace TCVV with spc db MW and phys constant
22 Jun 2016 - M. Yannetti
                           - Replace tracer pointer with species pointer
07 Jul 2016 - E. Lundgren
11 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code
```

7.9.4 get_noxcoeff

Subroutine GET_NOXCOEFF reads in O1D and O3P mixing ratios along with NO, NO2, NO3 and N2O J-rates from 2D data, interpolating onto the 3D grid and storing in NOX_O and NOX_J.

INTERFACE:

```
SUBROUTINE GET_NOXCOEFF( TARG_MONTH, Input_Opt, State_Met )
```

USES:

```
USE CHEMGRID_MOD, ONLY : ITS_IN_THE_CHEMGRID
USE CHEMGRID_MOD, ONLY : GET_CHEMGRID_LEVEL
USE ERROR_MOD, ONLY : ERROR_STOP
USE ERROR_MOD, ONLY : ALLOC_ERR
USE FILE_MOD, ONLY : IOERROR
USE Input_Opt_Mod, ONLY : OptInput
USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

REMARKS:

At some later point we should attempt to rewrite the parallel DO loop so that the loop order is L-J-I. Not sure how easy that is. (bmy, 2/14/14)

REVISION HISTORY:

```
26 Mar 2013 - S. D. Eastham - Initial version

14 Feb 2014 - R. Yantosca - Parallelize main DO loop

21 Feb 2014 - M. Sulprizio - Now pass Input_Opt and State_Met objects via the arg list

24 Feb 2014 - E. Lundgren - Replace GET_PCENTER, which retrieves wet air pressure, with State_Met%PMID and remove dependency on PRESSURE_MOD.
```

$7.9.5 \quad apply_2dtrac$

Subroutine APPLY_2DTRAC reads in and applies 2D data from AER 2D model output to the 3D GEOS-Chem grid. Zonally-averaged mixing ratios vary by month, but no interpolation is performed.

INTERFACE:

```
SUBROUTINE APPLY_2DTRAC( TRAC_ADD, STRAT_ONLY, SFC_ONLY, SCALEFAC, & Input_Opt, State_Met, State_Chm )
```

USES:

```
USE CHEMGRID_MOD, ONLY : ITS_IN_THE_STRATMESO
USE ERROR_MOD, ONLY : ERROR_STOP
USE FILE_MOD, ONLY : IOERROR
USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

```
LOGICAL,
               INTENT(IN)
                             :: TRAC_ADD
                                            ! Add (instead of overwrite)
LOGICAL,
               INTENT(IN)
                             :: STRAT_ONLY ! Only write to stratosphere
LOGICAL,
                             :: SFC_ONLY
                                            ! Only write to surface
               INTENT(IN)
                                              ! Future scaling factor
REAL(fp),
                 INTENT(IN)
                             :: SCALEFAC
TYPE(OptInput), INTENT(IN)
                             :: Input_Opt ! Input options
TYPE(MetState), INTENT(IN)
                             :: State_Met
                                            ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

REMARKS:

At some later point we should attempt to rewrite the parallel DO loop so that the loop order is L-J-I. Not sure how easy that is. (bmy, 2/14/14)

REVISION HISTORY:

```
26 Mar 2013 - S. D. Eastham - Initial version

14 Feb 2014 - R. Yantosca - Now parallelize main DO loop

21 Feb 2014 - M. Sulprizio - Now pass Input_Opt, State_Met, and State_Chm objects via the arg list

24 Feb 2014 - E. Lundgren - Replace GET_PCENTER, which retrieves wet air pressure, with State_Met%PMID and remove dependency on PRESSURE_MOD.

19 Mar 2015 - E. Lundgren - Change tracer units from kg to kg/kg

25 Jul 2016 - M. Yannetti - Pass State_Chem as argument to access spc db; Replace TCVV with spc db MW and phys constant

07 Jul 2016 - E. Lundgren - Replace tracer pointer with species pointer
```

7.9.6 emiss basic

Subroutine EMISS_BASIC sets surface mixing ratios of N2O, OCS and ozone-depleting substances covered by the Montreal protocol.

INTERFACE:

```
SUBROUTINE EMISS_BASIC( am_I_Root, Input_Opt, State_Met,
& State_Chm, RC )
```

USES:

```
USE ERROR_MOD, ONLY : GC_Error
USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState
USE TIME_MOD, ONLY : GET_MONTH
USE TIME_MOD, ONLY : GET_YEAR
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input options

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

REMARKS:

```
28 Mar 2013 - S. D. Eastham - Initial version

11 Feb 2014 - R. Yantosca - Rewrote DO loop to be more efficient

14 Feb 2014 - R. Yantosca - Now parallelize main DO loop

21 Feb 2014 - M. Sulprizio - Now pass Input_Opt, State_Met, and State_Chm objects via the arg list

10 Sep 2015 - E. Lundgren - Tracer units are now kg/kg dry air (prev v/v)

25 Jul 2016 - M. Yannetti - Pass State_Chm as arg for spc db access;
Replace TCVV with spc db MW and phys constant

07 Jul 2016 - E. Lundgren - Replace tracer pointer with species pointer

11 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code
```

7.9.7 read_sfc

Subroutine READ_SFC fills out the surface emissions for some species introduced as part of the unified chemistry upgrade.

INTERFACE:

```
SUBROUTINE READ_SFC( am_I_Root, Input_Opt )
```

USES:

```
USE GC_GRID_MOD, ONLY : GET_YMID
USE Input_Opt_Mod, ONLY : OptInput
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
!OUTPUT VARIABLES:
```

REVISION HISTORY:

```
04 Apr 2013 - S. D. Eastham - Initial version
21 Feb 2014 - M. Sulprizio - Now pass Input_Opt object via the arg list
```

7.9.8 set_montreal_ncdf

Subroutine SET_MONTREAL_NCDF calls GET_MONTREAL_NCDF for the surface mixing ratio for a specific year, and applies it to GRID_EMIT.

INTERFACE:

```
SUBROUTINE SET_MONTREAL_NCDF (TRAC_NAME, TARG_YR_NC, TARG_MO_NC, N)
```

USES:

INPUT PARAMETERS:

```
CHARACTER(LEN=20),INTENT(IN) :: TRAC_NAME INTEGER,INTENT(IN) :: TARG_YR_NC INTEGER,INTENT(IN) :: TARG_MO_NC
```

INTEGER, INTENT(IN) :: N

REVISION HISTORY:

```
10 Oct 2013 - S. D. Eastham - Wrapper built from edges of original GET 04 Mar 2014 - S. D. Eastham - Updated to NetCDF
```

7.9.9 get_montreal_ncdf

Function GET_MONTREAL_NCDF gets mean surface mixing ratio of a given species based on forecasts from WHO estimates. Values are interpolated between two monthly averages.

INTERFACE:

```
FUNCTION GET_MONTREAL_NCDF (TRAC_NAME, TARG_YR_NC, TARG_MO_NC) & RESULT (MEAN_MIXRATIO)
```

USES:

```
USE ERROR_MOD, ONLY : ERROR_STOP, ALLOC_ERR USE FILE_MOD, ONLY : IOERROR
```

INPUT PARAMETERS:

```
REAL(fp) :: MEAN_MIXRATIO
```

CHARACTER*(*), INTENT(IN) :: TRAC_NAME INTEGER, INTENT(IN) :: TARG_YR_NC INTEGER, INTENT(IN) :: TARG_MO_NC

REVISION HISTORY:

```
04 Apr 2013 - S. D. Eastham - Initial version
10 Oct 2013 - S. D. Eastham - Split into two routines (GET and SET)
04 Mar 2014 - S. D. Eastham - Added NetCDF compatibility
```

7.9.10 set_montreal

Subroutine SET_MONTREAL calls GET_MONTREAL for the surface mixing ratio for a specific year, and applies it to GRID_EMIT.

INTERFACE:

```
SUBROUTINE SET_MONTREAL (TRAC_NAME, TARG_LINE, N)
```

USES:

INPUT PARAMETERS:

```
CHARACTER(LEN=20), INTENT(IN) :: TRAC_NAME INTEGER, INTENT(IN) :: TARG_LINE
```

INTEGER, INTENT(IN) :: N

REVISION HISTORY:

10 Oct 2013 - S. D. Eastham - Wrapper built from edges of original GET

7.9.11 settle_strat_aer

Subroutine SETTLE_STRAT_AER performs gravitational settling of stratospheric aerosols. It is copied largely from GRAV_SETTLING in sulfate_mod.F. All of this is ignored if APM is active.

INTERFACE:

```
SUBROUTINE SETTLE_STRAT_AER( am_I_Root, Input_Opt, State_Met, State_Chm, RC)
```

USES:

```
USE CHEMGRID_MOD,
                            ONLY : ITS_IN_THE_STRATMESO
                         ONLY : ITS_IN_IRE_....
ONLY : ITS_IN_THE_CHEMGRID
USE CHEMGRID_MOD,
USE CHEMGRID_MOD,
USE CMN_DIAG_MOD
USE CMN_FJX_MOD,
                            ONLY: RAA, IND999
USE CMN_SIZE_MOD
                                  ! Size parameters
USE ErrCode_Mod
USE ERROR_MOD, ONLY : IT_IS_NAN,ERROR_STOP
USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod,
                          ONLY : MetState
USE TIME_MOD,
                           ONLY : GET_ELAPSED_SEC, GET_TS_CHEM
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input options

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
INTEGER, INTENT(INOUT) :: RC ! Return code
```

```
11 Apr 2013 - S. D. Eastham - Initial version
07 Feb 2014 - R. Yantosca - Add missing variables to !$OMP PRIVATE statement
07 Feb 2014 - R. Yantosca - Cosmetic changes
21 Feb 2014 - M. Sulprizio- Now pass Input_Opt, State_Met, and State_Chm
                            objects via the arg list
24 Feb 2014 - E. Lundgren - Replace GET_PCENTER and GET_PEDGE with
                            State_Met%PMID and State_Met%PEDGE
24 Feb 2014 - E. Lundgren - Remove dependency on PRESSURE_MOD
24 Feb 2014 - E. Lundgren - Use State_Met%DELP in place of PEDGE difference
08 Apr 2015 - R. Yantosca - Remove call to READ_PSC_FILE, this is
                            now done from DO_CHEMISTRY (chemistry_mod.F)
12 May 2016 - M. Sulprizio- Remove 1D arrays that depend on KLOOP. WERADIUS,
                            is now a pointer that point to 3D fields in
                            in State_Chm.
31 May 2016 - E. Lundgren - Replace Input_Opt%TRACER_MW_G with species
                            database emMW_g (emitted species g/mol)
16 Jun 2016 - S.D.Eastham - Remove references to tracerid_mod.F
15 Jul 2016 - E. Lundgren - Replace tracer pointer with species pointer
```

7.9.12 calc_h2so4_gas

Subroutine CALC_H2SO4_GAS calculates the fraction of strat. SO4 aerosol which can be considered to be gaseous H2SO4.

INTERFACE:

```
SUBROUTINE CALC_H2SO4_GAS( Input_Opt, State_Met, State_Chm )
```

USES:

```
USE CHEMGRID_MOD, ONLY: ITS_IN_THE_TROP
USE Input_Opt_Mod, ONLY: OptInput
USE State_Chm_Mod, ONLY: ChmState
USE State_Met_Mod, ONLY: MetState
```

INPUT PARAMETERS:

```
TYPE(OptInput), INTENT(IN) :: Input_Opt   ! Input options
TYPE(MetState), INTENT(IN) :: State_Met   ! Meteorology State object
TYPE(ChmState), INTENT(IN) :: State_Chm   ! Chemistry State object
```

```
11 Apr 2013 - S. D. Eastham - Initial version
07 Feb 2014 - R. Yantosca - Cosmetic changes
14 Feb 2014 - R. Yantosca - Changed parallel DO loop order to L-J-I,
which is the most efficient configuration
21 Feb 2014 - M. Sulprizio - Now pass Input_Opt, State_Met, and State_Chm
objects via the arg list
```

```
24 Feb 2015 - E. Lundgren - Replace GET_PCENTER with State_Met%PMID_DRY
24 Feb 2015 - E. Lundgren - Remove dependency on PRESSURE_MOD
26 Mar 2015 - E. Lundgren - Now use moist and dry air partial pressures
31 May 2016 - E. Lundgren - Replace Input_Opt%TRACER_MW_G with species database emMW_g (emitted species g/mol)
07 Jul 2016 - E. Lundgren - Replace tracer pointer with species pointer
```

7.9.13 so4_photfrac

FUNCTION SO4_PHOTFRAC returns the fraction of H2SO4 which is available for photolysis.

INTERFACE:

```
REAL(fp) FUNCTION SO4_PHOTFRAC(I,J,L)
```

INPUT PARAMETERS:

```
INTEGER,INTENT(IN) :: I,J,L ! Location indices
!OUTPUT VARIABLES:
    REAL(fp), INTENT(OUT) :: PHOTFRAC ! Gaseous fraction of H2SO4
```

REVISION HISTORY:

```
11 Apr 2013 - S. D. Eastham - Initial version
```

7.9.14 calc_strat_aer

Subroutine CALC_STRAT_AER calculates aerosol properties stratosphere using the thermodynamic parameterization described in Kirner et al. ('Simulation of polar stratospheric clouds in the chemistry-climate-model EMAC via the submodel PSC', Geosci. Mod. Dev., 4, 169-182, 2011).

INTERFACE:

```
SUBROUTINE CALC_STRAT_AER( am_I_Root, Input_Opt, & State_Met, State_Chm, RC )
```

USES:

```
USE CHEMGRID_MOD,
                        ONLY: ITS_IN_THE_STRATMESO
USE ErrCode_Mod
USE ERROR_MOD,
                        ONLY : DEBUG_MSG
USE ERROR_MOD,
                        ONLY : ERROR_STOP
USE ERROR_MOD,
                        ONLY : IS_SAFE_DIV
USE GC_GRID_MOD,
                        ONLY : GET_YMID
USE Input_Opt_Mod,
                        ONLY : OptInput
USE State_Chm_Mod,
                        ONLY : ChmState
USE State_Met_Mod,
                        ONLY : MetState
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?
```

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input options

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

```
13 Apr 2013 - S. D. Eastham - Initial version
```

06 Feb 2014 - R. Yantosca - Add missing variables to OpenMP loop

14 Feb 2014 - R. Yantosca - Make the L-loop the outermost DO loop

21 Feb 2014 - M. Sulprizio - Now pass Input_Opt, State_Met, and State_Chm

objects via the arg list

06 Nov 2014 - R. Yantosca - Now use State_Met%CLDF(I,J,L)

24 Feb 2014 - E. Lundgren - Replace GET_PCENTER, which retrieves wet air pressure, with State_Met%PMID_DRY and

remove dependency on PRESSURE_MOD.

08 Apr 2015 - R. Yantosca - Remove call to READ_PSC_FILE, this is

now done from DO_CHEMISTRY (chemistry_mod.F)

31 May 2016 - E. Lundgren - Replace Input_Opt%TRACER_MW_G with emMW_g

from species database (emitted species g/mol)

16 Jun 2016 - S. D. Eastham - Remove references to tracerid_mod.F

21 Jun 2016 - R. Yantosca - Now use module variables for species ID flags

07 Jul 2016 - E. Lundgren - Replace tracer pointer with species pointer

11 Aug 2016 - R. Yantosca - Remove temporary tracer removal code

7.9.15 kg_strat_aer

Function KG_STRAT_AER returns the calculated mass of a stratospheric aerosol. The routine is essentially just an interface to allow external routines to "see" the arrays.

INTERFACE:

REAL(fp) FUNCTION KG_STRAT_AER (I,J,L,IAER)

INPUT PARAMETERS:

INTEGER,INTENT(IN) :: I,J,L ! Grid indices
INTEGER,INTENT(IN) :: IAER ! Aerosol index

! 1 = SSA (pure H2SO4)

! 2 = STS

! 3 = Solid PSC

REVISION HISTORY:

18 Apr 2013 - S. D. Eastham - Initial version

7.9.16 rho_strat_aer

Function RHO_STRAT_AER returns the calculated stratospheric aerosol mass density.

INTERFACE:

```
REAL(fp) FUNCTION RHO_STRAT_AER (I,J,L,IAER)
```

INPUT PARAMETERS:

REVISION HISTORY:

```
18 Apr 2013 - S. D. Eastham - Initial version
```

7.9.17 get_strat_opt

Subroutine GET_STRAT_OPT returns local optical properties for a given stratospheric aerosol. The routine is essentially just an interface to allow external routines to "see" the arrays. However, local aerosol radius is adjusted from liquid to effective radius for aerosol optical depth calculations with liquid aerosols.

INTERFACE:

```
SUBROUTINE GET_STRAT_OPT (I,J,L,IAER,RAER,REFF,SAD,XSA)
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I, J, L ! Grid indices
INTEGER, INTENT(IN) :: IAER ! Aerosol index
! 1 = Liquid aerosols
! 2 = Solid PSC
!OUTPUT VARIABLES:
REAL(fp), INTENT(OUT) :: REFF ! Effective radius (cm)
REAL(fp), INTENT(OUT) :: RAER ! Physical radius (cm)
REAL(fp), INTENT(OUT) :: SAD ! Surface area density (cm2/cm3)
REAL(fp), INTENT(OUT) :: XSA ! X-S area density (m2/m3)
```

REMARKS:

Seb Eastham writes: "I would edit GET_STRAT_OPT so that, when SAD is less than some small value (say 1 nm2/cm3, which is a vanishingly small surface area), it returns SADSTRAT=XSASTRAT=0.d0 and RAER=REFF=0.1d0 for safety's sake. I think that will prevent code blow-up later on."

```
17 Apr 2013 - S. D. Eastham - Initial version
07 Apr 2015 - R. Yantosca
                            - Add error check to prevent div-by-zero errors
                              in other areas of GEOS-Chem caused by low SAD
```

7.9.18ternary

Subroutine TERNARY calculates the composition of SSA/STS aerosols using a paramaterization from Carslaw et al. "A Thermodynamic Model of the System HCl-HNO3-H2SO4-H2O, Including Solubilities of HBr, from ;200 to 328 K". The bulk of this code was taken directly from the Global Modeling Initiative implementation by David Considine.

INTERFACE:

```
SUBROUTINE TERNARY (PCENTER_IN, TCENTER_IN, H2OSUM_IN, H2SO4SUM,
                        HNO3SUM, HC1SUM, HOC1SUM, HBRSum, HOBrSUM,
      &
                        W_H2SO4, W_H2O, W_HNO3, W_HC1, W_HOC1, W_HBr, W_HOBr,
      &
      &
                        HNO3GASFRAC, HC1GASFRAC, HOC1GASFRAC,
      &
                        HBrGASFRAC,HOBrGASFRAC,SLA_VOL,SLA_RHO)
USES:
       ! Temporary - for debug
       USE ERROR_MOD,
                          ONLY : IT_IS_NAN, ERROR_STOP
                                                           ! Test for NaN
       USE ERROR_MOD,
                          ONLY : SAFE_EXP, SAFE_DIV, DEBUG_MSG
INPUT PARAMETERS:
       REAL(fp), INTENT(IN)
                                              ! Pressure (hPa)
                             :: PCENTER_IN
       REAL(fp), INTENT(IN)
                                              ! Temperature (K)
                             :: TCENTER_IN
       REAL(fp), INTENT(IN)
                                              ! Total H2O mixing ratio
                             :: H2OSUM_IN
       REAL(fp), INTENT(IN)
                                              ! Liquid H2SO4 mixing ratio
                             :: H2SO4SUM
       REAL(fp), INTENT(IN)
                                              ! Total HNO3 mixing ratio
                             :: HNO3SUM
       REAL(fp), INTENT(IN)
                                              ! Total HCl mixing ratio
                             :: HClSUM
       REAL(fp), INTENT(IN)
                                              ! Total HOCl mixing ratio
                             :: HOC1SUM
       REAL(fp), INTENT(IN)
                             :: HBrSUM
                                              ! Total HBr mixing ratio
       REAL(fp), INTENT(IN)
                                              ! Total HOBr mixing ratio
                            :: HOBrSUM
   !OUTPUT VARIABLES:
       REAL(fp), INTENT(OUT) :: W_H2SO4
                                              ! kg H2SO4/kg SLA
       REAL(fp), INTENT(OUT) :: W_H2O
                                              ! kg H2O /kg SLA
       REAL(fp), INTENT(OUT) :: W_HNO3
                                              ! kg HNO3 /kg SLA
       REAL(fp), INTENT(OUT) :: W_HCl
                                              ! kg HCl /kg SLA
       REAL(fp), INTENT(OUT) :: W_HOC1
                                              ! kg HOCl /kg SLA
       REAL(fp), INTENT(OUT) :: W_HBr
                                              ! kg HBr /kg SLA
       REAL(fp), INTENT(OUT) :: W_HOBr
                                              ! kg HOBr /kg SLA
       REAL(fp), INTENT(OUT) :: HNO3GASFRAC
                                              ! Gas fraction HNO3
       REAL(fp), INTENT(OUT) :: HClGASFRAC
                                              ! Gas fraction HCl
       REAL(fp), INTENT(OUT) :: HOC1GASFRAC
                                              ! Gas fraction HOCl
       REAL(fp), INTENT(OUT) :: HBrGASFRAC
                                              ! Gas fraction HBr
```

REVISION HISTORY:

```
19 Apr 2013 - S. D. Eastham - Initial version
16 Apr 2015 - M. Yannetti - Changed EXP to SAFE_EXP in H_HCL
01 Jan 2016 - E. Lundgren - Calculate R_ATM from global params
```

7.9.19 carslaw_density

Function CARSLAW_DENSITY determines the density of a sol'n through a relationship from Carslaw et al.. Result is in kg/m3.

INTERFACE:

```
REAL(fp) FUNCTION CARSLAW_DENSITY(CS,CN,T)
```

INPUT PARAMETERS:

REVISION HISTORY:

```
19 Apr 2013 - S. D. Eastham - Initial version
```

7.9.20 calc_fallvel

Function CALC_FALLVEL calculates the terminal velocity of a solid particle.

INTERFACE:

```
FUNCTION CALC_FALLVEL(DENSITY, RADIUS, TCENTER, PCENTER) RESULT(VEL)
```

USES:

```
USE ERROR_MOD, ONLY : ERROR_STOP
```

INPUT PARAMETERS:

```
REAL(fp),INTENT(IN) :: RADIUS ! Particle radius (cm)
REAL(fp),INTENT(IN) :: DENSITY ! Particle density (kg/m3)
REAL(fp),INTENT(IN) :: TCENTER ! Local temperature (K)
REAL(fp),INTENT(IN) :: PCENTER ! Local pressure (kPa)
!OUTPUT VARIABLES:
```

REAL(fp) :: VEL ! Fall velocity (m/s)

REMARKS:

(1) A remark

REVISION HISTORY:

```
11 Aug 2012 - S. D. Eastham - Initial version
```

7.9.21 cacl_sla_gamma

Subroutine CALC_SLA_GAMMA calculates 11 different sticking coefficients on the surface of local stratospheric liquid aerosols, relevant to each of the 11 reactions listed in Kirner's paper.

INTERFACE:

```
SUBROUTINE CALC_SLA_GAMMA( NDENS, T, P, WT_FRC, H2OSUM, HC1SUM, & HBrSUM, HOBrSUM, C1NO3SUM, BrNO3SUM, & RHO, ARAD, RXNGAMMA)
```

USES:

```
! Temporary - for debug
USE ERROR_MOD, ONLY : IT_IS_NAN,ERROR_STOP ! Test for NaN
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: NDENS
                                    ! Air number density (molec/cm3)
   REAL(fp), INTENT(IN) :: T
                                    ! Temperature (K)
                                  ! Pressure (hPa)
   REAL(fp), INTENT(IN) :: P
   REAL(fp), INTENT(IN) :: WT_FRC
                                    ! Weight fraction of H2SO4 (kg/kg)
   REAL(fp), INTENT(IN) :: H2OSUM
                                    ! H2O mixing ratio
   REAL(fp), INTENT(IN) :: HClSUM ! HCl mixing ratio
   REAL(fp), INTENT(IN) :: HBrSUM
                                    ! HBr mixing ratio
   REAL(fp), INTENT(IN) :: HOBrSUM ! HOBr mixing ratio
   REAL(fp), INTENT(IN) :: ClNO3SUM ! ClNO3 mixing ratio
   REAL(fp), INTENT(IN) :: BrNO3SUM ! BrNO3 mixing ratio
   REAL(fp), INTENT(IN) :: RHO
                                     ! STS density (g/cm3)
                                    ! SLA radius (cm)
   REAL(fp), INTENT(IN) :: ARAD
!OUTPUT VARIABLES:
   REAL(fp), INTENT(OUT) :: RXNGAMMA(11) ! Premultiplying factors
```

```
10 Oct 2012 - S. D. Eastham - Initial version
15 Apr 2015 - M. Yannetti - Adjustment to f8 from fp due to overflow concerns
```

7.9.22 molec_speed

Function MOLEC_SPEED calculates the mean velocity of gas phase particles based on temperature and molecular mass.

INTERFACE:

```
REAL(fp) FUNCTION MOLEC_SPEED(T,MOLMASS)
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: T ! Temperature (K)
REAL(fp), INTENT(IN) :: MOLMASS ! Molecular mass (g/mol)
```

REVISION HISTORY:

```
10 Oct 2012 - S. D. Eastham - Initial version
```

7.9.23 read_psc_file

Subroutine READ_PSC_FILE initializes PSC state information from a checkpoint file (binary punch file format).

INTERFACE:

```
SUBROUTINE READ_PSC_FILE( am_I_Root, State_Chm, RC )
```

USES:

```
USE ERROR_MOD, ONLY : ERROR_STOP

USE HCO_ERROR_MOD

USE HCO_RESTART_MOD, ONLY : HCO_RestartGet

USE HCO_CLOCK_MOD, ONLY : HcoClock_First

USE HCO_CLOCK_MOD, ONLY : HcoClock_Rewind

USE HCO_INTERFACE_MOD, ONLY : HcoState

USE State_Chm_Mod, ONLY : ChmState
```

INPUT PARAMETERS:

USE ErrCode_Mod

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
INTEGER, INTENT(INOUT) :: RC
```

```
28 Apr 2013 - S. D. Eastham - Initial version, based on READ_CSPEC_FILE

14 Feb 2014 - R. Yantosca - Reorder DO loops for efficiency

16 Apr 2014 - M. Sulprizio - Now get PSC restart file path from Input_Opt

23 Jul 2014 - R. Yantosca - Remove reference to obsolete CMN_mod.F

14 Jan 2015 - C. Keller - Now read from HEMCO

4 Mar 2015 - R. Yantosca - Declare pointer args to HCO_GetPtr w/ REAL(f4)

25 Mar 2015 - C. Keller - Now use HEMCO restart module

29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
```

7.9.24 set_clock_trac

Subroutine SET_CLOCK_TRAC sets the clock species mixing ratio within the bottom five grid levels, increasing by a fixed rate of 0.5 ppbv/day

INTERFACE:

```
SUBROUTINE SET_CLOCK_TRAC( STEPLEN, State_Chm )
```

USES:

```
USE CMN_SIZE_MOD
```

USE State_Chm_Mod, ONLY : ChmState

INPUT PARAMETERS:

OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(OUT) :: State_Chm ! Chemistry State object
```

REVISION HISTORY:

```
16 Oct 2013 - S. D. Eastham - Initial version
14 Feb 2014 - R. Yantosca - Reorder DO loop for efficiency
21 Feb 2014 - M. Sulprizio - Now pass State_Chm object via the arg list
```

7.9.25 set_h2o_trac

Subroutine SET_H2O_TRAC sets the H2O species throughout the selected domain (either troposphere only or the full grid).

INTERFACE:

```
SUBROUTINE SET_H2O_TRAC ( am_I_Root, SETSTRAT, Input_Opt,
& State_Met, State_Chm, RC )
```

USES:

```
USE CHEMGRID_MOD,
                             ONLY : ITS_IN_THE_TROP
      USE CMN_SIZE_MOD
      USE DAO_MOD,
                             ONLY : AIRQNT
      USE ErrCode_Mod
      USE ERROR_MOD
      USE Input_Opt_Mod,
                             ONLY : OptInput
      USE State_Chm_Mod,
                             ONLY : ChmState
      USE State_Met_Mod,
                             ONLY : MetState
      USE UnitConv_Mod
INPUT PARAMETERS:
      LOGICAL.
                     INTENT(IN)
                                   :: am_I_Root
                                                  ! Are we on the root CPU?
      LOGICAL,
                     INTENT(IN)
                                   :: SETSTRAT
                                                  ! Set strat H2O?
      TYPE(OptInput), INTENT(IN)
                                   :: Input_Opt
                                                 ! Input options
INPUT/OUTPUT PARAMETERS:
```

TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTENT(OUT) ! Success or failure? INTEGER, :: RC

REVISION HISTORY:

```
28 Mar 2013 - S. D. Eastham - Initial version
14 Feb 2014 - R. Yantosca
                            - Reordered DO loop for efficiency
21 Feb 2014 - M. Sulprizio - Now pass Input_Opt, State_Met, and State_Chm
                              objects via the arg list
                            - Replace GET_PCENTER with State_Met%PMID and
24 Feb 2015 - E. Lundgren
                              remove dependency on PRESSURE_MOD
24 Mar 2015 - E. Lundgren
                            - Change tracer units from kg to kg/kg
29 Apr 2015 - E. Lundgren
                            - Now pass am_I_Root and RC to SET_H2O_TRAC
29 Apr 2015 - E. Lundgren
                            - Now use grid box moist air mass ADMOIST
                              with SPHU since AD is now dry air mass
                            - Replace RH calculation method with Nordquist,
29 Apr 2015 - E. Lundgren
                              1973 and call AirQnt if moisture vars
                              are updated using H2O tracer concentration
28 Oct 2015 - E. Lundgren
                            - Tracer units are now kg/kg dry air
                            - Replace tracer pointer with species pointer
07 Jul 2016 - E. Lundgren
18 Jul 2016 - E. Lundgren
                            - Remove dependency on grid box mass
                            - Remove temporary tracer-removal code
11 Aug 2016 - R. Yantosca
```

7.9.26 ucx_h2so4phot

Subroutine UCX_H2SO4PHOT propagates the calculated H2SO4 photolysis (J) rate at the top of the chemistry grid through to the top of the transport grid, approximating H2SO4 photolysis in the mesosphere.

INTERFACE:

SUBROUTINE UCX_H2SO4PHOT(Input_Opt, State_Met, State_Chm)

USES:

```
USE CHEMGRID_MOD, ONLY : GET_CHEMGRID_LEVEL
USE CMN_FJX_MOD, ONLY : ZPJ

USE FAST_JX_MOD, ONLY : RXN_H2SO4

USE Input_Opt_Mod, ONLY : OptInput

USE State_Chm_Mod, ONLY : ChmState

USE State_Met_Mod, ONLY : MetState

USE TIME_MOD, ONLY : GET_TS_CHEM
```

INPUT PARAMETERS:

```
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

REMARKS:

(1) A remark

REVISION HISTORY:

```
17 Aug 2013 - S. D. Eastham - Initial version

14 Feb 2014 - R. Yantosca - Reorder DO loops for efficiency

21 Feb 2014 - M. Sulprizio - Now pass Input_Opt, State_Met, and State_Chm objects via the arg list

31 May 2016 - E. Lundgren - Replace Input_Opt%TRACER_MW_G with species database emMW_g (emitted species g/mol)

21 Jun 2016 - R. Yantosca - Remove reference to tracerid_mod.F

27 Jun 2016 - M. Sulprizio - Obtain photolysis rate directly from ZPJ array and remove reference to FJXFUNC and obsolete SMVGEAR variables like NKSO4PHOT, NAMEGAS, etc.

07 Jul 2016 - E. Lundgren - Replace tracer pointer with species pointer
```

7.9.27 get_ucx_ch4

Subroutine GET_UCX_CH4 retrieves zonal mean surface mixing ratios for 4 equal-area regions (90S-30S,30S-0,0-30N,30N-90N)

INTERFACE:

```
SUBROUTINE GET_UCX_CH4( CH4_YEAR, MR90S, MR30S, MR30N, MR90N, & am_I_Root, Input_Opt )
```

USES:

```
USE FUTURE_EMISSIONS_MOD, ONLY : GET_FUTURE_YEAR
USE Input_Opt_Mod, ONLY : OptInput
USE TIME_MOD, ONLY : GET_MONTH
USE TIME_MOD, ONLY : GET_YEAR
```

INPUT PARAMETERS:

REVISION HISTORY:

```
18 Dec 2013 - S. D. Eastham - Initial version
```

7.9.28 sfcmr_init

Subroutine SFCMR_INIT initializes the surface mixing ratio derived type object. This reads in all the mixing ratios from ASCII files and saves them in the SFCMR object.

INTERFACE:

```
SUBROUTINE SFCMR_INIT( am_I_Root, Input_Opt )
```

USES:

```
USE ERROR_MOD, ONLY : ALLOC_ERR
USE ERROR_MOD, ONLY : ERROR_STOP
USE Input_Opt_Mod, ONLY : OptInput
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Root CPU?
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input options
!OUTPUT VARIABLES:
```

```
05 Dec 2014 - C. Keller - Initial version
```

7.9.29 sfcmr_read

Subroutine SFCMR_READ reads the surface mixing rations from ASCII file and stores the values in the next available SFCMR object. The ascii file is expected to be in the following format: C2CL3F3 MIXING RATIO BOUNDARY CONDITIONS FOR WMO-2006 1.0E-12 time CFC113 1959.04 0.99 1959.12 1.00 1959.21 1.01 1959.29 1.02

INTERFACE:

```
SUBROUTINE SFCMR_READ( am_I_Root, Input_Opt, iName, iID, iMR )
```

USES:

```
USE ERROR_MOD, ONLY : ALLOC_ERR
USE ERROR_MOD, ONLY : ERROR_STOP
USE FILE_MOD, ONLY : IOERROR
USE Input_Opt_Mod, ONLY : OptInput
```

INPUT PARAMETERS:

```
) :: am_I_Root
                                                    ! Root CPU?
LOGICAL,
                  INTENT(IN
TYPE(OptInput),
                INTENT(IN
                             ) :: Input_Opt
                                                   ! Input options
CHARACTER(LEN=*),
                             ) :: iName
                                                    ! species name
                  INTENT(IN
                  INTENT(IN ) :: iID
                                                    ! species ID
INTEGER,
REAL(fp), OPTIONAL, INTENT(IN
                             ) :: iMR
                                                    ! fixed MR
```

REVISION HISTORY:

```
05 Dec 2014 - C. Keller - Initial version
```

$7.9.30 ext{sfcmr_get}$

Subroutine SFCMR_GET returns the surface mixing ratio of the given species for the given year and month. The value of the closest available date in the past is taken, and no interpolation between dates is performed.

INTERFACE:

```
FUNCTION SFCMR_GET( \ensuremath{\mathsf{TRAC}}\xspace_{\ensuremath{\mathsf{NAME}}}\xspace , \ensuremath{\mathsf{YEAR}}\xspace , \ensuremath{\mathsf{MONTH}}\xspace ) RESULT( \ensuremath{\mathsf{MR}}\xspace )
```

USES:

INPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(IN) :: TRAC_NAME ! species name INTEGER, INTENT(IN) :: YEAR ! desired year INTEGER, INTENT(IN) :: MONTH ! desired month !INPUT/OUTPUT VARIABLES:

REAL(fp) :: MR
```

```
05 Dec 2014 - C. Keller - Initial version
```

7.9.31 noxcoeff_init

Subroutine NOXCOEFF_INIT initializes the NOX 2D interpolation values.

INTERFACE:

```
SUBROUTINE NOXCOEFF_INIT ( am_I_Root, Input_Opt )
```

USES:

```
USE ERROR_MOD, ONLY : ALLOC_ERR
USE ERROR_MOD, ONLY : ERROR_STOP
USE FILE_MOD, ONLY : IOERROR
USE Input_Opt_Mod, ONLY : OptInput
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Root CPU?
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input options
!OUTPUT VARIABLES:
```

REVISION HISTORY:

```
05 Dec 2014 - C. Keller - Initial version
```

7.9.32 get_jjnox

Subroutine GET_JJNOX maps grid box at location IISIM, JJSIM of the simulation grid onto the latitude grid of the NOXCOEFF array. JJNOX can differ from JJSIM if it's not a 4x5 or 2x25 simulation.

This routine simply returns the index of the NOx latitude vector that covers the latitude value of interest. No grid box weighting, etc. is performed.

INTERFACE:

```
FUNCTION GET_JJNOX( IISIM, JJSIM ) RESULT ( JJNOX )
```

USES:

```
USE GC_GRID_MOD, ONLY : GET_YMID
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: IISIM ! Latitude index on simulation grid
INTEGER, INTENT(IN) :: JJSIM ! Latitude index on simulation grid
```

!OUTPUT VARIABLES:

INTEGER :: JJNOX ! Latitude index on NOXCOEFF grid

```
05 Dec 2014 - C. Keller - Initial version
```

7.9.33 init_ucx

Subroutine INIT_UCX initializes module arrays.

INTERFACE:

SUBROUTINE INIT_UCX(am_I_Root, Input_Opt, State_Chm)

USES:

```
USE ERROR_MOD,
                         ONLY : ALLOC_ERR
USE ERROR_MOD,
                         ONLY : IS_SAFE_DIV
                       ONLY : ERROR_STOP
ONLY : GET_YEDGE
USE ERROR_MOD,
USE GC_GRID_MOD,
USE Input_Opt_Mod,
                        ONLY : OptInput
USE PhysConstants,
                        ONLY : PI_180
USE State_Chm_Mod,
                        ONLY : ChmState
USE State_Chm_Mod,
                         ONLY : Ind_
USE TIME_MOD,
                         ONLY : GET_YEAR
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input options

TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object
```

REVISION HISTORY:

```
04 Apr 2013 - S. D. Eastham - Initial version
21 Jun 2016 - R. Yantosca - Now declare species ID's during INIT phase
21 Jun 2016 - R. Yantosca - Remove reference to tracerid_mod.F
24 Jun 2016 - R. Yantosca - Bug fix: get advected species index for H2
20 Sep 2016 - R. Yantosca - Now avoid using SIND, convert the argument to radians and use the SIN function instead
```

7.9.34 diaginit_ucx

Subroutine DIAGINIT_UCX initializes diagnostics containers for the UCX module.

INTERFACE:

```
SUBROUTINE DIAGINIT_UCX( am_I_Root, Input_Opt, State_Chm, RC )
```

USES:

```
USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP

USE HCO_RESTART_MOD, ONLY : HCO_RestartDefine

USE HCO_INTERFACE_MOD, ONLY : HcoState

USE HCO_ERROR_MOD

USE Input_Opt_Mod, ONLY : OptInput

USE State_Chm_Mod, ONLY : ChmState
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?!
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object
```

INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC ! Success or failure
```

REVISION HISTORY:

```
14 Jan 2015 - C. Keller - Initial version
25 Mar 2015 - C. Keller - Now use HEMCO restart module
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
```

7.9.35 write_state_psc

Subroutine WRITE_STATE_PSC saves the STATE_PSC array into diagnostics. This is only of relevance in an ESMF environment, where STATE_PSC is not automatically written into the HEMCO restart diagnostics but needs to be passed explicitly to the internal state. This should be done on every time step to make sure that replay simulations will always have the most current STATE_PSC values in the internal state (important for checkpointing!).

INTERFACE:

```
SUBROUTINE WRITE_STATE_PSC ( am_I_Root, State_Chm, RC )
```

USES:

```
USE ErrCode_Mod
   USE HCO_ERROR_MOD
   USE HCO_RESTART_MOD,
                           ONLY : HCO_RestartWrite
   USE HCO_INTERFACE_MOD, ONLY : HcoState
   USE State_Chm_Mod,
                           ONLY : ChmState
!INPUT ARGUMENTS:
   LOGICAL,
                    INTENT(IN)
                                  :: am_I_Root
!INPUT/OUTPUT ARGUMENTS:
   TYPE(ChmState), INTENT(INOUT) :: State_Chm
                                                 ! Chemistry State object
   INTEGER,
                   INTENT(INOUT) :: RC
```

```
08 May 2015 - C. Keller - Initial version
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
```

7.9.36 cleanup_ucx

Subroutine CLEANUP_UCX deallocates module variables.

INTERFACE:

```
SUBROUTINE CLEANUP_UCX ( am_I_Root )
!INPUT ARGUMENTS:
LOGICAL, INTENT(IN) :: am_I_Root
```

REVISION HISTORY:

```
04 Apr 2013 - S. D. Eastham - Initial version
13 Apr 2013 - S. D. Eastham - Added PSC arrays
```

7.10 Fortran: Module Interface bromocarb_mod.F

Module BROMOCARB_MOD contains variables and routines for the GEOS-Chem bromocarbon simulation.

INTERFACE:

MODULE BROMOCARB_MOD

USES:

```
USE PRECISION_MOD

IMPLICIT NONE
PRIVATE
```

PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: SET_CH3Br
PUBLIC :: SET_Br0
```

REMARKS:

HEMCO has made most of this routine obsolete. HEMCO reads in the data files in netCDF format and tracks them in its data structure.

```
13 Aug 2007 - J. Parrella - Initial version

22 May 2012 - M. Payer - Added ProTeX headers

27 Aug 2012 - M. Payer - Now parallelize DO loops

20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete

24 Jun 2014 - R. Yantosca - Removed code made obsolete by HEMCO

24 Jun 2014 - R. Yantosca - Removed INIT_BROMOCARB, CLEANUP_BROMOCARB

06 Nov 2015 - M. Yannetti - Added PRECISION_MOD

29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90
```

$7.10.1 \text{ set_ch3br}$

Subroutine SET_CH3Br set CH3Br Concentrations in the planetary boundary layer. Based on latitude bands (1) 90-55N, (2) 55N-0, (3) 0-55S, (4) 55-90S. Values for setting pbl flux were determined by surface measurements from NOAA 2006 data.

INTERFACE:

```
SUBROUTINE SET_CH3Br( am_I_Root, Input_Opt, State_Met, & State_Chm, RC )
```

USES:

```
USE CMN_SIZE_MOD

USE ErrCode_Mod

USE ERROR_MOD

USE GC_GRID_MOD, ONLY : GET_YMID

USE Input_Opt_Mod, ONLY : OptInput

USE PBL_MIX_MOD, ONLY : GET_FRAC_UNDER_PBLTOP

USE PhysConstants, ONLY : AIRMW

USE State_Chm_Mod, ONLY : ChmState

USE State_Chm_Mod, ONLY : Ind_
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

ONLY : MetState

INPUT/OUTPUT PARAMETERS:

USE State_Met_Mod,

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REMARKS:

1) Spc is converted back and forth between units of [kg] and [v/v]. Placement of the call to SET_CH3Br in main.f (it's with the emissions) means that it should be in [kg].

```
12 Feb 2008 - J. Parrella - Initial version
22 May 2012 - M. Payer - Added ProTeX headers
27 Aug 2012 - M. Payer - Added parallel DO loop
28 Aug 2012 - M. Payer - Add error check for CH3Br to avoid OOB error
09 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met derived type object
```

7.10.2 set_bro

Subroutine SET_BRO sets BrO concentrations in the planetary boundary layer. Based on latitude bands (1) 90-55N, (2) 55N-0, (3) 0-55S, (4) 55-90S. Values for setting pbl flux were determined by surface measurements from NOAA 2006 data.

INTERFACE:

```
SUBROUTINE SET_BRO( am_I_Root, Input_Opt, State_Met,
& State_Chm, RC )
```

USES:

```
USE CMN_SIZE_MOD
USE DAO_MOD,
                       ONLY : IS_WATER
USE ErrCode Mod
USE ERROR_MOD
USE Input_Opt_Mod,
                      ONLY : OptInput
USE PBL_MIX_MOD,
                       ONLY : GET_FRAC_UNDER_PBLTOP
USE PhysConstants,
                      ONLY : AIRMW
USE State_Chm_Mod,
                      ONLY : ChmState
USE State_Chm_Mod,
                       ONLY : Ind_
USE State_Met_Mod,
                       ONLY : MetState
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Met State object
```

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

1) Spc is converted back and forth between units of [kg] and [v/v]. Placement of the call to SET_Bro in main.f (it's with the emissions) means that it should be in [kg].

REVISION HISTORY:

```
12 Feb 2008 - J. Parrella - Initial version

22 May 2012 - M. Payer - Added ProTeX headers

27 Aug 2012 - M. Payer - Added parallel DO loop

28 Aug 2012 - M. Payer - Add error check for BrO to avoid OOB error

09 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met derived type object

27 Nov 2012 - R. Yantosca - Replace SUNCOS with State_Met%SUNCOS

24 Jun 2014 - R. Yantosca - Remove IJLOOP, it's not used anymroe

06 Nov 2014 - M. Yannetti - Changed REAL*8 to REAL(fp)

10 Sep 2015 - E. Lundgren - Modification for State_Chm%TRACERS units now in kg/kg dry air (previously kg/box)

10 Sep 2015 - E. Lundgren - Remove passed argument 'unitflag'

30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

25 Jul 2016 - M. Yannetti - Replaced TCVV with MW from spec db and phys const
```

7.11 Fortran: Module Interface cldice_hbrhobr_rxn.F

Subroutine CLDICE_HBrHOBr_RXN calculates the rate constants for HBr and HOBr pseudo-reactions with ice.

INTERFACE:

```
SUBROUTINE CLDICE_HBrHOBr_RXN( I, J, L, DENAIR, & QI, hbr, hobr, & k_hbr, k_hobr, AREA, State_Met )
```

USES:

```
USE ERROR_MOD, ONLY : IS_SAFE_DIV, IT_IS_NAN

USE ERROR_MOD, ONLY : GEOS_CHEM_STOP

USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

USE State_Met_Mod, ONLY : MetState
```

IMPLICIT NONE

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I ! Longitude index
INTEGER, INTENT(IN) :: J ! Latitude index
INTEGER, INTENT(IN) :: L ! Altitude index
```

```
INTENT(IN) :: DENAIR
       REAL(fp),
                                               ! Density of air
                                                                        [\#/cm3]
      REAL(fp),
                      INTENT(IN) :: QI
                                               ! Cloud ice mixing ratio [kg/kg]
                                                                        [#/cm3]
      REAL(fp),
                                               ! Concentration of HBr
                      INTENT(IN) :: hbr
      REAL(fp),
                      INTENT(IN) :: hobr
                                             ! Concentration of HOBr [#/cm3]
      TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
OUTPUT PARAMETERS:
       REAL(fp),
                      INTENT(OUT) :: k_hbr
                                               ! Rate constant for HBr + ice
                                                   pseudo-rxn [cm3/s]
                                               ! Rate constant for HOBr + ice
                      INTENT(OUT) :: k_hobr
      REAL(fp),
                                                   pseudo-rxn [cm3/s]
                                               ! Surface area [cm2/cm3]
                      INTENT(OUT) :: AREA
      REAL(fp),
REMARKS:
    The rate constant is calculated assuming:
     1. A sticking coefficient of 0.1 [JPL 2006], Abbatt [1994],
        Chai et al. [2000]
     2. An effective radius is assumed as a function of (i) temperature and
        ice water content (IWC). This relationship is taken from Wyser [1998].
    ** Calculations of a 1st order rate constent are borrowed from the
       subroutine arsl1k.F. Below are comments from that code:
        The 1st-order loss rate on wet aerosol (Dentener's Thesis, p. 14)
        is computed as:
          ARSL1K [1/s] = area / [ radius/dfkg + 4./(stkcf * nu) ]
                   = Mean molecular speed [cm/s] = sqrt(8R*TK/pi/M) for Maxwell
              DFKG = Gas phase diffusion coeff [cm2/s] (order of 0.1)
REVISION HISTORY:
    16 Jun 2011 - J. Parrella - Initial version
    22 May 2012 - M. Payer - Added ProTeX headers
   26 Sep 2012 - R. Yantosca - For now, comment out debug print statements
   23 Oct 2012 - R. Yantosca - Add better error checks to prevent div-by-zero
    09 Nov 2012 - M. Payer
                             - Replaced all met field arrays with State_Met
                               derived type object
   20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
   05 Sep 2013 - R. Yantosca - Now exit if IWC <= 0, this will cause the
                               logarithm to choke
   26 Sep 2013 - R. Yantosca - Renamed GEOS_57 Cpp switch to GEOS_FP
```

19 Dec 2014 - R. Yantosca - Now perform internal computations w/ REAL*8 11 Aug 2015 - R. Yantosca - MERRA2 behaves the same way as GEOS-FP

06 Nov 2014 - R. Yantosca - Now use State_Met%CLDF(I,J,L)

04 Jan 2016 - E. Lundgren - Remove grid box area-dependence

7.12 Fortran: Module Interface get_global_ch4.F

Subroutine GET_GLOBAL_CH4 computes the latitudinal gradient in CH4 corresponding to year.

INTERFACE:

```
SUBROUTINE GET_GLOBAL_CH4( THISYEAR, VARIABLE_CH4, & A3090S, A0030S, & A0030N, A3090N, & am_I_Root, Input_Opt )
```

USES:

```
USE FUTURE_EMISSIONS_MOD, ONLY : GET_FUTURE_SCENARIO
USE Input_Opt_Mod, ONLY : OptInput
USE PRECISION_MOD
```

IMPLICIT NONE

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: THISYEAR ! Current year
LOGICAL, INTENT(IN) :: VARIABLE_CH4 ! =T: Use time-varying CH4
! =F: Use constant CH4
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

OUTPUT PARAMETERS:

REMARKS:

- (1) 2007 was the prior default year for CH4 emissions. This has now been changed to 2013.
- (2) The FUTURE_SCENARIO option is probably now obsolete, as most scale factors are now handled by HEMCO. But we shall leave this intact until further notice.

```
03 Jan 2001 - J. Wang - Initial version
```

- (1) GET_GLOBAL_CH4 only has to be called at the start of the new year, as long as A3090S, A0030S, A0030N, A3090N are saved in the calling program (bmy, 1/3/01)
- (2) Also need to compute yearly gradients for CH4 beyond 1997 -- will do this later (bmy, 1/3/01)
- (3) Bug fix: add missing comma to FORMAT statement (bmy, 3/23/03)

- (4) Place WRITE statments w/in an !\$OMP CRITICAL block, so as to make sure that only one processor at a time writes them. Also now use F90 REPEAT intrinsic function. Also replaced old CH4 gradient values with updated values for 1983-2001. Use data for 2001 as a proxy for years past 2001, since data for those years has not been reported yet. (mje, bmy, 7/7/03)
- (5) Split off from module "global_ch4_mod.f". Updated for IPCC future emissions scenarios. (swu, bmy, 5/30/06)
- (6) Add the preindustrial CH4 scenarios. Also set 2001 as the default in case we are running 2030 or 2050 met but present-day emissions. (swu, havala, bmy, 1/25/08)
- (7) Updated CH4 vales with version 2008-07-02 for 1983-2007. Also use 2007 for years past 2007 (jaf, 4/15/09)
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 05 Mar 2013 R. Yantosca Now use Input_Opt%LFUTURE instead of LFUTURE from logical_mod.F
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 13 Nov 2014 M. Yannetti Added PRECISION_MOD
- 06 Jan 2015 R. Yantosca Initial version
- 12 May 2015 K. Travis Updated CH4 values with Version: 2014-06-24 for 2008-2013.
- 12 May 2015 R. Yantosca Added ProTeX headers

7.13 Fortran: Module Interface strat_chem_mod.F90

Module STRAT_CHEM_MOD contains variables and routines for performing a simple linearized chemistry scheme in the stratosphere, using archived 3D monthly climatological production rates and loss frequencies are applied from the GMI combo model.

In the original schem code (schem.F), only the following species were destroyed by photolysis in the stratosphere: PAN, H2O2, ACET, MEK, ALD2, RCHO, MVK, MACR, R4N2, CH2O, N2O5, HNO4, MP and by reaction with OH: ALK4, ISOP, H2O2, ACET, MEK, ALD2, RCHO, MVK, MACR, PMN, R4N2, PRPE, C3H8, CH2O, C2H6, HNO4, MP The updated code includes at least all of these, and many more. The code is flexible enough to automatically apply the rate to any new species for future simulations that share the name in species_mod with the GMI name. (See Documentation on wiki).

The prod rates and loss frequencies are now read via HEMCO. They are stored in a data structure of flexible length (PLVEC). The file containing the prod rates and loss frequencies need to be specified in the HEMCO configuration file for each species of interest. They are then automatically read and remapped onto the simulation grid. The field names assigned to the production and loss fields are expected to be 'GMI_PROD_XXX' and 'GMI_LOSS_XXX', respectively, where XXX is the species name. Production rates must be given in units of v/v/s, and loss frequencies in s-1. The module variable PLMUSTFIND (set below) determines the behavior if no production rates and/or loss frequencies can be found for any of the GMI species defined in this module. IF PLMUSTFIND is set to TRUE, the code stops with an error if no entry is found. Otherwise, stead-state values are used for all species with no explicitly given values.

The (monthly) OH concentrations are also obtained through HEMCO. The field name must be 'STRAT_OH', and values must be in v/v.

INTERFACE:

```
MODULE Strat_Chem_Mod
```

USES:

```
for precisions
USE HCO_Error_Mod
USE Precision_Mod ! For GEOS-Chem Precision (fp, f4, f8)

IMPLICIT NONE
PRIVATE
```

PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: Init_Strat_Chem

PUBLIC :: Do_Strat_Chem

PUBLIC :: Cleanup_Strat_Chem
```

PUBLIC :: Calc_STE

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: Set_BryPointers
PRIVATE :: Set_PLVEC
PRIVATE :: Do_Synoz

PUBLIC DATA MEMBERS:

REMARKS:

References:

(1)

```
01 Feb 2011 - L. Murray - Initial version
20 Jul 2012 - R. Yantosca - Reorganized declarations for clarity
20 Jul 2012 - R. Yantosca - Correct compilation error in GET_RATES_INTERP
07 Aug 2012 - R. Yantosca - Fix parallelization problem in Bry do loop
05 Oct 2012 - R. Yantosca - Add bug fix for IFORT 12 compiler in CALC_STE
                         - Replace Ox with O3 as part of removal of NOx-Ox
14 Mar 2013 - M. Payer
                            partitioning
20 Nov 2014 - M. Yannetti - Added PRECISION_MOD
30 Dec 2014 - C. Keller - Now read Bry data through HEMCO
16 Jan 2015 - C. Keller - Now read all prod/loss fields and OH conc.
                           through HEMCO.
4 Mar 2015 - R. Yantosca - Declare pointer args for HCO_GetPtr as REAL(f4)
06 Apr 2016 - C. Keller - Add Minit_Is_Set and SET_MINIT.
03 Oct 2016 - R. Yantosca - Now dynamically allocate BrPtrDay, BrPtrNight
03 Oct 2016 - R. Yantosca - Dynamically allocate BrPtrDay, BrPtrNight
```

7.13.1 Do_Strat_Chem

Function DO_STRAT_CHEM is the driver routine for computing the simple linearized stratospheric chemistry scheme.

INTERFACE:

```
SUBROUTINE DO_STRAT_CHEM( am_I_Root, Input_Opt,
                          State_Met, State_Chm, errCode )
```

USES:

```
USE CHEMGRID_MOD,
                        ONLY : GET_TPAUSE_LEVEL
                        ONLY : ITS_IN_THE_CHEMGRID
USE CHEMGRID_MOD,
USE CHEMGRID_MOD,
                        ONLY : ITS_IN_THE_TROP
```

USE CMN_SIZE_MOD USE ErrCode_Mod USE ERROR_MOD

USE Input_Opt_Mod, ONLY : OptInput USE LINOZ_MOD, ONLY : DO_LINOZ

ONLY : XNUMOLAIR, AIRMW

USE LINUZ_MOD,
USE PhysConstants,
USE State_Chm_Mod,
Grate Met_Mod, ONLY : ChmState ONLY : MetState USE TIME_MOD, ONLY : GET_MONTH

USE TIME_MOD, ONLY : TIMESTAMP_STRING

USE UnitConv_Mod

IMPLICIT NONE

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root
TYPE(OptInput), INTENT(IN) :: Input_Opt
                                                    ! Is this the root CPU?
                                                    ! Input Options object
TYPE(MetState), INTENT(IN) :: State_Met
                                                    ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTENT(INOUT) :: errCode
                                         ! Success or failure
INTEGER,
```

REMARKS:

```
01 Feb 2011 - L. Murray - Initial version
18 Jul 2012 - R. Yantosca - For compatibility w/ the GEOS-5/GCM, we cannot
                            assume a minimum tropopause level anymore
18 Jul 2012 - R. Yantosca - Make sure I is the innermost DO loop
                            wherever expedient
20 Jul 2012 - R. Yantosca - Reorganized declarations for clarity
30 Jul 2012 - R. Yantosca - Now accept am_I_Root as an argument when
                            running with the traditional driver main.F
07 Aug 2012 - R. Yantosca - Make BEFORE a local variable for parallel loop
26 Oct 2012 - R. Yantosca - Now pass the Chemistry State object for GIGC
09 Nov 2012 - R. Yantosca - Now pass the Input Options object for GIGC
15 Nov 2012 - M. Payer
                          - Replaced all met field arrays with State_Met
                            derived type object
27 Nov 2012 - R. Yantosca - Replace SUNCOS with State_Met%SUNCOS
14 Mar 2013 - M. Payer
                          - Replace Ox with O3 as part of removal of NOx-Ox
                            partitioning
18 Mar 2013 - R. Yantosca - Now pass Input_Opt via the arg list
19 Mar 2013 - R. Yantosca - Now only copy Input_Opt%TCVV(1:N_TRACERS)
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
30 Dec 2014 - C. Keller - Now get Bry data through HEMCO.
24 Mar 2015 - E. Lundgren - Replace dependency on tracer_mod with
                            CMN_GTCM_MOD for XNUMOLAIR
30 Sep 2015 - E. Lundgren - Now use UNITCONV_MOD for unit conversion
05 Mar 2016 - C. Keller
                        - Allow O3 P/L be done by GMI if both LINOZ and
                            SYNOZ are disabled. This is primarily for
                            testing/data assimilation applications.
16 Jun 2016 - M. Yannetti - Replaced TRACERID_MOD.\
20 Jun 2016 - R. Yantosca - Now make species ID flags module variables
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected
                            species ID from State_Chm%Map_Advect.
01 Jul 2016 - R. Yantosca - Now rename species DB object ThisSpc to SpcInfo
12 Jul 2016 - R. Yantosca - Bug fix: ISBR2 should be held !$OMP PRIVATE
18 Jul 2016 - M. Yannetti - Replaced TCVV with spec db and phys constant
10 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code
```

7.13.2 Set_BryPointers

Subroutine SET_BryPointers gets the Bry stratospheric data read by HEMCO. The pointers only need to be established once. Target data is automatically updated through HEMCO.

INTERFACE:

SUBROUTINE Set_BryPointers(am_I_Root, Input_Opt, State_Chm, State_Met, RC)
USES:

USE ErrCode_Mod
USE ERROR_MOD, ONLY : ERROR_STOP

```
USE HCO_INTERFACE_MOD, ONLY : HcoState
USE HCO_EMISLIST_MOD, ONLY : HCO_GetPtr
USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState
```

IMPLICIT NONE

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorological State object
```

INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC ! Success or failure
```

REVISION HISTORY:

```
30 Dec 2014 - C. Keller - Initial version
```

7.13.3 Set_Plvec

Subroutine SET_PLVEC gets the production and loss terms of all strat chem species from HEMCO. The pointers only need to be established once. Target data is automatically updated through HEMCO.

INTERFACE:

```
SUBROUTINE Set_PLVEC ( am_I_Root, Input_Opt, State_Chm, State_Met, RC )
```

USES:

```
USE ERROR_MOD, ONLY : ERROR_STOP
USE HCO_INTERFACE_MOD, ONLY : HcoState
USE HCO_EMISLIST_MOD, ONLY : HCO_GetPtr
USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState
```

IMPLICIT NONE

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorological State object
```

INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC ! Success or failure

REVISION HISTORY:

16 Jan 2015 - C. Keller - Initial version

7.13.4 Calc_Ste

Subroutine CALC_STE estimates what the stratosphere-to- troposphere exchange flux must have been since the last time it was reset

INTERFACE:

```
SUBROUTINE Calc_STE( am_I_Root, Input_Opt, State_Chm, State_Met, RC )
```

USES:

```
USE CMN_SIZE_MOD
USE ErrCode_Mod
```

USE ERROR_MOD, ONLY : GC_Error USE Input_Opt_Mod, ONLY : OptInput

USE Species_Mod, ONLY : Species
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState

USE TIME_MOD, ONLY : GET_TAU, GET_NYMD, GET_NHMS, EXPAND_DATE

USE UnitConv_Mod

IMPLICIT NONE

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

```
28 Apr 2012 - L. Murray - Initial version
```

18 Jul 2012 - R. Yantosca - Make sure I is the innermost DO loop

(wherever expedient)

20 Jul 2012 - R. Yantosca - Reorganized declarations for clarity

30 Jul 2012 - R. Yantosca - Now accept am_I_Root as an argument when

```
running with the traditional driver main.F

05 Oct 2012 - R. Yantosca - Bug fix for IFORT 12: extend the #if statement to avoid including code for nested-grid sims

25 Mar 2013 - R. Yantosca - Now accept Input_Opt, State_Chm, RC arguments

20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete

10 Aug 2015 - E. Lundgren - Input tracer concentration units are now [kg/kg]

25 May 2016 - E. Lundgren - Replace input_opt%TRACER_MW_KG with species database field emMW_g (emitted species g/mol)

30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

01 Jul 2016 - R. Yantosca - Now rename species DB object ThisSpc to SpcInfo

10 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code
```

7.13.5 Init_Strat_Chem

Subroutine INIT_STRAT_CHEM allocates all module arrays. It also opens the necessary rate files.

INTERFACE:

```
SUBROUTINE INIT_STRAT_CHEM( am_I_Root, Input_Opt, State_Chm, State_Met, RC )
```

USES:

```
USE CMN_SIZE_MOD
USE ErrCode_Mod
                       ONLY : ALLOC_ERR, GC_Error
USE ERROR_MOD,
USE Input_Opt_Mod,
                       ONLY : OptInput
USE Species_Mod,
                       ONLY : Species
USE State_Chm_Mod,
                       ONLY : ChmState
USE State_Chm_Mod,
                       ONLY : Ind
USE State_Met_Mod,
                       ONLY : MetState
USE TIME_MOD,
                       ONLY : GET_TAU
USE TIME_MOD,
                       ONLY : GET_NYMD
                       ONLY : GET_NHMS
USE TIME_MOD,
USE TIME_MOD,
                       ONLY : GET_TS_CHEM
```

INPUT PARAMETERS:

IMPLICIT NONE

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REVISION HISTORY:

```
01 Feb 2011 - L. Murray - Initial version
30 Jul 2012 - R. Yantosca - Now accept am_I_Root as an argument when
                            running with the traditional driver main.F
26 Oct 2012 - R. Yantosca - Now pass Chemistry State object for GIGC
09 Nov 2012 - R. Yantosca - Now pass Input Options object for GIGC
05 Nov 2013 - R. Yantosca - Now update tracer flags for tagOx simulation
03 Apr 2014 - R. Yantosca - PROD, LOSS, STRAT_OH, MINIT, SCHEM_TEND are
                            now REAL*4, so use 0e0 to initialize
11 Aug 2015 - E. Lundgren - Tracer units are now kg/kg and are converted
                            kg for assignment of MInit
16 Jun 2016 - M. Yannetti - Replaced TRACERID_MOD.
20 Jun 2016 - R. Yantosca - Now save species ID flags as module variables
                            and only define them in the INIT phase.
12 Jul 2016 - R. Yantosca - Now also store advected species ID's
11 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code
20 Sep 2016 - R. Yantosca - Rewrote GMI_TrName statement for Gfortran
```

7.13.6 Set_Minit

Sets the MINIT array to current values in State_Chm

INTERFACE:

```
SUBROUTINE SET_MINIT( am_I_Root, Input_Opt, State_Met, State_Chm, RC )
```

USES:

```
USE ERROR_MOD, ONLY : GC_ERROR
USE ErrCode_Mod
USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState
USE UnitConv_Mod
```

IMPLICIT NONE

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REVISION HISTORY:

```
06 Apr 2016 - C. Keller - Initial version: moved outside of INIT_STRAT_CHEM so that it can be called from within DO_STRAT_CHEM (for ESMF applications).
```

7.13.7 Cleanup_Strat_Chem

Subroutine CLEANUP_STRAT_CHEM deallocates all module arrays.

INTERFACE:

SUBROUTINE CLEANUP_STRAT_CHEM

USES:

IMPLICIT NONE

REVISION HISTORY:

```
01 Feb 2011 - L. Murray - Initial version
03 Oct 2016 - R. Yantosca - Deallocate BrPtrDay and BrPtrNight
05 Oct 2016 - R. Yantosca - Now make deallocations more robust
```

7.13.8 Do_Synoz

Subroutine Do_Synoz establishes the flux boundary condition for Ozone coming down from the stratosphere, using the Synoz algorithm of McLinden et al, 2000.

INTERFACE:

USE CHEMGRID_MOD,

IMPLICIT NONE

```
SUBROUTINE Do_Synoz( am_I_Root, Input_Opt, State_Met, State_Chm, RC )
```

ONLY : GET_TPAUSE_LEVEL

```
USE CMN_SIZE_MOD

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP

USE Input_Opt_Mod, ONLY : OptInput

USE PhysConstants

USE State_Chm_Mod, ONLY : ChmState

USE State_Met_Mod, ONLY : MetState

USE TIME_MOD, ONLY : GET_TS_CHEM, GET_YEAR
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

Reference:

C. A. McLinden, S. Olsen, B. Hannegan, O. Wild, M. J. Prather, and J. Sundet, "Stratospheric Ozone in 3-D models: A simple chemistry and the cross-tropopause flux".

REVISION HISTORY:

- 13 Dec 1999 Q. Li, R. Martin Initial version
- (1) The parameter RdgO from "CMN_GCTM" = R / gO = 28.97.
- (2) Pass PW = PS PTOP to UPBDFLX via "CMN".
- (3) Now pass IORD, JORD, KORD as arguments (bmy, 12/6/00)
- (4) Now compute the proper value of PO3_vmr that will yield 475 Tg O3/yr for various settings of IORD, JORD, KORD (rvm, bey, bmy, 12/5/00)

- (5) Added to "upbdflx_mod.f". Also updated comments and made some cosmetic changes. (bmy, 6/28/01)
- (6) Now reference CMN_SETUP for LSPLIT. Also store strat 03 into tracer #11 for multi-tracer 0x run. (amf, bmy, 7/3/01)
- (7) Removed IREF, JREF -- these are obsolete. Also T(IREF, JREF, L) is now T(I,J,L). (bmy, 9/27/01)
- (8) Also replace PW(I,J) with P(I,J) (bmy, 10/3/01)
- (9) Removed obsolete commented out code from 9/01 (bmy, 10/24/01)
- (10) Removed obsolete commented out code from 7/01 (bmy, 11/26/01)

- (11) Now write file names to stdout (bmy, 4/3/02)
- (12) Replaced all instances of IM with IIPAR and JM with JJPAR, in order to prevent namespace confusion for the new TPCORE (bmy, 6/25/02)
- (13) Now use GET_PEDGE and GET_PCENTER from "pressure_mod.f" to compute the pressure at the bottom edge and center of grid box (I,J,L).

 Also removed obsolete, commented-out code. Removed G_SIG and G_SIGE from the arg list. (dsa, bdf, bmy, 8/21/02)
- (14) Now reference BXHEIGHT and T from "dao_mod.f". Also reference routine ERROR_STOP from "error_mod.f". Now references IDTOX from F90 module "tracerid_mod.f" instead of from "comtrid.h". (bmy, 11/6/02)
- (15) Now define J30S and J30N for 1x1 nested grid (bmy, 3/11/03)
- (16) Make sure to pass AD via "dao_mod.f" for GEOS-1 (bnd, bmy, 4/14/03)
- (17) On the first timestep, print how much 03 flux is coming down from the stratosphere in Tg/yr. (mje, bmy, 8/15/03)
- (18) Change O3 flux to 500 Tg/yr for GEOS-3 (mje, bmy, 9/15/03)
- (19) Now calls routine ADD_STRAT_POX from "tagged_ox_mod.f" in order to pass stratospheric flux of Ox to the proper tagged tracer w/o resorting to hardwiring w/in this routine. (bmy, 8/18/03)
- (20) Add GEOS_4 to the #if defined block. (bmy, 1/29/04)
- (21) Activated parallel DO-loops. Now made STFLUX a local array in order to facilitate parallelization. (bmy, 4/15/04)
- (22) Removed IORD, JORD, KORD from the arg list. Now reference STT and ITS_A_TAGOX_SIM from "tracer_mod.f". (bmy, 7/20/04)
- (23) Use an #ifdef block to comment out an EXIT statement from w/in a parallel loop for COMPAQ compiler. COMPAQ seems to have some problems with this. Now supports 1x125 grid. (auvray, bmy, 12/1/04)
- (24) Now modified for GEOS-5 and GCAP met fields (swu, bmy, 5/25/05)
- (25) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (26) Now set J30S and J30N for GEOS-5 nested grid (yxw, dan, bmy, 11/6/08)
- (27) Remove support for COMPAQ compiler (bmy, 7/8/09)
- (28) Now do not call ADD_STRAT_POx for tagged Ox (dbj, bmy, 10/16/09)
- 13 Aug 2010 R. Yantosca Treat MERRA like GEOS-5 (bmy, 8/13/10)
- 02 Dec 2010 R. Yantosca Added ProTeX headers
- 08 Feb 2012 R. Yantosca Treat GEOS-5.7.2 in the same way as MERRA
- 10 Feb 2012 R. Yantosca Modified for 0.25 x 0.3125 grids
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 28 Apr 2012 L. Murray Moved from upbdflx_mod.F to here, modified to F90, renamed from UPBDFLX_03 to DO_SYNOZ. Use chem timestep now. Also, removed INIT_UPBDFLX, which was last used for GEOS-3.
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 04 Feb 2013 M. Payer Replace all JJPAR with values for nested grids since JJPAR is no longer a parameter
- 14 Mar 2013 M. Payer Replace Ox with O3 as part of removal of NOx-Ox partitioning
- 25 Mar 2013 R. Yantosca Now use explicit numbers for J30S, J30N
- 31 May 2013 R. Yantosca Now pass Input_Opt, RC as arguments

```
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
26 Sep 2013 - R. Yantosca - Remove SEAC4RS C-preprocessor switch
26 Sep 2013 - R. Yantosca - Renamed GEOS_57 Cpp switch to GEOS_FP
05 Nov 2013 - R. Yantosca - Rename IDTOxStrt to id_O3Strat
23 Jan 2014 - M. Sulprizio- Linoz does not call UPBDFLX_03. Synoz does.
                            Now uncomment ADD_STRAT_POx (jtl,hyl,dbj,11/3/11)
26 Feb 2015 - E. Lundgren - Replace GET_PEDGE and GET_PCENTER with
                            State_Met%PEDGE and State_Met%PMID. Remove
                            dependency on pressure_mod.
03 Mar 2015 - E. Lundgren - Use virtual temperature in hypsometric eqn
12 Aug 2015 - R. Yantosca - Add placeholder values for 0.5 x 0.625 grids
16 Jun 2016 - M. Yannetti - Replaced TRACERID_MOD.
20 Jun 2016 - R. Yantosca - Now make species ID flags module variables
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected
                            species ID from State_Chm%Map_Advect.
12 Jul 2016 - R. Yantosca - Remove references to ADD_STRAT_POX
```

7.14 Fortran: Module Interface linoz_mod.F

Module LINOZ_MOD contains routines to perform the Linoz stratospheric ozone chemistry.

INTERFACE:

MODULE LINOZ_MOD

USES:

```
USE ERROR_MOD, ONLY: DEBUG_MSG ! Routine for debug output
USE PRECISION_MOD ! For GEOS-Chem Precision (fp, f4, f8)

IMPLICIT NONE
PRIVATE
!PRIVATE DATA MEMBERS:
REAL(fp), ALLOCATABLE :: TLSTT(:,:,:,:)
```

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: CLEANUP_LINOZ
PUBLIC :: DO_LINOZ
PUBLIC :: INIT_LINOZ
PUBLIC :: LINOZ_READ

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: LINOZ_CHEM3
PRIVATE :: LINOZ_STRATL
PRIVATE :: LINOZ_STRT2M
PRIVATE :: LINOZ_SOMLFQ
PRIVATE :: LINOZ_INTPL

REMARKS:

LINOZ Climatology:

The LINOZ stratospheric chemistry tables for ozone consist of:

7 tables, each a function of:

- 12 months,
- 18 latitudes (-85 to 85 in 10 deg. increments)
- 25 altitudes (z*=10-58 km in 2 km increments)

The 7 data fields are:

- 1- ozone (Logan climatology), v/v
- 2- Temperature climatology, K
- 3- Column ozone climatology, Logan ozone integrated above box, DU
- 4- ozone (P-L) for climatological ozone, v/v/s
- 5- d(P-L) / d03, 1/s
- 6- d(P-L) / dT, v/v/s/K
- 7- d(P-L) / d(column 03), v/v/s/DU

Implementation notes:

Dylan Jones (dbj@atmosp.physics.utoronto.ca) wrote:

Testing this code [in v8-02-04] was more difficult that I thought. I began by trying to compare the output of v8-02-04 with our previous runs with v8-02-01. I accounted for the changes in the transport_mod.f and I tried to undo the changes in when the diagnostics are archived in v8-02-04, but I was still getting large differences between v8-02-04 and v8-02-01. I finally gave up on this since I may have made a mistake in reverting to the old way of doing the diagnostics in v8-02-04. In the end I took the new linoz code from v8-02-04 and used it in v8-02-01. I ran two GEOS-5 full chemistry simulations for 2007 and the output were consistent over the full year.

I think that it is safe to release [Linoz in v8-02-04]. However, we should acknowledge that it was [only] tested in v8-02-01, since I was not able to assess the quality of the output in v8-02-04.

Bob Yantosca (yantosca@seas.harvard.edu) wrote:

We have also modified the code for use within the GEOS-5 GCM. We now declare the TPARM array as part of the Input_Opt object. The LINOZ climatology ASCII file is now read on the root CPU and MPI-broadcasted to the non-root CPUs. Also, the INIT_LINOZ routine is now called not on the first chemistry timestep but rather in the initialization phase at the start of the run. (bmy, 3/18/13)

```
REVISION HISTORY:
 23 Mar 2000 - P. Cameron-Smith - Initial version adapted heavily
                                    from McLinden's original file.
 24 Jun 2003 - B. Field & D. Jones - Further updates for GEOS-Chem
 28 May 2009 - D. Jones
                                 - Further modifications
 18 Nov 2009 - D. Jones
                                  - Further modifications
 01 Mar 2012 - R. Yantosca - Now reference new grid_mod.F90
 01 Aug 2012 - R. Yantosca - Add reference to findFreeLUN from inqure_mod.F90
 15 Mar 2013 - R. Yantosca - Now use fields from Input_Opt and made other
                            modifications for GIGC interface to GEOS-5 GCM
 18 Mar 2013 - R. Yantosca - Comment out STRAT_INIT, it's not called
 20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
 17 Nov 2014 - M. Yannetti - Added PRECISION_MOD
 19 Oct 2015 - C. Keller - TLSTT is now 4D to work on curvilinear grids
 29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90
```

7.14.1 do_linoz

Subroutine DO_LINOZ is the main driver for the Linoz stratospheric Ozone chemistry package.

INTERFACE:

```
SUBROUTINE DO_LINOZ( am_I_Root, Input_Opt,
& State_Met, State_Chm, RC )
```

USES:

```
USE ErrCode_Mod

USE Input_Opt_Mod, ONLY : OptInput

USE State_Chm_Mod, ONLY : ChmState

USE State_Met_Mod, ONLY : MetState

USE TIME_MOD, ONLY : GET_MONTH

USE TIME_MOD, ONLY : GET_TS_CHEM
```

INPUT PARAMETERS:

USE CMN_SIZE_MOD

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

7.14.2 linoz_chem3

Subroutine LINOZ_CHEM3 applies linearized chemistry based on tables from PRATMO model using climatological T, O3, time of year

INTERFACE:

```
SUBROUTINE LINOZ_CHEM3( DTCHEM, am_I_Root, Input_Opt, & State_Met, State_Chm, RC )
```

USES:

```
ONLY : GET_CHEMGRID_LEVEL
USE CHEMGRID_MOD,
USE CHEMGRID_MOD,
                        ONLY : GET_MAX_CHEMGRID_LEVEL
USE CMN_SIZE_MOD
USE ErrCode_Mod
USE GC_GRID_MOD,
                        ONLY : GET_AREA_CM2
USE Input_Opt_Mod,
                        ONLY : OptInput
USE PhysConstants,
                        ONLY: AIRMW, AVO
USE State_Chm_Mod,
                        ONLY : ChmState
USE State_Chm_Mod,
                        ONLY : Ind_
USE State_Met_Mod,
                        ONLY : MetState
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: DTCHEM ! Time step [seconds]
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object !OUTPUT PARAMETERS
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REMARKS:

Replace fields from tracer_mod.f with fields from Input_Opt. When we use GEOS-Chem within the GEOS-5 GCM, the fields within Input_Opt will be read on the root CPU and MPI-broadcasted to all other CPUs.

```
24 Jun 2003 - B. Field & D. Jones - Further updates for GEOS-Chem
18 Nov 2009 - D. Jones
                                 - For now, set tagged stratospheric
                                    tracer to total O3 in the overworld
                                    to avoid issues with spin ups
08 Feb 2010 - R. Yantosca
                                 - Deleted obsolete local variables
22 Oct 2010 - R. Yantosca
                                 - Added OMP parallel loop
01 Mar 2012 - R. Yantosca - Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
30 Jul 2012 - R. Yantosca - Now accept am_I_Root as an argument when
                           running with the traditional driver main.F
09 Nov 2012 - M. Payer
                          - Replaced all met field arrays with State_Met
                            derived type object
14 Mar 2013 - M. Payer
                          - Replace Ox with O3 as part of removal of NOx-Ox
                            partitioning
18 Mar 2013 - R. Yantosca - Now accept Input_Opt, RC as arguments
19 Mar 2013 - R. Yantosca - Now copy Input_Opt%TCVV(1:N_TRACERS)
                         - Now pass State_Chm object via the arg list
25 Mar 2013 - M. Payer
06 Nov 2013 - R. Yantosca - Now activate the parallel loop. Unit testing
                           revealed that this no longer causes errors.
26 Feb 2015 - E. Lundgren - Replace GET_PCENTER and GET_PEDGE with
                            State_Met%PMID and State_Met%PEDGE. Remove
                            dependency on pressure_mod.
19 Oct 2015 - C. Keller - TLSTT is now 4D to work on curvilinear grids
06 Jan 2016 - E. Lundgren - Use global physical parameters
16 Jun 2016 - R. Silvern - Now define species ID of 03 with Ind_ function
17 Jun 2016 - R. Yantosca - Only look up species ID of 03 on first call
22 Jun 2016 - M. Yannetti - Replace TCVV with spc db and physical constant
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected
                            species ID from State_Chm%Map_Advect.
11 Jul 2016 - R. Yantosca - Bug fix: SPC now points to State_Chm%Species
```

7.14.3 linoz_stratl

Subroutine LINOZ_STRATL performs a monthly fixup of chemistry parameters for the Linoz stratospheric ozone chemistry.

INTERFACE:

SUBROUTINE LINOZ_STRATL(am_I_Root, Input_Opt, RC)

USES:

```
USE CMN_SIZE_MOD

USE ErrCode_Mod

USE GC_GRID_MOD, ONLY : GET_YMID

USE Input_Opt_Mod, ONLY : OptInput

USE PRESSURE_MOD

USE TIME_MOD, ONLY : GET_MONTH
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

Replace size fields NLAT_LINOZ etc. with fields from Input_Opt. When we use GEOS-Chem within the GEOS-5 GCM, the fields within Input_Opt will be read on the root CPU and MPI-broadcasted to all other CPUs.

The LINOZ climatology array is $Input_Opt\%LINOZ_TPARM(25,18,12,N)$, which has the following dimensions

- * 25 layers from 58 km to 10 km by 2 km intervals
- * 18 latitudes (85S, 75S, ...85N)
- * 12 months
- * N fields (currently N=7)

REVISION HISTORY:

7.14.4 linoz_strt2m

Subroutine LINOZ_STRT2M interpolates quantities from the LINOZ vertical grid to the GEOS-Chem vertical grid. It also computes the 1st & 2nd moments of the distribution.

INTERFACE:

```
SUBROUTINE LINOZ_STRT2M( am_I_Root, Input_Opt, NSTRT, & STRTX, POL, STRTOL, & STRT1L, STRT2L, RC )
```

USES:

```
USE CMN_SIZE_MOD
USE ErrCode_Mod
```

INPUT PARAMETERS:

```
! am_I_Root : Are we on the root CPU?
      ! Input_Opt : Input Options object
      ! NSTRT : # of levels in the GEOS-Chem grid (= LLPAR)
      ! STRTX
               : Quantity on the LINOZ vertical grid
                 (i.e. fields #1-7 of the LINOZ climatology)
      ! POL : Pressure edges on the GEOS-Chem grid
      I-----
                   INTENT(IN) :: am_I_Root
      LOGICAL,
      TYPE(OptInput), INTENT(IN) :: Input_Opt
      INTEGER, INTENT(IN) :: NSTRT
                  INTENT(IN) :: STRTX(Input_Opt%LINOZ_NLEVELS)
INTENT(IN) :: POL(LLPAR+1)
      REAL(fp),
      REAL(fp),
OUTPUT PARAMETERS:
      ! STRTOL : Oth moment of distribution, on GEOS-Chem grid edges
      ! STRT1L : 1st moment of distribution, on GEOS-Chem grid edges
      ! RC : Success or failure?
      I-----
      REAL(fp),
                    INTENT(OUT) :: STRTOL(LLPAR+1)
                 INTENT(OUT) :: STRT1L(LLPAR+1)
INTENT(OUT) :: STRT2L(LLPAR+1)
      REAL(fp),
     REAL(fp),
                 INTENT(OUT) :: RC
      INTEGER,
REMARKS:
   Comments from Chris McLinden to Peter Cameron-Smith:
   ______
   CALL SOMLFQ(P1,P2,F0,F1,F2,PS,F,NL)
   - P1,P2 are the pressure EDGES for the CTM layer onto which the
     coefficients will be mapped. [P1>P2 I believe {PJC}]
   - F0,F1,F2 are the CTM layer vertical moments determined in SOMLFQ
   - PS are the pressure layer edges of the original [ie Linox] grid
   - F is the column of coefficients (on the original grid); note
     F is flipped relative to STRTX and since the coefficients begin
     at z*=10, F(1)=F(2)=...=F(5)=0
   - NL is 30; size of F()
    The box model calculations were performed at z*=10km, 12km, ... and
    so these would represent the centres with the corresponding edges at
    9,11km; 11,13km; ...
    PS() represents the edges (although PS(1) is set to 1000mb).
    The first few values are:
      PS(1)=1000
      PS(2)=874.947105 (note PS(2) is not quite 1000 exp(-1/16) as the
     PS(3)=656.117767 the average pressure is used - not the pressure
```

!-----

```
PS(4)=492.018914 at the average z*)
PS(5)=368.96213
PS(6)=276.68257
PS(7)=207.48266
...
PS(30)=0.276682568
PS(31)=0.0

F(1) spans PS(1)-PS(2)
F(2) spans PS(2)-PS(3)
...
F(30) spans PS(30)-PS(31)
```

REVISION HISTORY:

```
24 Jun 2003 - B. Field & D. Jones - Further updates for GEOS-Chem

18 Mar 2013 - R. Yantosca - Now pass am_I_root, Input_Opt, RC arguments

18 Mar 2013 - R. Yantosca - Rearrange argument list so that inputs are

all listed before outputs

18 Mar 2013 - R. Yantosca - Now make NL a local variable and set its

value from Input_Opt%LINOZ_NLEVELS
```

7.14.5 linoz_somlfq

subroutine LINOZ_SOMLFQ calculates loss freq moments from a set of loss frequencies at std z*, given a CTM model interval pressure range: P1; P2 (decreasing up)

INTERFACE:

```
SUBROUTINE LINOZ_SOMLFQ(P1,P2,F0,F1,F2,PS,F,NL)
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NL
REAL(fp), INTENT(IN) :: F(NL)
REAL(fp), INTENT(IN) :: PS(NL+1)
REAL(fp), INTENT(IN) :: P1
REAL(fp), INTENT(IN) :: P2
```

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT) :: F0
REAL(fp), INTENT(OUT) :: F1
REAL(fp), INTENT(OUT) :: F2
REMARKS:
The pressure levels BETWEEN z* values are:
    PS(i) > PS(i+1) bounds z*(i)
```

REVISION HISTORY:

```
24 Jun 2003 - B. Field & D. Jones - Further updates for GEOS-Chem 19 Mar 2013 - R. Yantosca - P1, P2 are now declared as INTENT(IN)
```

7.14.6 linoz_read

Subroutine LINOZ_READ reads the input data file for the Linoz stratospheric ozone chemistry.

INTERFACE:

```
SUBROUTINE LINOZ_READ( am_I_Root, Input_Opt, RC )
```

USES:

```
USE ErrCode_Mod

USE FILE_MOD, ONLY : IOERROR

USE Input_Opt_Mod, ONLY : OptInput

USE InquireMod, ONLY : findFreeLun
```

INPUT PARAMETERS:

USE CMN_SIZE_MOD

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(OptInput), INTENT(INOUT) :: Input_Opt ! Input Options object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

 $\label{linoz_READ} LINOZ_READ is called from "main.f" at the start of the simulation. \\ LINOZ_READ will also call INIT_LINOZ to initialize the arrays.$

```
24 Jun 2003 - B. Field & D. Jones - Further updates for GEOS-Chem
16 Oct 2009 - R. Yantosca - Now use IU_FILE instead of IU_LINOZ
16 Oct 2009 - R. Yantosca - Read file from DATA_DIR_1x1
01 Aug 2012 - R. Yantosca - Add reference to findFreeLUN from inqure_mod.F90
03 Aug 2012 - R. Yantosca - Move calls to findFreeLUN out of DEVEL block
15 Mar 2013 - R. Yantosca - Now call INIT_LINOZ from GIGC_Init_Extra
5 Mar 2015 - R. Yantosca - Now read data relative to ExtData/CHEM_INPUTS
```

7.14.7 linoz_intpl

Subroutine LINOZ_INTPL does some kind of interpolation.

INTERFACE:

SUBROUTINE LINOZ_INTPL(KE, IE, ND, NE, XI, XN, YI, YN)

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: KE
INTEGER, INTENT(IN) :: IE
INTEGER, INTENT(IN) :: ND
INTEGER, INTENT(IN) :: NE
REAL(fp), INTENT(IN) :: XI(IE)
REAL(fp), INTENT(IN) :: XN(ND)
REAL(fp), INTENT(IN) :: YI(KE,IE)
```

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT) :: YN(KE,ND)
```

REVISION HISTORY:

```
24 Jun 2003 - B. Field & D. Jones - Further updates for GEOS-Chem
```

7.14.8 init_linoz

Subroutine INIT_LINOZ allocates and zeroes the module arrays used in the Linoz stratospheric ozone algorithm.

INTERFACE:

```
SUBROUTINE INIT_LINOZ( am_I_Root, Input_Opt, RC )
```

```
USE CMN_SIZE_MOD

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ALLOC_ERR

USE Input_Opt_Mod, ONLY : OptInput
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REVISION HISTORY:

```
16 Oct 2009 - R. Yantosca - Initial version

18 Mar 2013 - R. Yantosca - Remove TPARM array since that is now carried within the Input_Opt object.

18 Mar 2013 - R. Yantosca - Accept am_I_Root, Input_Opt, RC arguments

14 Mar 2013 - M. Payer - Replace Ox with O3 for full-chemistry simulation

19 Oct 2015 - C. Keller - TLSTT is now 4D to work on curvilinear grids
```

7.14.9 cleanup_linoz

Subroutine CLEANUP_LINOZ deallocates all module arrays.

INTERFACE:

SUBROUTINE CLEANUP_LINOZ

REVISION HISTORY:

```
16 Oct 2009 - R. Yantosca - Initial version
```

8 Aerosol modules

These modules contain routines to perform chemistry or removal of the various aerosol species.

8.1 Fortran: Module Interface aerosol_mod.F

Module AEROSOL_MOD contains variables and routines for computing optical properties for aerosols which are needed for both the FAST-J photolysis and ND21 optical depth diagnostics. (bmy, 7/20/04, 2/10/09)

INTERFACE:

MODULE AEROSOL_MOD

USE PRECISION_MOD

IMPLICIT NONE PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: AEROSOL_CONC
PUBLIC :: CLEANUP_AEROSOL
PUBLIC :: INIT_AEROSOL

PUBLIC :: RDAER

PUBLIC DATA MEMBERS:

```
! BCPI
              : Hydrophilic black carbon aerosol
                                                   [kg/m3]
! BCPO
              : Hydrophobic black carbon aerosol
                                                   [kg/m3]
! OCPI
              : Hydrophilic organic carbon aerosol [kg/m3]
! OCPO
              : Hydrophilic organic carbon aerosol
                                                  [kg/m3]
! OCPISOA
              : Hydrophilic OC + SOA aerosol
                                                   [kg/m3]
! SALA
              : Accumulation mode seasalt aerosol
                                                   [kg/m3]
              : Coarse mode seasalt aerosol
                                                   [kg/m3]
! SALC
! SO4_NH4_NIT : Lumped SO4-NH4-NIT aerosol
                                                   [kg/m3]
              : Sulfate aerosol
                                                   [kg/m3]
! NH4
              : Ammonium aerosol
                                                   [kg/m3]
! NIT
              : Inorganic nitrate aerosol
                                                   [kg/m3]
! SOILDUST
              : Mineral dust aerosol from soils
                                                   [kg/m3]
              : Stratospheric liquid aerosol
! SLA
                                                   [kg/m3]
              : Stratospheric particulate aerosol
! SPA
                                                   [kg/m3]
                                                   [kg/m3]
! TSOA
              : Terpene SOA
! ISOA
              : Isoprene SOA
                                                   [kg/m3]
! ASOA
              : Aromatic + IVOC SOA
                                                   [kg/m3]
              : Aerosol product of SVOC oxidation
                                                   [kg/m3]
! OPOA
! SOAG
              : SOA product of GLYX
                                                   [kg/m3]
              : SOA product of MYLY
                                                   [kg/m3]
! SOAM
! PM25
              : Particulate matter < 2.5 um
                                                   [kg/m3]
REAL(fp), ALLOCATABLE, PUBLIC :: BCPI(:,:,:)
REAL(fp), ALLOCATABLE, PUBLIC :: BCPO(:,:,:)
REAL(fp), ALLOCATABLE, PUBLIC :: OCPI(:,:,:)
REAL(fp), ALLOCATABLE, PUBLIC :: OCPO(:,:,:)
REAL(fp), ALLOCATABLE, PUBLIC :: OCPISOA(:,:,:)
REAL(fp), ALLOCATABLE, PUBLIC :: SALA(:,:,:)
REAL(fp), ALLOCATABLE, PUBLIC :: SALC(:,:,:)
REAL(fp), ALLOCATABLE, PUBLIC :: SO4_NH4_NIT(:,:,:)
REAL(fp), ALLOCATABLE, PUBLIC :: SO4(:,:,:)
REAL(fp), ALLOCATABLE, PUBLIC :: NH4(:,:,:)
REAL(fp), ALLOCATABLE, PUBLIC :: NIT(:,:,:)
REAL(fp), ALLOCATABLE, PUBLIC :: FRAC_SNA(:,:,:,:)
```

```
REAL(fp), ALLOCATABLE, PUBLIC :: SOILDUST(:,:,:,:)

REAL(fp), ALLOCATABLE, PUBLIC :: SLA(:,:,:)

REAL(fp), ALLOCATABLE, PUBLIC :: SPA(:,:,:)

REAL(fp), ALLOCATABLE, PUBLIC :: TSOA(:,:,:)

REAL(fp), ALLOCATABLE, PUBLIC :: ISOA(:,:,:)

REAL(fp), ALLOCATABLE, PUBLIC :: ASOA(:,:,:)

REAL(fp), ALLOCATABLE, PUBLIC :: OPOA(:,:,:)

REAL(fp), ALLOCATABLE, PUBLIC :: SOAG(:,:,:)

REAL(fp), ALLOCATABLE, PUBLIC :: SOAM(:,:,:)

REAL(fp), ALLOCATABLE, PUBLIC :: PM25(:,:,:)
```

DEFINED PARAMETERS:

REMARKS:

References:

(1) Pye, H.O.T., and J.H. Seinfeld, "A global perspective on aerosol from low-volatility organic compounds", Atmos. Chem. & Phys., Vol 10, pp 4377-4401, 2010.

- (1) Added AEROSOL_RURALBOX routine (bmy, 9/28/04)
- (2) Now convert ABSHUM from absolute humidity to relative humidity in AEROSOL_RURALBOX, using the same algorithm as in "gasconc.f". (bmy, 1/27/05)
- (3) Now references "tropopause_mod.f" (bmy, 8/22/05)
- (4) Now add contribution of SOA4 into Hydrophilic OC (dkh, bmy, 5/18/06)
- (5) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (6) Add support for variable tropopause (bdf, phs, 9/14/06)
- (7) Now set OCF=2.1 in AEROSOL_CONC for consistency w/ carbon_mod.f $(\mbox{tmf, }2/\mbox{10}/\mbox{09})$
- (8) Add WTAREA and WERADIUS for dicarbonyl SOA production. WTAREA is the same as TAREA, but excludes dry dust, BCPO and OCPO; use same units as TAREA. WERADIUS is same as ERADIUS, but excludes dry dust, BCPO and OCPO;

```
use same units as ERADIUS. (tmf, 3/2/09)

(9 ) Add SOAG and SOAM species. (tmf, ccc, 3/2/09)

(10) Modify AOD output to wavelength specified in jv_spec_aod.dat (clh, 05/07/10)

22 Dec 2011 - M. Payer - Added ProTeX headers

05 Mar 2013 - R. Yantosca - Now make INIT_AEROSOL a public routine

20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
```

8.1.1 aerosol_conc

Subroutine AEROSOL_CONC computes aerosol concentrations in kg/m3 from the tracer mass in kg in the Species array. These are needed to compute optical properties for photolysis, for the optical depth diagnostics, and for the SOA concentration diagnostics. (bmy, 7/20/04, 2/10/09)

INTERFACE:

```
SUBROUTINE AEROSOL_CONC( am_I_Root, Input_Opt, & State_Met, State_Chm, RC )
```

USES:

```
USE CHEMGRID_MOD,
                              ONLY : ITS_IN_THE_TROP
     USE CMN_FJX_MOD,
                              ONLY: REAA
     USE CMN_SIZE_MOD
     USE ErrCode_Mod
     USE ERROR_MOD
     USE Input_Opt_Mod,
                              ONLY : OptInput
     USE State_Met_Mod,
                              ONLY : MetState
     USE State_Chm_Mod,
                              ONLY : ChmState
     USE UCX_MOD,
                              ONLY : KG_STRAT_AER
     USE UnitConv_Mod
#if
     defined( TOMAS )
     USE TOMAS_MOD,
                             ONLY : IBINS
#endif
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure
```

REMARKS:

This code was originally included in "chemdr.f", but the same computation also needs to be done for offline aerosol simulations. Therefore, we have split this code off into a separate subroutine which can be called by both fullchem and offline aerosol simulations.

REVISION HISTORY:

```
(1) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
(2) Now add contribution from SOA4 into Hydrophilic OC (dkh, bmy, 5/18/06)
(3 ) Now set OCF=2.1 to be consistent w/ "carbon_mod.f" (tmf, 2/10/09)
22 Dec 2011 - M. Payer
                          - Added ProTeX headers
30 Jul 2012 - R. Yantosca - Now accept am_I_Root as an argument when
                            running with the traditional driver main.F
13 Nov 2012 - R. Yantosca - Now pass am_I_Root, Input_Opt, RC as arguments
15 Nov 2012 - M. Payer
                          - Replaced all met field arrays with State_Met
                            derived type object
05 Mar 2013 - R. Yantosca - Remove call to INIT_AEROSOL, this is now done
                            in the initialization stage
                          - Now pass State_Chm object via the arg list
25 Mar 2013 - M. Payer
13 Aug 2013 - M. Sulprizio- Add modifications for updated SOA and SOA +
                            semivolatile POA simulations (H. Pye)
                          - Now allow bulk dust in TOMAS simulations
17 Jun 2014 - J. Pierce
07 Apr 2015 - R. Yantosca - Add check to prevent div-by-zero errors
25 Jun 2015 - E. Lundgren - Use L. Zhang dust size distribution params for
                            mineral dust aerosols (non-TOMAS)
13 Aug 2015 - E. Lundgren - Convert tracer units to kg if input units are
                            mixing ratio
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected
                            species ID from State_Chm%Map_Advect.
10 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code
18 Nov 2016 - M. Sulprizio- Move calculation of SOA and PM2.5 concentrations
                            here from diag42_mod.F
22 Nov 2016 - M. Sulprizio- Add online calculation of aerosol growth factors
                            at 35% RH
```

8.1.2 rdaer

Subroutine RDAER reads global aerosol concentrations as determined by Mian Chin. Calculates optical depth at each level for "set_prof.f". Also calculates surface area for heterogeneous chemistry. It uses aerosol parameters in FAST-J input file "jv_spec.dat" for these calculations. (rvm, rjp, tdf, bmy, 11/04/01, 7/20/04)

INTERFACE:

```
SUBROUTINE RDAER( am_I_Root, Input_Opt, State_Met, State_Chm, & RC, MONTH, YEAR, ODSWITCH )
```

USE CHEMGRID_MOD, ONLY : ITS_IN_THE_CHEMGRID
USE CHEMGRID_MOD, ONLY : ITS_IN_THE_NOCHEMGRID

USE CMN_DIAG_MOD
USE CMN_FJX_MOD

USE CMN_SIZE_MOD

USE DIAG_MOD, ONLY : AD21

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP
USE Input_Opt_Mod, ONLY : OptInput
USE PhysConstants, ONLY : CONSVAP
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState

USE TIME_MOD, ONLY : ITS_A_NEW_MONTH
USE TIME_MOD, ONLY : SYSTEM_TIMESTAMP

USE TRANSFER_MOD, ONLY : TRANSFER_3D
USE UCX_MOD, ONLY : GET_STRAT_OPT
USE UCX_MOD, ONLY : NDENS_AER

IMPLICIT NONE

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on root CPU? TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State INTEGER, OPTIONAL :: MONTH ! # of current month

INTEGER, OPTIONAL :: YEAR ! 4-digit year INTEGER, OPTIONAL :: ODSWITCH ! Logical indicator

! Logical indicator ! = 0: AOD computed

! at 999 nm ! = 1: AOD computed

! at wavelength set ! in Radiation Menu

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

- (1) At the point in which "rdaer.f" is called, ABSHUM is actually absolute humidity and not relative humidity (rvm, bmy, 2/28/02)
- (2) Now force double-precision arithmetic by using the "D" exponent. (bmy, 2/28/02)
- (3) At present aerosol growth is capped at 90% RH. The data in jv_spec.dat could be used to allow a particle to grow to 99% RH if desired. (rvm, 3/15/02)

- (4) Bug fix: TEMP2 needs to be sized (IIPAR, JJPAR, LLPAR) (bmy, 5/30/02)
- (5) Now reference BXHEIGHT from "dao_mod.f". Also references ERROR_STOP from "error_mod.f". Delete local declaration of TIME, since that is also declared w/in comode.h -- this causes compile-time errors on the ALPHA platform. (gcc, bmy, 11/6/02)
- (6) Now use the online SO4, NH4, NIT aerosol, taken from the STT array, and passed via SO4_NH4_NIT argument if sulfate chemistry is turned on. Otherwise, read monthly mean sulfate from disk. (rjp, bmy, 3/23/03)
- (7) Now call READ_BPCH2 with QUIET=.TRUE., which prevents info from being printed to stdout. Also made cosmetic changes. (bmy, 3/27/03)
- (8) Add BCPI, BCPO, OCPI, OCPO to the arg list. Bug fix: for online sulfate & carbon aerosol tracers, now make sure these get updated every timestep. Now references "time_mod.f". Now echo info about which online/offline aerosols we are using. Updated comments. (bmy, 4/9/04)
- (9) Add SALA, SALC to the arg list (rjp, bec, bmy, 4/20/04)
- (10) Now references DATA_DIR from "directory_mod.f". Now references LSULF, LCARB, LSSALT from "logical_mod.f". Added minor bug fix for conducting the appropriate scaling for optical depth for ND21 diagnostic. Now make MONTH and YEAR optional arguments. Now bundled into "aerosol_mod.f". (rvm, aad, clh, bmy, 7/20/04)
- (11) Now remove FWET from extinction efficiency computation (avd, 8/3/10)
- (12) Include third input argument to determine the wavelength at which the AOD should be computed. This will set the optical properties that are used for the calculation of the AOD. The ND21 diagnostic should only be updated when WAVELENGTH = 1. (skim, 02/03/11)
- 09 Mar 2011 R. Yantosca Set MSDENS(2) = 1800 for APM (G. Luo)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 13 Nov 2012 R. Yantosca Now pass Input_Opt, RC arguments for GIGC
- 15 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 27 Mar 2013 S.D. Eastham- Upgraded from Fast-J to Fast-JX
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 17 Dec 2014 R. Yantosca Leave time/date variables as 8-byte
- 05 Mar 2015 R. Yantosca Remove DO_READ_DATA option. We can no longer have binary punch input in HPC environments.
- 31 Mar 2015 R. Yantosca Bug fix: Declare LINTERP as !\$OMP PRIVATE
- 07 Apr 2015 R. Yantosca Bug fix: Add error check to JLOOP do-loop so that we cycle if JLOOP <= 0
- 24 Jun 2015 M. Sulprizio- Update organic aerosol density MSDENS(3) from 1800 to 1300 kg/m3 (E. Marais, M. Hammer)
- 15 Oct 2015 C. Keller Empty ODAER before refilling.
- 12 May 2016 M. Sulprizio- Remove 1D arrays that depend on JLOOP. ABSHUM is now a 3D field in State_Met. ERADIUS, TAREA WERADIUS, WTAREA are now pointers that point to 3D fields in State_Chm.

```
16 May 2016 - M. Sulprizio- Remove JLOOP entirely and loop over LLPAR, JJPAR,
IIPAR instead.

28 Jun 2016 - M. Sulprizio- Make IOUT a local variable to remove dependence
on comode_loop_mod.F

22 Nov 2016 - M. Sulprizio- Now define aerosol densities in species database
```

and use SpcData%Info%Density to populate MSDENS

8.1.3 init_aerosol

Subroutine INIT_AEROSOL allocates and zeroes module arrays

INTERFACE:

```
SUBROUTINE INIT_AEROSOL( am_I_Root, Input_Opt, RC )
```

USES:

```
USE CMN_SIZE_MOD

USE ErrCode_Mod

USE ERROR MOD. ONLY
```

USE ERROR_MOD, ONLY : ALLOC_ERR
USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : Ind_

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

INPUT/OUTPUT PARAMETERS:

INTEGER. INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

```
20 Jul 2004 - R. Yantosca - Initial version
22 Dec 2011 - M. Payer - Added ProTeX headers
05 Mar 2013 - R. Yantosca - Now accept am_I_Root, Input_Opt, RC arguments
17 Jun 2016 - R. Yantosca - Now use locally-defined species ID flags,
```

8.1.4 cleanup_aerosol

Subroutine CLEANUP_AEROSOL deallocates all module arrays (bmy, 7/20/04)

INTERFACE:

SUBROUTINE CLEANUP_AEROSOL

```
22 Dec 2011 - M. Payer - Added ProTeX headers
```

8.2 Fortran: Module Interface carbon_mod.F

Module CARBON_MOD contains arrays and routines for performing a carbonaceous aerosol simulation. Original code taken from Mian Chin's GOCART model and modified accordingly. (rjp, bmy, 4/2/04, 6/30/10)

INTERFACE:

MODULE CARBON_MOD

USES:

USE AEROSOL_MOD, ONLY : OCFPOA, OCFOPOA

USE HCO_ERROR_MOD ! For HEMCO error reporting

USE PhysConstants ! Physical constants

USE PRECISION_MOD ! For GEOS-Chem Precisions

IMPLICIT NONE

PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: CHEMCARBON
PUBLIC :: EMISSCARBON
PUBLIC :: CLEANUP_CARBON
PUBLIC :: INIT_CARBON

#if defined (TOMAS)

PUBLIC :: EMISSCARBONTOMAS

#endif

PUBLIC DATA MEMBERS:

! SOAupdate: for branching ratio diagnostic (hotp 5/24/10)

PUBLIC :: BETANOSAVE

! Make BIOG_SESQ array public so that it can be used by HEMCO

! (ckeller, 05/19/14)
PUBLIC :: BIOG_SESQ

REMARKS:

4 Aerosol species : Organic and Black carbon

: hydrophilic (soluble) and hydrophobic of each

For secondary organic aerosol (SOA) simulation orginal code developed by Chung and Seinfeld [2002] and Hong Liao from John Seinfeld's group at Caltech was taken and further modified accordingly (rjp, bmy, 7/15/04)

SOAupdate: Traditional SOA simulation updated by hotp 7/2010

New code treats semivolatile or nonvolatile POA, aerosol from IVOCs,

and has updated biogenic SOA

For more detailes on the updated SOA/POA simulation, see comments

in SOA_CHEMISTRY, Pye and Seinfeld ACP 2010, Pye et al. in prep for ACP 2010 $\,$

Note that modifications were made throughout the code for SOAupdate

References:

- (1) Bond, T.C., E. Bhardwaj, R. Dong, R. Jogani, S. Jung, C. Roden, D.G. Streets, and N.M. Trautmann, "Historical emissions of black and organic carbon aerosol from energy-related combustion, 1850-2000", Global Biogeochem. Cycles, 21, GB2018, doi:10.1029/2006GB002840, 2007.
- (2) Chan, A.W.H., K.E. Kautzman, P.S. Chhabra, J.D. Surratt, M.N. Chan, J.D. Crounse, A. Kurten, P.O. Wennberg, R.C. Flagan, and J.H. Seinfeld, "Secondary orgains aerosol formation from photooxidation of naphthlene and alkylnaphthalenes: implications for oxidation of intermediate volatility orgains compounds (IVOCs)", Atmos. Chem. Phys, Vol 9, 3049-3060, doi:10.5194/acp-9-3049-2009, 2009.
- (3) Chung, S.H., and J.H. Seinfeld. "Global distribution and climate forcing of carbonaceous aerosols", J. Geophys. Res., Vol 107(D19), 4407, doi:10.1029/2001JD001397, 2002.
- (4) Grieshop, A.P., J.M. Logue, N.M. Donahue, and A.L. Robinson, "Laboratory investigation of photochemical oxidation of organic aerosol deom wood fires 1: Measurement and simulation of organic aerosol evolution", Atmos. Chem. Phys., Vol 9, 1263-1277, doi:10.5194/acp-9-1263-2009, 2009.
- (5) Griffin, R.J., D.R. Cocker, R.C. Flagan, and J.H. Seinfeld, "Orgainc aerosol formation from the oxidation of biogenic hydrocarbons", J. Geophys. Res., 104(D3), 3555-3567, 1999.
- (6) Henze, D.K., and J.H. Seinfeld, "Global secondary organic aerosol from isoprene oxidation", Geophys. Res. Lett., Vol 33, L09812, doi:10.1029/2006GL025976, 2006.
- (7) Henze, D.K., J.H. Seinfeld, N.L. Ng, J.H. Kroll, T.-M. Fu, D.J. Jacob, and C.L. Heald, "Global modeling of secondary orgains aerosol formation from aromatic hydrocarbons: high vs. low-yield pathways", Atmos. Chem. Phys., Vol 8, 2405-2420, doi:10.5194/acp-8-2405-2008, 2008.
- (8) Kroll, J.H., N.L. Ng, S.M. Murphy, R.C. Flagan, and J.H. Seinfeld, "Secondary orgains aerosol formation from isoprene photooxidation", Environ. Sci. Technol, Vol 40, 1869-1877, doi:10.1021/Es0524301, 2006.
- (9) Liao, H., D.K. Henze, J.H. Seinfeld, S.L Wu, and L.J. Mickley, "Biogenic secondary aerosol over the United States: Comparison of climatological simulations with observations, J. Geophys. Res. Vol 112, D06201, doi:10.1029/2006JD007813, 2007.
- (10) Ng, N.L., P.S. Chhabra, A.W.H. Chan, J.D. Surratt, J.H. Kroll, A.J. Kwan, D.C. McCabe, P.O. Wennberg, A. Sorooshian, S.M. Murphy, N.F. Dalleska, R.C. Flagan, and J.H. Seinfeld, "Effect of NOx level on secondary orgainc aerosol (SOA) formation from the photooxidation of terpenes", Atmos. Chem. Phys., Vol 7, 5159-5174, doi:10.5194/acp-7-5195-2007, 2007a.

- (11) Ng, N.L., J.H. Kroll, A.W.H. Chan, P.S. Chhabra, R.C. Flagan, and J.H. Seinfeld, "Secondary orgains aerosol formation from m-xylene, toluele, and benzene", Atmos. Chem. Phys., Vol 7, 3909-3922, doi:10.5194/acp-7-3909-2007, 2007b.
- (12) Ng, N.L., A.J. Kwan, J.D. Surratt, A.W.H. Chan, P.S. Chhabra, A. Sorooshian, H.O.T. Pye, J.D. Crounse, P.O. Wennberg, R.C. Flagan, and J.H. Seinfeld, "Secondary organic aerosol (SOA) formation from reaction of isoprene with nitrate radicals (NO3)", Atmos. Chem. Phys., Vol 8, 4117-4140, doi:10.5194/acp-8-4117-2008, 2008.
- (13) Pye, H.O.T., and J.H. Seinfeld, "A global perspective on aesorol from low-volatility orgnaic compounds", Atmos. Chem. Phys., Vol 10, 4377-4401, doi:10.5194/acp-10-4377-2010, 2010.
- (14) Pye. H.O.T., A.W.H Chan, M.P. Barkley, and J.H. Seinfeld, "Global modeling of organic aerosol: The importance of reactive nitrogen (NOx and NO3)", Atmos. Chem. Phys., Vol 10, 11261-11276, doi:10.5194/acp-10-11261-2010, 2010.
- (15) Shilling, J.E., Q. Chen, S.M. King, T. Rosenoern, J.H. Kroll, D.R. Worsnop, K.A. McKinney, S.T., Martin, "Particle mass yield in secondary orgainc aerosol formed by the dark ozonolysis of a-pinene", Atmos Chem Phys, Vol 8, 2073-2088, doi: 10.5194/acp-8-2073-2008, 2008.
- (16) Shrivastava, M.K., E.M. Lipsky, C.O. Stanier, A.L. Robinson, "Modeling semivolatile organic mass emissions from combustion systems", Environ. Sci. Technol., Vol 40, 2671-2677, doi:10.1021/ES0522231, 2006.
- (17) Zhang, J.Y., K.E.H. Hartz, S.N. Pandis, N.M. Donahue, "Secondary organic aerosol formation from limonene ozonolysis: Homogeneous and heterogeneous influences as a function of NOx", J. Phys. Chem. A, Vol 110, 11053-11063, doi:10.1021/Jp06286f, 2006.

Base Year is 2000. More at http://www.hiwater.org

- (1) Added code from the Caltech group for SOA chemistry (rjp, bmy, 7/15/04)
- (3) Now read data from carbon_200411/ subdir of DATA_DIR. Also added some extra debug output. Now read T. Bond yearly emissions as default, but overwrite N. America with the monthly Cooke/RJP emissions. Added module variables I1_NA, I2_NA, J1_NA, J2_NA. (rjp, bmy, 12/1/04)
- (4) Now can read seasonal or interannual BCPO, OCPO biomass emissions.

 Also parallelize loop in OHNO3TIME. (rjp, bmy, 1/18/05)
- (5) Now references "pbl_mix_mod.f". Bug fix: now make sure only to save up to LD07 levels for the ND07 diagnostic in SOA_LUMP. (bmy, 3/4/05)
- (6) Now can read data for both GEOS and GCAP grids (bmy, 8/16/05)
- (7) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (8) Now references "megan_mod.f". Also now references XNUMOL and XNUMOLAIR from "tracer_mod.f" (tmf, bmy, 10/25/05)
- (9) Bug fix for GCAP in BIOGENIC_OC (bmy, 4/11/06)

- (10) Updated for SOA production from ISOP (dkh, bmy, 5/22/06)
- (11) Updated for IPCC future emission scale factors. Also added function GET_DOH to return ISOP that has reacted w/ OH. (swu, dkh, bmy, 6/1/06)
- (12) Now add SOG condensation onto SO4, NH4, NIT (rjp, bmy, 8/3/06)
- (13) Minor fix for 20 carbon tracers. (phs, 9/14/06)
- (14) Now remove reading of biomass emissions from "carbon_mod.f", since they are better done in gc_biomass_mod.f. This will allow us to standardize treatment of GFED2 or default BB emissions. Also applied a typo fix in SOA_LUMP. (tmf, bmy, 10/16/06)
- (15) Prevent seg fault error in BIOMASS_CARB_GEOS (bmy, 11/3/06)
- (16) Corrected typos in SOA_LUMP. Now also save GPROD and APROD to disk for each new diagnostic interval. (dkh, tmv, havala, bmy, 2/6/07)
- (17) Modifications for 0.5 x 0.666 nested grids (yxw, dan, bmy, 11/6/08)
- (18) Now account for various GFED2 products (yc, phs, 12/23/08)
- (19) Now add future scaling to BIOMASS_CARB_GEOS (hotp, swu, 2/19/09)
- (20) Added SOA production from dicarbonyls (tmf, 3/2/09)
- (21) Bugfix: cleanup ORVC_TERP and ORVC_SESQ (tmf, 3/2/09)
- (22) Replace USE_MONTHLY_BIOB with USE_BOND_BIOBURN, since this hardwired flag is a switc b/w annual Bond biomass burning emissions, and default GC source, which can be monthly/8 days/3hr.

 Implement changes for reading new Bond files (eml, phs, 5/18/09)
- (23) Add option for non-local PBL scheme (lin, 06/09/08)
- (24) Now added NESTED_EU grid. Updated formulation of SOG condensation onto OC aerosol, according to recommendations of Aerosol Working Group. (amv, clh, bmy, 12/21/09)
- (25) Bug fix for EMIS_SAVE in EMITHIGH (bmy, 1/11/10)
- (26) Modifications for TOMAS (win, bmy, 1/25/10)
- (27) Bug fix: call SOA_PARA_INIT (ensberg, bmy, 6/30/10)
- (28) Modified to include GFED3 (psk, 1/5/11)
- 01 Mar 2012 R. Yantosca Now reference new grid_mod.F90
- 30 Jul 2012 R. Yantosca Modifications for grid-independence
- 28 Nov 2012 R. Yantosca Replace SUNCOS array with State_Met%SUNCOS and SUNCOS_MID array with State_Met%SUNCOSmid
- 04 Mar 2013 R. Yantosca Now call INIT_CARBON from the init stage which facilitates connection to GEOS-5 GCM
- 05 Mar 2013 R. Yantosca Remove reference to LNLPBL from logical_mod.F and replace with Input_Opt%LNLPBL
- 13 Aug 2013 M. Sulprizio- Add modifications for updated SOA and SOA + semivolatile POA simulations (H. Pye)
- 20 Aug 2013 M. Sulprizio- Added ProTeX headers
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 20 Jun 2014 R. Yantosca Removed obsolete code; we now use HEMCO
- 23 Sep 2014 M. Sulprizio- Get OH, NO3, and O3 fields for offline aerosol simulation from HEMCO
- 06 Nov 2014 M. Yannetti Added PRECISION_MOD
- 13 Nov 2014 C. Keller Added EMISSCARBON to make sure that SESQ and POA emissions are properly passed from HEMCO.
- 05 Jan 2016 E. Lundgren Use global physical parameters (AIRMW and AVO)

```
14 Jan 2016 - M. Sulprizio- POAEMISS(:,:,:,1) now represents POG1 and
                            POAEMISS(:,:,:,2) now represents POG2
17 Jun 2016 - J.D.Maaasakkers - Now use Ind_ to define species ID's
17 Jun 2016 - R. Yantosca - Now declare all species ID's as module
                            variables, and initialize them at startup
28 Jun 2016 - M. Sulprizio- Add species ID's for L*RO2N/H and LISOP* to
                            replace uses of IL*RO2N/H and ILISOP* from
                            comode_loop_mod.F
```

8.2.1 chemcarbon

Subroutine CHEMCARBON is the interface between the GEOS-Chem main program and the carbon aerosol chemistry routines that calculates dry deposition, chemical conversion between hydrophilic and hydrophobic, and SOA production.

INTERFACE:

```
SUBROUTINE CHEMCARBON( am_I_Root, Input_Opt,
&
                        State_Met, State_Chm, RC )
```

```
USES:
      USE CMN_SIZE_MOD
      USE ErrCode_Mod
      USE ERROR_MOD,
                               ONLY : DEBUG_MSG
      USE ERROR_MOD,
                               ONLY : ERROR_STOP
      USE HCO_INTERFACE_MOD, ONLY : HcoState
      USE HCO_EMISLIST_MOD,
                               ONLY : HCO_GetPtr
      USE Input_Opt_Mod,
                               ONLY : OptInput
      USE State_Chm_Mod,
                               ONLY : ChmState
      USE State_Met_Mod,
                               ONLY : MetState
      USE TIME_MOD,
                               ONLY : ITS_A_NEW_MONTH
 #if
       defined( TOMAS )
       USE TOMAS_MOD,
                               ONLY : IBINS
                                                                   !(win, 1/25/10)
 #endif
```

INPUT PARAMETERS:

```
:: am_I_Root ! Is this the root CPU?
LOGICAL,
               INTENT(IN)
TYPE(OptInput), INTENT(IN)
                             :: Input_Opt
                                            ! Input Options object
TYPE(MetState), INTENT(IN)
                             :: State_Met
                                            ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm
                                            ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER,
               INTENT(OUT) :: RC
                                           ! Success or failure?
```

REMARKS:

REVISION HISTORY:

```
01 Apr 1994 - R. Park - Initial version
```

- (1) Added code from the Caltech group for SOA chemistry. Also now reference "global_oh_mod.f", "global_o3_mod.f", "global_no3_mod.f". (rjp, bmy, 7/8/04)
- (2) Now reference LSOA and LEMIS from CMN_SETUP. Now only call OHNO3TIME if it hasn't been done before w/in EMISSCARBON. (rjp, bmy, 7/15/04)
- (3) Now reference LSOA, LEMIS, LPRT from "logical_mod.f". Now reference STT and ITS_AN_AEROSOL_SIM from "tracer_mod.f" (bmy, 7/20/04)
- (4) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (5) Now updated for SOA production from ISOP. (dkh, bmy, 6/1/06)
- (6) Bug fix for aerosol sim w/ 20 tracers (phs, 9/14/06)
- (7) Add subroutine call AGING_CARB for converting H-phobic 30-bin EC or OC to H-philic EC or OC. (win, 1/25/10)
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 14 Nov 2012 R. Yantosca Add am_I_Root, Input_Opt, RC as arguments
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 15 Nov 2012 R. Yantosca Added ProTeX headers
- 04 Mar 2013 R. Yantosca Remove call to INIT_CARBON
- 04 Mar 2013 R. Yantosca Now pass Input_Opt to SOA_CHEMISTRY
- 25 Mar 2013 M. Payer Now pass State_Chm object via the arg list
- 13 Aug 2013 M. Sulprizio- Add modifications for updated SOA and SOA + semivolatile POA simulations (H. Pye)
- 23 Oct 2013 R. Yantosca Now pass objects to GET_GLOBAL_OH routine
- 23 Sep 2014 M. Sulprizio- Get OH, NO3, and O3 fields for offline aerosol simulation from HEMCO
- 16 Jun 2016 J.D.Maasakkers- Now define species ID's with Ind_ function
- 23 Jun 2016 R. Yantosca Add more error checks to make sure each id_* species flag is defined before using it
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.
- 10 Aug 2016 R. Yantosca Remove temporary tracer-removal code

8.2.2 chem_bcpo

Subroutine CHEM_BCPO converts hydrophobic BC to hydrophilic BC and calculates the dry deposition of hydrophobic BC.

INTERFACE:

```
SUBROUTINE CHEM_BCPO( am_I_Root, Input_Opt, TC, RC)
```

```
USE CMN_DIAG_MOD
USE CMN_SIZE_MOD
```

USE DIAG_MOD, ONLY : ADO7_BC

USE ErrCode_Mod

USE Input_Opt_Mod, ONLY : OptInput
USE TIME_MOD, ONLY : GET_TS_CHEM

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options

INPUT/OUTPUT PARAMETERS:

REAL(fp), INTENT(INOUT) :: TC(IIPAR, JJPAR, LLPAR) ! H-phobic BC [kg]

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success?

REMARKS:

Drydep is now applied in mixing_mod.F90.

REVISION HISTORY:

- 01 Apr 2004 R. Park Initial version
- (1) Remove reference to "CMN", it's obsolete (bmy, 7/20/04)
- (2) Replace PBLFRAC from "drydep_mod.f" with GET_FRAC_UNDER_PBLTOP from "pbl_mix_mod.f" (bmy, 2/17/05)
- (3) Now references XNUMOL from "tracer_mod.f" (bmy, 10/25/05)
- (4) Add option for non-local PBL scheme (lin, 06/09/08)
- 01 Mar 2012 R. Yantosca Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
- 14 Nov 2012 R. Yantosca Add am_I_Root, Input_Opt, RC as arguments
- 26 Nov 2012 R. Yantosca Added ProTeX headers
- 05 Mar 2013 R. Yantosca Now use Input_Opt%LNLPBL
- 19 Mar 2013 R. Yantosca Now copy Input_Opt%XNUMOL(1:N_TRACERS)
- 04 Mar 2015 C. Keller Now do dry dep in mixing_mod.F90
- 12 Jun 2015 R. Yantosca Remove orphaned ND44 drydep variables
- 12 Jun 2015 R. Yantosca Drydep is now handled in mixing_mod.F90,

so we can greatly collapse this code

23 Sep 2015 - R. Yantosca - Remove reference to DRYBCPO, it's obsolete

8.2.3 chem_bcpi

Subroutine CHEM_BCPI calculates dry deposition of hydrophilic BC.

INTERFACE:

SUBROUTINE CHEM_BCPI(am_I_Root, Input_Opt, TC, RC)

USES:

```
USE CMN_DIAG_MOD

USE CMN_SIZE_MOD

USE ErrCode_Mod

USE Input_Opt_Mod, ONLY : OptInput
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options
```

INPUT/OUTPUT PARAMETERS:

```
REAL(fp), INTENT(INOUT) :: TC(IIPAR, JJPAR, LLPAR) ! H-philic BC [kg]
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success?
```

REMARKS:

Drydep is now applied in mixing_mod.F90.

REVISION HISTORY:

- 01 Apr 2004 R. Park Initial version
- (1) Remove reference to "CMN", it's obsolete (bmy, 7/20/04)
- (3) Now references XNUMOL from "tracer_mod.f" (bmy, 10/25/05)
- 01 Mar 2012 R. Yantosca Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
- 14 Nov 2012 R. Yantosca Add am_I_Root, Input_Opt, RC as arguments
- 26 Nov 2012 R. Yantosca Added ProTeX Headers
- 05 Mar 2013 R. Yantosca Now use Input_Opt%LNLPBL
- 19 Mar 2013 R. Yantosca Now copy Input_Opt%XNUMOL(1:N_TRACERS)
- 04 Mar 2015 C. Keller Now do dry dep in mixing_mod.F90
- 12 Jun 2015 R. Yantosca Remove orphaned ND44 drydep variables
- 12 Jun 2015 R. Yantosca Drydep is now handled in mixing_mod.F90,

so we can greatly collapse this code

23 Sep 2015 - R. Yantosca - Remove reference to DRYBCPI, it's obsolete

8.2.4 chem_ocpo

Subroutine CHEM_OCPO converts hydrophobic OC to hydrophilic OC and calculates the dry deposition of hydrophobic OC.

INTERFACE:

```
SUBROUTINE CHEM_OCPO( am_I_Root, Input_Opt, TC, RC)
```

USES:

USE CMN_DIAG_MOD
USE CMN_SIZE_MOD

USE DIAG_MOD, ONLY : ADO7_OC

USE ErrCode_Mod

USE Input_Opt_Mod, ONLY : OptInput
USE TIME_MOD, ONLY : GET_TS_CHEM

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Root CPU?
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options

INPUT/OUTPUT PARAMETERS:

REAL(fp), INTENT(INOUT) :: TC(IIPAR, JJPAR, LLPAR) ! H-phobic OC [kg]

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success?

REMARKS:

REVISION HISTORY:

- 01 Apr 2004 R. Park Initial version
- (1) Remove reference to "CMN", it's obsolete (bmy, 7/20/04)
- (2) Replace PBLFRAC from "drydep_mod.f" with GET_FRAC_UNDER_PBLTOP from "pbl_mix_mod.f" (bmy, 2/17/05)
- (3) Now references XNUMOL from "tracer_mod.f" (bmy, 10/25/05)
- 01 Mar 2012 R. Yantosca Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
- 14 Nov 2012 R. Yantosca Add am_I_Root, Input_Opt, RC as arguments
- 26 Nov 2012 R. Yantosca Added ProTeX headers
- 05 Mar 2013 R. Yantosca Now use Input_Opt%LNLPBL
- 19 Mar 2013 R. Yantosca Now copy Input_Opt%XNUMOL(1:N_TRACERS)
- 04 Mar 2015 C. Keller Now do dry dep in mixing_mod.F90
- 12 Jun 2015 R. Yantosca Remove orphaned ND44 drydep variables
- 23 Sep 2015 R. Yantosca Remove reference to DRYOCPO, it's obsolete

8.2.5 chem_ocpi

Subroutine CHEM_BCPI calculates dry deposition of hydrophilic OC.

INTERFACE:

SUBROUTINE CHEM_OCPI(am_I_Root, Input_Opt, TC, RC)

USE CMN_DIAG_MOD USE CMN_SIZE_MOD USE ErrCode_Mod

USE Input_Opt_Mod, ONLY : OptInput
USE TIME_MOD, ONLY : GET_TS_CHEM

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Root CPU?
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options

INPUT/OUTPUT PARAMETERS:

REAL(fp), INTENT(INOUT) :: TC(IIPAR, JJPAR, LLPAR) ! H-philic OC [kg]

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success?

REMARKS:

REVISION HISTORY:

- 01 Apr 2004 R. Park Initial version
- (1) Remove reference to "CMN", it's obsolete (bmy, 7/20/04)
- (2) Replace PBLFRAC from "drydep_mod.f" with GET_FRAC_UNDER_PBLTOP from "pbl_mix_mod.f" (bmy, 2/17/05)
- (3) Bug fix: add BL_FRAC to the PRIVATE list (mak, bmy, 10/3/05)
- (4) Now refrerences XNUMOL from "tracer_mod.f" (bmy, 10/25/05)
- 01 Mar 2012 R. Yantosca Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
- 14 Nov 2012 R. Yantosca Add am_I_Root, Input_Opt, RC as arguments
- 26 Nov 2012 R. Yantosca Added ProTeX headers
- 05 Mar 2013 R. Yantosca Now use Input_Opt%LNLPBL
- 19 Mar 2013 R. Yantosca Now copy Input_Opt%XNUMOL(1:N_TRACERS)
- 04 Mar 2015 C. Keller Now do dry dep in mixing_mod.F90
- 12 Jun 2015 R. Yantosca Remove orphaned ND44 drydep variables
- 23 Sep 2015 R. Yantosca Remove reference to DRYOCPI, it's obsolete

8.2.6 aging_carb

Subroutine AGING_CARB converts the size-resolved hydrophobic EC or OC to hydrophilic EC or OC with an assumed e-folding time. (win, 9/11/07)

INTERFACE:

SUBROUTINE AGING_CARB(MIL, MOB)

```
USE CMN_SIZE_MOD
```

USE TIME_MOD,

ONLY : IBINS USE TOMAS_MOD,

INPUT/OUTPUT PARAMETERS:

```
REAL(fp), INTENT(INOUT) :: MIL(IIPAR, JJPAR, LLPAR, IBINS)
REAL(fp), INTENT(INOUT) :: MOB(IIPAR, JJPAR, LLPAR, IBINS)
```

REMARKS:

```
20 Aug 2013 - M. Sulprizio- Added ProTeX headers
```

8.2.7soag_liggio_diff

Subroutine SOAG_LIGGIO_DIFF produces SOA on aqueous aerosol surfaces from GLYX following the uptake model used for N2O5, and the gamma from Liggio et al. [2005]. (tmf, 5/30/06)

INTERFACE:

```
SUBROUTINE SOAG_LIGGIO_DIFF( am_I_Root, Input_Opt,
                             State_Met, State_Chm, RC )
```

USES:

```
USE CMN_DIAG_MOD
USE CMN_03_MOD
USE CMN_SIZE_MOD
```

USE DIAG_MOD, ONLY : ADO7_SOAGM

USE ErrCode_Mod

USE Input_Opt_Mod, ONLY: DEBUG_MSG
USE State_Met_Mod, ONLY: OptInput
USE State_Met_Mod, ONLY: " ONLY : DEBUG_MSG USE State_Chm_Mod, ONLY : ChmState

USE TIME_MOD, ONLY : GET_TS_CHEM, GET_MONTH

INPUT PARAMETERS:

```
LOGICAL.
               INTENT(IN)
                              :: am_I_Root
                                            ! Are we on the root CPU?
TYPE(OptInput), INTENT(IN)
                              :: Input_Opt    ! Input Options object
TYPE(MetState), INTENT(IN)
                              :: State_Met
                                             ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTENT(OUT) :: RC ! Success or failure? INTEGER,

REMARKS:

(1) SOAG (SOA product of GLYX is produced at existing hydrophilic aerosol surface.

REVISION HISTORY:

```
09 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met
derived type object
25 Mar 2013 - M. Payer - Now pass State_Chm object via the arg list
20 Aug 2013 - M. Sulprizio- Added ProTeX headers
21 Dec 2015 - M. Sulprizio- Get air density directly from State_Met
12 May 2016 - M. Sulprizio- Remove 1D arrays that depend on JLOOP. WERADIUS,
WTAREA are now pointers that point to 3D fields
in State_Chm.
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected
species ID from State_Chm%Map_Advect.
```

8.2.8 soam_liggio_diff

Subroutine SOAM_LIGGIO_DIFF produces SOA on aqueous aerosol surfaces from GLYX following the uptake model used for N2O5, and the gamma from Liggio et al. [2005]. (tmf, 5/30/06)

INTERFACE:

```
SUBROUTINE SOAM_LIGGIO_DIFF( am_I_Root, Input_Opt,
& State_Met, State_Chm, RC )
```

USES:

```
USE CMN_O3_MOD

USE CMN_SIZE_MOD

USE DIAG_MOD, ONLY : ADO7_SOAGM

USE ErrCode_Mod

USE ERROR_MOD, ONLY : DEBUG_MSG

USE Input_Opt_Mod, ONLY : OptInput

USE State_Met_Mod, ONLY : MetState

USE State_Chm_Mod, ONLY : ChmState

USE TIME_MOD, ONLY : GET_TS_CHEM, GET_MONTH
```

INPUT PARAMETERS:

USE CMN_DIAG_MOD

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

(1) SOAM (SOA product of MGLY) is produced at existing hydrophilic aerosol surface.

REVISION HISTORY:

```
09 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met derived type object

5 Mar 2013 - R. Yantosca - Now accept am_I_Root, Input_Opt arguments

25 Mar 2013 - M. Payer - Now pass State_Chm object via the arg list

20 Aug 2013 - M. Sulprizio- Added ProTeX headers

21 Dec 2015 - M. Sulprizio- Get air density directly from State_Met

12 May 2016 - M. Sulprizio- Remove 1D arrays that depend on JLOOP. WERADIUS, WTAREA are now pointers that point to 3D fields in State_Chm.

30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.
```

8.2.9 soa_chemistry

Subroutine SOA_CHEMISTRY performs SOA formation. This code is from the Caltech group (Hong Liao, Serena Chung, et al) and was modified for GEOS-CHEM. (rjp, bmy, 7/8/04, 12/21/09)

ONLY : ITS_IN_THE_NOCHEMGRID

INTERFACE:

```
SUBROUTINE SOA_CHEMISTRY( am_I_Root, Input_Opt,
& State_Met, State_Chm, RC )
```

USES:

```
USE CMN_DIAG_MOD
USE CMN_03_MOD
USE CMN_SIZE_MOD
USE DIAG_MOD,
                        ONLY: ADO7_HC
USE ErrCode_Mod
USE ERROR_MOD,
                        ONLY : DEBUG_MSG
USE Input_Opt_Mod,
                        ONLY : OptInput
USE State_Met_Mod,
                        ONLY : MetState
                        ONLY : ChmState
USE State_Chm_Mod,
USE TIME_MOD,
                        ONLY : GET_TS_CHEM,
                                                 GET_MONTH
USE TIME_MOD,
                        ONLY : ITS_TIME_FOR_BPCH
```

INPUT PARAMETERS:

USE CHEMGRID_MOD,

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

Procedure:

- (1) Read in NO3, O3, OH in CHEM_SOA
- (2) Scales these fields using OHNO3TIME in sulfate_mod.f (see GET_OH)
- (3) Calculate reaction rates (Serena's OCHEMPARAETER)
- (4) CALCULATE DELHC
- (5) get TOM gas products
- (6) equilibrium calculation

As of 5/20/10: Havala's New formulation

The parent hydrocarbons are lumped into 5 semivolatile systems:

TSOA/G: the lumped semivolatile oxidation products of monoterpene and sesquiterpene oxidation

ISOA/G: the lumped semivolatile oxidation products of isoprene ox ASOA/G: the lumped semivolatile (and nonvolatile) products of

benzene, toluene, xylene, and naphthalene (IVOC surrogate)

oxidation

POA/G : the lumped primary semivolatile emissions

OPOA/G: the lumped products of primary semivolatile oxidation

Parent HC	Oxidized by	Products
=========	===========	
MTPA	OH, O3, NO3	TSOA/GO-3
LIMO	OH, O3, NO3	TSOA/G1-3
MTPO	OH, O3, NO3	TSOA/GO-3
SESQ	OH, O3, NO3	TSOA/G1-3
ISOP	OH, NO3	ISOA/G1-3
BENZ	OH, (+NO,HO2)	ASOAN, ASOA/G1-3

TOLU	OH, (+NO,HO2)	ASOAN, ASOA/G1-3
XYLE	OH, (+NO,HO2)	ASOAN, ASOA/G1-3
SVOC/POA	OH	POA/G1-2
O-SVOC/OPOA	OH	OPOA/G1-2
NAP	OH, (+NO,HO2)	ASOAN, ASOA/G1-3

Species that must be defined in input.geos (in addition to standard full chem species) (34 additional):

_ u u	Proces,	(0				
TSOA1	TSOG1	ISOA1	ISOG1	ASOA1	ASOG1	
TSOA2	TSOG2	ISOA2	ISOG2	ASOA2	ASOG2	
TSOA3	TSOG3	ISOA3	ISOG3	ASOA3	ASOG3	
ASOAN	TSOAO	TSOGO				
BENZ	TOLU	XYLE	MTPA	LIMO	MTPO	
NAP						
POA1	POG1	POA2	POG2			
OPOA1	OPOG1	OPOA2	OPOG2			

The following should NOT be defined for semivol POA: OCPI, OCPO

Two non-volatile, traditional primary OC species exist:

OCPO: hydrophobic POA OCPI: hydrophillic POA

The parent hydrocarbons are lumped into 3 semivolatile systems:

TSOA/G: the lumped semivolatile oxidation products of monoterpene and sesquiterpene oxidation

ISOA/G: the lumped semivolatile oxidation products of isoprene ox ASOA/G: the lumped semivolatile (and nonvolatile) products of benzene, toluene, and xylene oxidation

Parent HC	Oxidized by	Products
=========	=======================================	
MTPA	OH, O3, NO3	TSOA/GO-3
LIMO	OH, O3, NO3	TSOA/G1-3
MTPO	OH, O3, NO3	TSOA/GO-3
SESQ	OH, O3, NO3	TSOA/G1-3
ISOP	OH, NO3	ISOA/G1-3
BENZ	OH, (+NO,HO2)	ASOAN, ASOA/G1-3
TOLU	OH, (+NO,HO2)	ASOAN, ASOA/G1-3
XYLE	OH, (+NO,HO2)	ASOAN, ASOA/G1-3

Species that must be defined in input.geos (in addition to standard

```
full chem species) (25 additional):
TSOA1
          TSOG1
                     ISOA1
                                ISOG1
                                           ASOA1
                                                     ASOG1
                                TSOG2
TSOA2
          TSOG2
                     TSOA2
                                           ASOA2
                                                     ASDG2
TSOA3
          TSOG3
                     ISOA3
                                ISOG3
                                           ASOA3
                                                     ASOG3
ASOAN
          TSOAO
                     TSOGO
BENZ
          TOLU
                     XYLE
                                          LIMO
                                MTPA
                                                     MTPO
The following should NOT be defined for traditional POA:
   NAP, POA/G OPOA/G
References (see above for full citations):
_____
Monoterpenes and sesquiterpenes:
  Experimental Data:
   Griffin et al. 1999 JGR
                                (sesquiterps low NOx)
                                (a-pinene ozonolysis for MTPO/MTPA)
   Shilling et al. 2008 ACP
   Zhang et al. 2006 JPhysChemA (limonene ozonolysis)
   Ng et al. 2007 ACP
                                (data for NOx effect on sesq aerosol)
  Modeling:
                                (original formulation in GEOS-Chem)
   Chung and Seinfeld 2002 JGR
                                (comparison to measurements)
   Liao et al. 2007 JGR
                                (new lumping scheme, NOx effect)
   Pye et al. in prep 2010
Isoprene
   Kroll et al. 2006 ES&T
                                (low NOx experiments)
   Ng et al. 2008 ACP
                                (isoprene + NO3 experiments)
   Henze et al. 2006 GRL
                                (low NOx isoprene modeling in GEOS-Chem)
   Pye et al. in prep 2010
                                (new lumping scheme and isop+no3 modeling)
Aromatics: benz, tolu, xyle
   Ng et al. 2007 ACP
                                (experiments)
   Henze et al. 2008 ACP
                                (global modeling)
POA/OPOA
   Shrivastava et al. 2006 ES&T (POA experiments)
   Grieshop et al. 2009 ACP
                                (POA/SVOC oxidation experiments)
   Pye and Seinfeld 2010 ACP
                                (global modeling)
IVOC/Naphthalene
   Chan et al. 2009 ACP
                                (experiments)
                                (global modeling)
   Pye and Seinfeld 2010 ACP
```

- (1) Now references STT from "tracer_mod.f" (bmy, 7/20/04)
- (2) Now modified for SOG4, SOA4 -- products of oxidation by isoprene. (dkh, bmy, 6/1/06)
- (3) Now consider SOG condensation onto SO4, NH4, NIT aerosols (if SO4, NH4, NIT are defined as tracers). (rjp, bmy, 8/3/06)
- (4) Updated formulation of SOG condensation onto OC aerosol, according to recommendations of Aerosol Working Group (clh, bmy, 12/21/09)
- (5) Now only print out debug info when LPRT=T (bmy, 4/21/10)

```
(6) Bug fix: call SOA_PARA_INIT (ensberg, bmy, 6/30/10)
05 Oct 2011 - R. Yantosca - SUNCOS is not needed, so remove
30 Jul 2012 - R. Yantosca - Now accept am_I_Root as an argument when
                            running with the traditional driver main.F
09 Nov 2012 - M. Payer
                          - Replaced all met field arrays with State_Met
                            derived type object
05 Mar 2013 - R. Yantosca - Now pass Input_Opt to SOA_DEPO
05 Mar 2013 - R. Yantosca - Now use Input_Opt%LPRT
                         - Now pass State_Chm object via the arg list
25 Mar 2013 - M. Payer
13 Aug 2013 - M. Sulprizio- Add modifications for updated SOA and SOA +
                            semivolatile POA simulations (H. Pye)
20 Aug 2013 - M. Sulprizio- Added ProTeX headers
12 Jun 2015 - R. Yantosca - Removed SOA_DEPO; ND44 is now done in mixing_mod
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected
                            species ID from State_Chm%Map_Advect.
```

8.2.10 soa_equil

Function SOA_EQUIL solves SOAeqn=0 to determine Mnew (= mass) See Eqn (27) on page 70 of notes. Originally written by Serena Chung at Caltech, and modified for inclusion into GEOS-CHEM. (rjp, bmy, 7/8/04)

INTERFACE:

```
FUNCTION SOA_EQUIL( MASS, MPOC, AEROSOL, GAS, KOM )
& RESULT( SOA_MASS )
```

INPUT/OUTPUT PARAMETERS:

RETURN VALUE:

REAL(fp) :: SOA_MASS

REMARKS:

This version does NOT assume that the gas and aerosol phases are in equilibrium before chemistry; therefore, gas phase concentrations are needed explicitly. The gas and aerosol phases are assumed to be in equilibrium after chemistry.

Note: Unlike FUNCTION SOA, this function assumes no reactions. It only considers the partitioning of existing products of VOC oxidation.

```
HC_JHC + OXID_IOXID - >
     alpha(1,IOXID,JHC) [SOAprod_gas(1,IOXID,JHC)+SOAprod(1,IOXID,JHC)]+
     alpha(2,IOXID,JHC) [SOAprod_gas(2,IOXID,JHC)+SOAprod(2,IOXID,JHC)]
   SOAprod_gas(IPR,IOXID,JHC) <--> SOAprod(IPR,IOXID,JHC)
                                            (aerosol phase)
   w/ equilibrium partitioning:
                                    SOAprod(IPR, IOXID, JHC)
     SOAprod_gas(IPR,IOXID,JHC) = -----
                                      Kom(IPR,IOXID,JHC)
   NOTES:
   13 Aug 2013 - M. Sulprizio- Add modifications for updated SOA and SOA +
                               semivolatile POA simulations (H. Pye)
    20 Aug 2013 - M. Sulprizio- Added ProTeX headers
8.2.11 zeroin
Function ZEROIN computes a zero of the function f(x) in the interval ax,bx.
INTERFACE:
      FUNCTION ZEROIN(AX, BX, TOL, MPOC, AEROSOL, GAS, KOM) RESULT( MNEW )
INPUT PARAMETERS:
      REAL(fp), INTENT(IN) :: ax
      REAL(fp), INTENT(IN) :: bx
      REAL(fp), INTENT(IN) :: tol
      REAL(fp), INTENT(IN) :: Mpoc
      REAL(fp), INTENT(IN) :: Aerosol(MPROD,MSV)
      REAL(fp), INTENT(IN) :: Gas(MPROD,MSV)
      REAL(fp), INTENT(IN) :: Kom(MPROD,MSV)
RETURN VALUE:
      REAL(fp)
                     :: MNEW
REMARKS:
  NOTE: This function may be problematic -- it uses GOTO's, which are not
  good for parallelization. (bmy, 7/8/04)
  shc I got this code from http://www.netlib.org
```

a zero of the function f(x) is computed in the interval ax,bx.

input..

ax left endpoint of initial interval

bx right endpoint of initial interval

f function subprogram which evaluates f(x) for any x in the interval ax,bx

tol desired length of the interval of uncertainty of the final result (.ge. 0.0e+0_fp)

output..

zeroin abcissa approximating a zero of f in the interval ax,bx

it is assumed that f(ax) and f(bx) have opposite signs without a check. zeroin returns a zero x in the given interval ax,bx to within a tolerance 4*macheps*abs(x) + tol, where macheps is the relative machine precision.

this function subprogram is a slightly modified translation of the algol 60 procedure zero given in richard brent, algorithms for minimization without derivatives, prentice - hall, inc. (1973).

REVISION HISTORY:

- (1) Change dabs to ABS and dsign to SIGN, in order to avoid conflicts with intrinsic function names on the PGI compiler. (bmy, 12/2/04)
- 13 Aug 2013 M. Sulprizio- Add modifications for updated SOA and SOA + semivolatile POA simulations (H. Pye)
- 20 Aug 2013 M. Sulprizio- Added ProTeX headers

8.2.12 rtbis

Function RTBIS finds the root of the function SOA_EQUIL via the bisection method. Original algorithm from "Numerical Recipes" by Press et al, Cambridge UP, 1986. Modified for inclusion into GEOS-CHEM. (bmy, 7/8/04)

INTERFACE:

```
FUNCTION RTBIS( X1, X2, XACC, & MPOC, AEROSOL, GAS, KOM ) RESULT( ROOT )
```

USES:

USE ERROR_MOD, ONLY : ERROR_STOP

INPUT PARAMETERS:

REAL(fp), INTENT(IN) :: X1 ! Endpoint #1

```
REAL(fp), INTENT(IN) :: X2 ! Endpoint #2

REAL(fp), INTENT(IN) :: XACC ! Desired accuracy of solution

REAL(fp), INTENT(IN) :: MPOC ! POA mass [ug/m3]

REAL(fp), INTENT(IN) :: AEROSOL(MPROD,MSV) ! Aerosol concentration [ug/m3]

REAL(fp), INTENT(IN) :: GAS(MPROD,MSV) ! Gas-phase concentration [ug/m3]

REAL(fp), INTENT(IN) :: KOM(MPROD,MSV) ! Equilibrium gas-aerosol

! partition coeff. [m3/ug]
```

RETURN VALUE:

REAL(fp) :: ROOT

REVISION HISTORY:

```
13 Aug 2013 - M. Sulprizio- Add modifications for updated SOA and SOA + semivolatile POA simulations (H. Pye)
20 Aug 2013 - M. Sulprizio- Added ProTeX headers
```

8.2.13 soa_para

Subroutine SOA_PARA gves mass-based stoichiometric coefficients for semi-volatile products from the oxidation of hydrocarbons. It calculates secondary organic aerosol yield parameters. Temperature effects are included. Original code from the CALTECH group and modified for inclusion to GEOS-CHEM. (rjp, bmy, 7/8/04, 6/30/08)

INTERFACE:

```
SUBROUTINE SOA_PARA( TEMP, KO3, KOH, KNO3, KOM, & II, JJ, LL, KRO2NO, KRO2HO2, State_Met )
```

USES:

USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

```
! Arguments

INTEGER, INTENT(IN) :: II ! Longitude index

INTEGER, INTENT(IN) :: JJ ! Latitude index

INTEGER, INTENT(IN) :: LL ! Altitude index

REAL(fp), INTENT(IN) :: TEMP ! Temperature [k]

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

OUTPUT PARAMETERS:

REAL(fp),	<pre>INTENT(OUT) :: KO3(MHC)</pre>	! Rxn rate for HC oxidation
		! by O3 [cm3/molec/s]
REAL(fp),	<pre>INTENT(OUT) :: KOH(MHC)</pre>	! Rxn rate for HC oxidation
		! by OH [cm3/molec/s]
REAL(fp),	<pre>INTENT(OUT) :: KNO3(MHC)</pre>	! Rxn rate for HC oxidation
		! by NO3 [cm3/molec/s]

REAL(fp), INTENT(OUT) :: KOM(MPROD, MSV) ! Equilibrium gas-aerosol ! partition coeff [m3/ug]

! RO2+NO, HO2 rate constants (hotp 5/7/10)

REAL(fp), INTENT(OUT) :: KRO2NO ! RO2+NO rate constant REAL(fp), INTENT(OUT) :: KRO2HO2 ! RO2+HO2 rate constant

REMARKS:

References:

PHOTO-OXIDATION RATE CONSTANTS OF ORGANICS come from:

- (1) Atkinson, el al., Int. J. Chem. Kinet., 27: 941-955 (1995)
- (2) Shu and Atkinson, JGR 100: 7275-7281 (1995)
- (3) Atkinson, J. Phys. Chem. Ref. Data 26: 215-290 (1997)
- (4) Some are reproduced in Table 1 of Griffin, et al., JGR 104: 3555-3567
- (5) Chung and Seinfeld (2002)

ACTIVATION ENERGIES come from:

- (6) Atkinson, R. (1994) Gas-Phase Tropospheric Chemistry of Organic Compounds. J. Phys. Chem. Ref. Data, Monograph No.2, 1-216.
- (7) They are also reproduced in Tables B.9 and B.10 of Seinfeld and Pandis (1988).

PARAMETERS FOR ISOPRENE:

- (8) Kroll et al., GRL, 109, L18808 (2005)
- (9) Kroll et al., Environ Sci Tech, in press (2006)
- (10) Henze and Seinfeld, GRL, submitted (2006)

- (1) Now use temporary variables TMP1, TMP2, TMP3 to pre-store the values of exponential terms outside of DO-loops (bmy, 7/8/04)
- (2) Add parameters for isoprene. Now include grid cell location in subroutine arguments. Define a reference temperature at 295. Now use ITS_IN_THE_TROP to determine if we are in a tropospheric grid box. Now pass II, JJ, LL via the argument list. (dkh, bmy, 5/22/06)
- (3) Corrected confusing documentation. (clh, bmy, 6/30/08)
- (4) Add paramters for aromtics. Add high NOx low NOx index to every parameter, NNOX (dkh, 10/29/06)
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 13 Aug 2013 M. Sulprizio- Add modifications for updated SOA and SOA + semivolatile POA simulations (H. Pye)
- 20 Aug 2013 M. Sulprizio- Added ProTeX headers

8.2.14 soa_para_init

Subroutine SOA_PARA_INIT initializes the ALPHAS and KOMS, the latter at their reference temperature. It is faster to define these separately as it only needs to be done once. (dkh, 11/12/06)

INTERFACE:

```
SUBROUTINE SOA_PARA_INIT( Input_Opt )
```

USES:

INPUT PARAMETERS:

```
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

REMARKS:

NOTE: REFT for KOM_REF depends on hydrocarbon.

REVISION HISTORY:

```
20 Aug 2013 - M. Sulprizio- Added ProTeX headers
```

8.2.15 chem_nvoc

Subroutine CHEM_NVOC computes the oxidation of Hydrocarbon by O3, OH, and NO3. This comes from the Caltech group (Hong Liao, Serena Chung, et al) and was incorporated into GEOS-CHEM. (rjp, bmy, 7/6/04,6/1/06)

INTERFACE:

```
SUBROUTINE CHEM_NVOC( I, J, L, & KO3, KOH, KNO3, & GMO, KNO, KHO2, & Input_Opt, State_Met, State_Chm, RC)
```

USES:

```
USE CMN_DIAG_MOD

USE CMN_SIZE_MOD

USE DIAG_MOD, ONLY : ADO7_HC

USE ErrCode_Mod

USE Input_Opt_Mod, ONLY : OptInput

USE State_Met_Mod, ONLY : MetState

USE State_Chm_Mod, ONLY : ChmState

USE TIME_MOD, ONLY : GET_TS_CHEM, GET_MONTH
```

INPUT PARAMETERS:

```
INTEGER,
               INTENT(IN)
                              :: I
                                              ! Longitude index
INTEGER,
               INTENT(IN)
                              :: J
                                              ! Latitude index
INTEGER,
                             :: L
                                              ! Altitude index
               INTENT(IN)
                                              ! Rxn rate for HC oxidation
REAL(fp),
               INTENT(IN) :: KO3(MHC)
                                              ! by O3 [cm3/molec/s]
REAL(fp),
               INTENT(IN)
                             :: KOH(MHC)
                                              ! Rxn rate for HC oxidation
                                              ! by OH [cm3/molec/s]
                                              ! Rxn rate for HC oxidation
REAL(fp),
               INTENT(IN)
                             :: KNO3(MHC)
                                              ! by NO3 [cm3/molec/s]
! RO2+NO, RO2+HO2 rate constants (hotp 5/7/10)
REAL(fp),
               INTENT(IN)
                             :: KNO
                                              ! RO2+NO rate constant
REAL(fp),
               INTENT(IN)
                             :: KHO2
                                              ! RO2+HO2 rate constant
TYPE(OptInput), INTENT(IN)
                             :: Input_Opt
                                              ! Input Options object
                                              ! Meteorology State object
TYPE(MetState), INTENT(IN)
                             :: State_Met
```

INPUT/OUTPUT PARAMETERS:

```
REAL(fp), INTENT(INOUT) :: GMO(MPROD, MSV)! Gas mass for HCs and ! oxidation products [kg]
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

```
SVOCs should immediately partition upon emission
SVOCs also react in the gas-phase
If SVOCs were emitted before reactions, we wouldn't know how
much to put in each phase
H.O.T. Pye decided to emit them after the existing SVOCs
react in the gas-phase. Thus the order of operations is:
    SVOC + OH in gas-phase
    SVOC emission (added to gas-phase GMO)
    partitioning
    dry dep
    wet dep
    etc
```

- (1) Now references STT from "tracer_mod.f" (bmy, 7/20/04)
- (2) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (3) Updated for SOA from isoprene. Now calls GET_DOH. (dkh, bmy, 6/1/06)
- (4) Updated for SOA from aromatics. (dkh, 10/29/06)
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 13 Aug 2013 M. Sulprizio- Add modifications for updated SOA and SOA + semivolatile POA simulations (H. Pye)

```
20 Aug 2013 - M. Sulprizio- Added ProTeX headers

12 Dec 2014 - M. Yannetti - Changed DEXP to EXP for compatability

30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

22 Sep 2016 - R. Yantosca - Avoid array size mismatch for GLOB_DARO2
```

8.2.16 soa_partition

Subroutine SOA_PARTITION partitions the mass of gas and aerosol species according to five Hydrocarbon species and three oxidants. (rjp, bmy, 7/7/04, 5/22/06)

Revised purpose: SOA_PARTITION assigns the mass in the chemical species array to the GM0 and AM0 arrays (hotp 5/13/10)

INTERFACE:

```
SUBROUTINE SOA_PARTITION( I, J, L, GMO, AMO, State_Chm )
```

USES:

```
USE CMN_SIZE_MOD
USE State_Chm_Mod, ONLY : ChmState
```

INPUT PARAMETERS:

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT) :: GMO(MPROD, MSV) ! Gas mass for HCs and ! oxidation products [kg] REAL(fp), INTENT(OUT) :: AMO(MPROD, MSV) ! Aer mass for HCs and ! oxidation products [kg]
```

INPUT/OUTPUT PARAMETERS:

REMARKS:

NOTE: GPROD and APROD are mass ratios of individual oxidation products of gas/aerosol to the sum of all.

- (1) Now references STT from "tracer_mod.f" (bmy, 7/20/04)
- (2) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (3) Updated for SOG4, SOA4 (bmy, 5/22/06)
- 13 Aug 2013 M. Sulprizio- Add modifications for updated SOA and SOA +

semivolatile POA simulations (H. Pye)

- 20 Aug 2013 M. Sulprizio- Added ProTeX headers
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

8.2.17 soa_lump

Subroutine SOA_LUMP returns the organic gas and aerosol back to the STT array. (rjp, bmy, 7/7/04, 2/6/07)

INTERFACE:

SUBROUTINE SOA_LUMP(I, J, L, GMO, AMO, State_Chm)

USES:

USE CMN_DIAG_MOD

USE CMN_SIZE_MOD

USE DIAG_MOD, ONLY : ADO7_HC
USE State_Chm_Mod, ONLY : ChmState

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: I ! Longitude index
INTEGER, INTENT(IN) :: J ! Latitude index
INTEGER, INTENT(IN) :: L ! Altitude index

REAL(fp), INTENT(IN) :: GMO(MPROD, MSV) ! Gas mass for HCs and

! oxidation products [kg]

REAL(fp), INTENT(IN) :: AMO(MPROD, MSV) ! Aer mass for HCs and

! oxidation products [kg]

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

- (1) Now references STT from "tracer_mod.f" (bmy, 7/20/04)
- (2) Bug fix: make sure L <= LD07 before saving into AD07 array, or else we will get an out-of-bounds error. (bmy, 3/4/05)
- (3) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (4) Updated for SOG4, SOA4 (dkh, bmy, 5/22/06)
- (5) Typo fix: GPROD should be APROD in a couple places (tmf, bmy, 10/16/06)
- (6) Bug fix: For SOA4, GPROD and APROD should have default values of 0.5, instead of 1.0 (dkh, bmy, 2/6/07)
- 13 Aug 2013 M. Sulprizio- Add modifications for updated SOA and SOA + semivolatile POA simulations (H. Pye)
- 20 Aug 2013 M. Sulprizio- Added ProTeX headers
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

8.2.18 emitsgc

Subroutine EMITSGC calculates sub-grid coagulation for the size distribution of emission. (win, 10/6/07)

INTERFACE:

```
SUBROUTINE EMITSGC( EMISMASS, CTYPE, & Input_Opt, State_Met, State_Chm )
```

USES:

```
USE CMN_SIZE_MOD
USE CMN_DIAG_MOD
                             ! ND59
USE DIAG_MOD,
                        ONLY : AD59_ECIL,
                                            AD59_ECOB
USE DIAG_MOD,
                      ONLY : AD59_OCIL,
                                            AD59_OCOB
                       ONLY : AD59_NUMB
USE DIAG_MOD,
                     ONLY : IT_IS_NAN
ONLY : OptInput
ONLY : GET_FRAC_OF_PBL, GET_PBL_MAX_L
USE ERROR_MOD,
USE Input_Opt_Mod,
USE PBL_MIX_MOD,
USE State_Chm_Mod,
                        ONLY : ChmState
USE State_Met_Mod,
                       ONLY : MetState
USE TOMAS_MOD,
                       ONLY : IBINS,
                                                             IDIAG
                                        AVGMASS, ICOMP,
USE TOMAS_MOD,
                        ONLY: SRTECIL, SRTECOB, SRTOCIL
                      ONLY : SRTOCOB, SRTSO4,
USE TOMAS_MOD,
                                                   SRTNH4
USE TOMAS_MOD,
                      ONLY : SRTH2O,
                                         MNFIX
USE TOMAS_MOD,
                       ONLY : SUBGRIDCOAG
USE TOMAS_MOD,
                        ONLY: NH4BULKTOBIN
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: EMISMASS(IIPAR, JJPAR, IBINS)

INTEGER, INTENT(IN) :: CTYPE ! 1 = EC and 2 = OC

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

```
09 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met
derived type object
20 Aug 2013 - M. Sulprizio- Added ProTeX headers
26 Feb 2015 - E. Lundgren - Replace GET_PCENTER with State_Met%PMID and
remove dependency on pressure_mod.
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected
species ID from State_Chm%Map_Advect.
```

8.2.19 scalecarb

Function SCALECARB split the carbonaceous emission from each source into the TOMAS aerosol size bins using different mass distribution for fossil fuel and biomass burning+biofuel. The mass size distributions are different for EC and OC. (win, 9/4/07)

INTERFACE:

FUNCTION SCALECARB(BULKEMIS, STYPE, CTYPE) RESULT(VALUE)

USES:

```
USE CMN_SIZE_MOD
USE TOMAS_MOD, ONLY : IBINS
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: BULKEMIS(IIPAR, JJPAR)
INTEGER, INTENT(IN) :: STYPE, CTYPE
```

RETURN VALUE:

```
REAL(fp) :: VALUE(IIPAR, JJPAR, IBINS)
```

REMARKS:

```
STYPE (source type): 1 = Fossil fule

2 = Biofuel

3 = Biomass burning

CTYPE (carbon type): 1 = EC

2 = OC
```

Array ECSCALE30 and OCSCALE100 specify how mass is distributed into bins for a 30 nm number peak and a 100 nm peak. Similary for OC size split.

This function is adapted from emisOCbond.f and emisBCbond.f by Jeff Pierce (Jan, 2007) used in GISS GCM-II'. Introduced to GEOS-Chem by Win T.(9/4/07)

REVISION HISTORY:

```
20 Aug 2013 - M. Sulprizio- Added ProTeX headers
```

8.2.20 emisscarbon

Subroutine EMISSCARBON is the emissions routine for the carbon module. All carbon emissions, incl. SESQ and SVOC, are calculated through HEMCO and this module simply makes sure that the SESQ and SVOC emissions (if defined) are properly passed to the internal arrays.

INTERFACE:

```
SUBROUTINE EMISSCARBON( am_I_Root, Input_Opt, & State_Met, RC)
```

USES:

USE CMN_SIZE_MOD, ONLY : IIPAR, JJPAR

USE ErrCode_Mod

USE GC_GRID_MOD, ONLY : GET_AREA_M2

USE HCO_INTERFACE_MOD, ONLY : HcoState, GetHcoID, GetHcoVal

USE HCO_ERROR_MOD

USE Input_Opt_Mod, ONLY : OptInput
USE PBL_MIX_MOD, ONLY : GET_PBL_MAX_L
USE PBL_MIX_MOD, ONLY : GET_FRAC_OF_PBL

USE State_Met_Mod, ONLY : MetState
USE TIME_MOD, ONLY : GET_TS_EMIS

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC ! Failure?

REMARKS:

SVOC emissions are expected to be fully calculated by HEMCO, i.e. its emissions need be specified in the HEMCO configuration file. In the original code, the emissions were calculated by scaling anthropogenic, biofuel and biomass burning OC emissions. The same behavior can be achieved in HEMCO by assigning the desired SVOC species name to the given source type, e.g.: O BOND_ANTH_POG1 Bond_fossil.nc OC 2000/1-12/1/0 C xy kg/m2/s POG1 74 1 1 All POG1 emissions (anthropogenic + biofuel + biomass burning) will go into POAEMISS(:,:,:,1) and all POG2 emissions will go into POAEMISS(:,:,:,2). SVOC emissions are assigned to POG1 and POG2 in HEMCO using a ratio of 0.49:0.51. We no longer separate anthropogenic from biofuel and biomass burning since this appears to have been done only for debugging purposes. Routine CHEM_NVOC handles passing POAEMISS to the two gas-phase semivolatile species in the GMO array.

IMPORTANT: The SVOC emissions scale factor should be applied through HEMCO. In the example above, scale factor 74 represents the scale factor POGSCAL. The SCALING_POG1 scale factor is applied to the GFED biomass burning extensions. The two scale factors should be set to the same value in the HEMCO configuration file. The recommended value is 1.27.

REVISION HISTORY:

```
11 Nov 2014 - C. Keller - Initial version
```

11 Sep 2015 - E. Lundgren - Remove State_Chm from arguments since not used

```
14 Jan 2016 - M. Sulprizio- Emit SVOC emissions as POG1 and POG2 (not POA1
                            and POG1) in HEMCO to better reflect that these
                            emissions are added to the gas-phase species
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
```

emisscarbontomas 8.2.21

Subroutine emisscarbontomas scales BULK HEMCO emissions into TOMAS arrays. Only use for TOMAS simulations. This is essential a re-write of the TOMAS portions of the v9 emisscarbon (JKodros 6/2/15)

INTERFACE:

```
SUBROUTINE EMISSCARBONTOMAS( am_I_Root, Input_Opt,
                              State_Met, State_Chm, RC )
&
```

USES:

```
USE CMN_DIAG_MOD
   USE CMN_SIZE_MOD
   USE ErrCode_Mod
   USE ERROR_MOD
   USE GC_GRID_MOD,
                            ONLY : GET_XOFFSET, GET_YOFFSET
                            ONLY : OptInput
   USE Input_Opt_Mod,
   USE State_Chm_Mod,
                            ONLY : ChmState
   USE State_Met_Mod,
                            ONLY : MetState
   USE UnitConv_Mod
TOMAS DIAGNs:
                            ONLY : GET_PCENTER
   USE PRESSURE_MOD,
   USE TOMAS_MOD,
                            ONLY : IBINS,
                                              AVGMASS, SOACOND
                                              IDIAG, xSOA
   USE TOMAS_MOD,
                            ONLY : ICOMP,
    ! HEMCO update
```

USE HCO_INTERFACE_MOD, ONLY : HcoState, GetHcoDiagn

INPUT PARAMETERS:

```
! Are we on the root CPU?
LOGICAL.
               INTENT(IN)
                              :: am_I_Root
TYPE(OptInput), INTENT(IN)
                              :: Input_Opt    ! Input Options object
TYPE(MetState), INTENT(IN)
                              :: State_Met
                                             ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm
                                            ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER,
                INTENT(OUT)
                               :: RC
                                              ! Success or failure?
```

```
12 Jun 2015 - J. Kodros - Initial version
12 Jun 2015 - R. Yantosca - Bug fix: also add reference to DEBUG_MSG
10 Jul 2015 - R. Yantosca - Fixed typo in ProTeX header
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
```

8.2.22 emithigh2

Subroutine EMITHIGH2 mixes species completely from the surface to the PBL top. This is a copy of subroutine EMITHIGH modified to work with 30-bin EC and OC mass and also aerosol number. (win, 9/4/07)

INTERFACE:

```
SUBROUTINE EMITHIGH2( BCSRC, OCSRC, NUMBSRC, & Input_Opt, State_Chm)
```

USES:

```
USE CMN_SIZE_MOD

USE Input_Opt_Mod, ONLY : OptInput

USE PBL_MIX_MOD, ONLY : GET_FRAC_OF_PBL, GET_PBL_MAX_L

USE State_Chm_Mod, ONLY : ChmState

USE TOMAS_MOD, ONLY : IBINS
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: BCSRC(IIPAR, JJPAR, IBINS, 2) !Total BC [kg]
REAL(fp), INTENT(IN) :: OCSRC(IIPAR, JJPAR, IBINS, 2) !Total OC [kg]
REAL(fp), INTENT(IN) :: NUMBSRC(IIPAR, JJPAR, IBINS)
TYPE(OptInput), INTENT(IN) :: Input_Opt !Input Options
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

- (1) Now also mix ALPH, LIMO, ALCO tracers (rjp, bmy, 7/8/04)
- (2) Now reference STT from "tracer_mod.f" (bmy, 7/20/04)
- (3) Remove references to "dao_mod.f", "pressure_mod.f", and "error_mod.f".
 Rewrote for computational expediency using routines from
 "pbl_mix_mod.f". (bmy, 2/17/05)
- 20 Aug 2013 M. Sulprizio- Added ProTeX headers
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

8.2.23 ohno3time

Subroutine OHNO3TIME computes the sum of cosine of the solar zenith angle over a 24 hour day, as well as the total length of daylight. This is needed to scale the offline OH and NO3 concentrations. (rjp, bmy, 12/16/02, 1/18/05)

INTERFACE:

SUBROUTINE OHNOSTIME

USES:

```
USE CMN_SIZE_MOD

USE GC_GRID_MOD, ONLY : GET_XMID, GET_YMID_R

USE TIME_MOD, ONLY : GET_NHMSb, GET_ELAPSED_SEC

USE TIME_MOD, ONLY : GET_TS_CHEM, GET_DAY_OF_YEAR, GET_GMT
```

REVISION HISTORY:

- (1) Copy code from COSSZA directly for now, so that we don't get NaN values. Figure this out later (rjp, bmy, 1/10/03)
- (2) Now replace XMID(I) with routine GET_XMID from "grid_mod.f". Now replace RLAT(J) with routine GET_YMID_R from "grid_mod.f". Removed NTIME, NHMSb from the arg list. Now use GET_NHMSb, GET_ELAPSED_SEC, GET_TS_CHEM, GET_DAY_OF_YEAR, GET_GMT from "time_mod.f". (bmy, 3/27/03)
- (3) Now store the peak SUNCOS value for each surface grid box (I,J) in the COSZM array. (rjp, bmy, 3/30/04)
- (4) Also added parallel loop over grid boxes (bmy, 1/18/05)
- 01 Mar 2012 R. Yantosca Now use GET_XMID(I,J,L) from grid_mod.F90
- 01 Mar 2012 R. Yantosca Now use GET_YMID_R(I,J,L) from grid_mod.F90
- 20 Aug 2013 M. Sulprizio- Added ProTeX headers
- 16 May 2016 M. Sulprizio- Remove IJLOOP and change SUNTMP array dimensions from (MAXIJ) to (IIPAR, JJPAR)

8.2.24 get_oh

Function GET_OH returns OH from State_Chmcoupled runs) or monthly mean OH (for offline runs). Imposes a diurnal variation on OH for offline simulations. (bmy, 7/9/04)

INTERFACE:

```
FUNCTION GET_OH( I, J, L, Input_Opt, State_Chm, State_Met )
& RESULT( OH_MOLEC_CM3 )
USES:
```

```
USE CHEMGRID_MOD, ONLY : ITS_IN_THE_CHEMGRID USE CMN_SIZE_MOD
```

```
USE ERROR_MOD, ONLY: ERROR_STOP
USE Input_Opt_Mod, ONLY: OptInput
USE State_Chm_Mod, ONLY: ChmState
USE State_Met_Mod, ONLY: MetState
USE TIME_MOD, ONLY: GET_TS_CHEM
```

```
INTEGER, INTENT(IN) :: I ! Longitude index
INTEGER, INTENT(IN) :: J ! Latitude index
INTEGER, INTENT(IN) :: L ! Altitude index
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object
TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

RETURN VALUE:

REAL(fp) :: OH_MOLEC_CM3

REVISION HISTORY:

```
(1) We assume SETTRACE has been called to define IDOH (bmy, 11/1/02)
```

- (2) Now use function GET_TS_CHEM from "time_mod.f" (bmy, 3/27/03)
- (3) Now reference inquiry functions from "tracer_mod.f" (bmy, 7/20/04)
- 28 Nov 2012 R. Yantosca Replace SUNCOS with State_Met%SUNCOS
- 28 Nov 2012 R. Yantosca Add State_Met to the argument list
- 4 Mar 2013 R. Yantosca Add Input_Opt to the argument list
- 20 Aug 2013 M. Sulprizio- Added ProTeX headers
- 23 Sep 2014 M. Sulprizio- Now get OH for offline aerosol sim from HEMCO
- 22 Dec 2015 M. Sulprizio- Replace CSPEC with State_Chm%Species
- 07 Sep 2016 M. Sulprizio- Bug fix: Convert State_Chm%Species from kg to molec/cm3

8.2.25 get_no3

Function GET_NO3 returns NO3 from State_Chmcoupled runs) or monthly mean OH (for offline runs). For offline runs, the concentration of NO3 is set to zero during the day. (rjp, bmy, 12/16/02, 7/20/04)

INTERFACE:

```
FUNCTION GET_NO3( I, J, L, Input_Opt, State_Chm, State_Met )
& RESULT( NO3_MOLEC_CM3 )
```

USES:

```
USE CHEMGRID_MOD, ONLY : ITS_IN_THE_CHEMGRID
```

USE CMN_SIZE_MOD

USE ERROR_MOD, ONLY : ERROR_STOP

```
USE Input_Opt_Mod, ONLY: OptInput
USE State_Chm_Mod, ONLY: ChmState
USE State_Met_Mod, ONLY: MetState
```

```
INTEGER, INTENT(IN) :: I ! Longitude index
INTEGER, INTENT(IN) :: J ! Latitude index
INTEGER, INTENT(IN) :: L ! Altitude index
```

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object
TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

RETURN VALUE:

REAL(fp) :: NO3_MOLEC_CM3

REVISION HISTORY:

- (1) Now references ERROR_STOP from "error_mod.f". We also assume that SETTRACE has been called to define IDNO3. Now also set NO3 to zero during the day. (rjp, bmy, 12/16/02)
- (2) Now reference inquiry functions from "tracer_mod.f" (bmy, 7/20/04)
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 28 Nov 2012 R. Yantosca Replace SUNCOS with State_Met%SUNCOS
- 04 Mar 2013 R. Yantosca Add Input_Opt to the argument list
- 20 Aug 2013 M. Sulprizio- Added ProTeX headers
- 23 Jul 2014 R. Yantosca Remove reference to obsolete CMN_MOD
- 24 Jul 2014 R. Yantosca Now compute BOXVL internally
- 23 Sep 2014 M. Sulprizio- Now get NO3 for offline aerosol sims from HEMCO
- 22 Dec 2015 M. Sulprizio- Replace CSPEC with State_Chm%Species
- 28 Jul 2016 R. Yantosca Now convert NO3 from kg to molec/cm3
- 07 Sep 2016 M. Sulprizio- Get MolecRatio and NO3_MW_kg from species DB

$8.2.26 \quad \text{get_o3}$

Function GET_O3 returns monthly mean O3 for offline sulfate aerosol simulations. (bmy, 12/16/02, 7/20/04)

INTERFACE:

```
FUNCTION GET_03( I, J, L, Input_Opt, State_Chm, State_Met )
& RESULT( 03_MOLEC_CM3 )
```

USES:

```
USE CHEMGRID_MOD, ONLY : ITS_IN_THE_CHEMGRID USE CMN_SIZE_MOD
```

```
USE ERROR_MOD, ONLY: ERROR_STOP
USE Input_Opt_Mod, ONLY: OptInput
USE State_Chm_Mod, ONLY: ChmState
USE State_Met_Mod, ONLY: MetState
USE TIME_MOD, ONLY: GET_TS_CHEM
```

```
INTEGER, INTENT(IN) :: I ! Longitude index
INTEGER, INTENT(IN) :: J ! Latitude index
INTEGER, INTENT(IN) :: L ! Altitude index
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object
TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

RETURN VALUE:

REAL(fp) :: 03_MOLEC_CM3

REVISION HISTORY:

```
(1) We assume SETTRACE has been called to define IDO3. (bmy, 12/16/02)
(2) Now reference inquiry functions from "tracer_mod.f" (bmy, 7/20/04)
(3 ) Now reference XNUMOLAIR from "tracer_mod.f" (bmy, 10/20/05)
09 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met
                            derived type object
28 Nov 2012 - R. Yantosca - Replace SUNCOS with State_Met%SUNCOS
04 Mar 2013 - R. Yantosca - Add Input_Opt to the argument list
20 Aug 2013 - M. Sulprizio- Added ProTeX headers
24 Jul 2014 - R. Yantosca - Now compute BOXVL internally
18 Sep 2014 - M. Sulprizio- Now get 03 for offline aerosol sim from HEMCO
24 Mar 2015 - E. Lundgren - Replace dependency on tracer_mod with
                            CMN_GTCM_MOD for XNUMOLAIR
22 Dec 2015 - M. Sulprizio- Replace CSPEC with State_Chm%Species
06 Jan 2016 - E. Lundgren - Use global physical parameter AVO
28 Jul 2016 - R. Yantosca - Now convert O3 from kg to molec/cm3
07 Sep 2016 - M. Sulprizio- Get MolecRatio and NO3_MW_kg from species DB
```

8.2.27 get_daro2

Function GET_DARO2 returns the amount of aromatic peroxy radical that reacted with HO2 or NO during the last chemistry timestep. (dkh, 11/10/06)

INTERFACE:

```
FUNCTION GET_DARO2( I, J, L, NOX, JHC, Input_Opt,
& State_Chm, State_Met )
& RESULT( DARO2 )
```

USES:

USE CHEMGRID_MOD, ONLY : ITS_IN_THE_CHEMGRID
USE CMN_O3_MOD

USE CMN_SIZE_MOD

USE ERROR_MOD, ONLY : ERROR_STOP

USE Input_Opt_Mod, ONLY : OptInput

USE PhysConstants, ONLY : AVO

USE State_Chm_Mod, ONLY : ChmState

USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

```
INTEGER,
             INTENT(IN) :: I
                                        ! Longitude index
INTEGER.
                                        ! Latitude index
             INTENT(IN) :: J
INTEGER,
             INTENT(IN) :: L
                                        ! Altitude index
INTEGER,
             INTENT(IN) :: NOX
INTEGER,
              INTENT(IN) :: JHC
                                         ! Input Options object
TYPE(OptInput), INTENT(IN) :: Input_Opt
TYPE(ChmState), INTENT(IN) :: State_Chm
                                         ! Chemistry State object
TYPE(MetState), INTENT(IN) :: State_Met
                                         ! Meteorology State object
```

RETURN VALUE:

REAL(fp) :: DARO2

REVISION HISTORY:

```
04 Mar 2013 - R. Yantosca - Add Input_Opt to the argument list
13 Aug 2013 - M. Sulprizio- Add NAP for SOA + semivolatile POA (H. Pye)
20 Aug 2013 - M. Sulprizio- Added ProTeX headers
21 Dec 2015 - M. Sulprizio- Get grid box volume directly from State_Met
22 Dec 2015 - M. Sulprizio- Replace CSPEC with State_Met%Species
17 May 2016 - R. Yantosca - Now get MolecRatio from species database
31 May 2016 - E. Lundgren - Now get molecular weight from species database
07 Sep 2016 - M. Sulprizio- Bug fix: Convert State_Chm%Species from kg LARO2 to kg AROM
```

$8.2.28 \text{ get_doh}$

Function GET_DOH returns the amount of isoprene [kg] that has reacted with OH during the last chemistry time step. (dkh, bmy, 6/01/06)

INTERFACE:

```
FUNCTION GET_DOH( I, J, L, Input_Opt, State_Chm, State_Met ) & RESULT( DOH )
```

USES:

USE CHEMGRID_MOD, ONLY : ITS_IN_THE_CHEMGRID

USE CMN_SIZE_MOD

USE ERROR_MOD, ONLY : ERROR_STOP
USE Input_Opt_Mod, ONLY : OptInput
USE PhysConstants, ONLY : AVO
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: I ! Longitude index
INTEGER, INTENT(IN) :: J ! Latitude index
INTEGER, INTENT(IN) :: L ! Altitude index

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object
TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

RETURN VALUE:

REAL(fp) :: DOH

REVISION HISTORY:

04 Mar 2013 - R. Yantosca - Now use fields from Input_Opt object

20 Aug 2013 - M. Sulprizio- Added ProTeX headers

21 Dec 2015 - M. Sulprizio- Get grid box volume directly from State_Met

17 May 2016 - R. Yantosca - Now get MolecRatio from species database

31 May 2016 - E. Lundgren - Now get molecular weight from species database

07 Sep 2016 - M. Sulprizio- Bug fix: Convert State_Chm%Species from kg ISOPOH to kg ISOP

8.2.29 get_vcldf

Subroutine GET_VCLDF computes the volume cloud fraction for SO2 chemistry. (rjp, bdf, bmy, 9/23/02)

INTERFACE:

SUBROUTINE GET_VCLDF(State_Met)

USES:

USE CMN_SIZE_MOD

INPUT PARAMETERS:

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

REMARKS:

References:

(1) Sundqvist et al. [1989]

REVISION HISTORY:

- (1) Copied from 'sulfate_mod.f' for cloud uptake of GLYX and MGLY (tmf, 2/26/07)
- 14 Jan 2011 R. Yantosca Return if VCLDF is not allocated
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 20 Aug 2013 M. Sulprizio- Added ProTeX headers
- 26 Feb 2015 E. Lundgren Replace GET_PEDGE and GET_PCENTER with State_Met%PEDGE and State_Met%PMID.

 Remove dependency on pressure_mod.

$8.2.30 \text{ get_lwc}$

Function GET_LWC returns the cloud liquid water content [g H2O/m3 air] at a GEOS-CHEM grid box as a function of temperature. (rjp, bmy, 10/31/02, 1/14/03)

INTERFACE:

```
FUNCTION GET_LWC( T ) RESULT( LWC )
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: T   ! Temperature [K]
```

RETURN VALUE:

```
REAL(fp) :: LWC ! Cloud liquid water content [g H2O/m3 air]
```

REVISION HISTORY:

- (1) Copied from 'sulfate_mod.f' for cloud uptake of GLYX and MGLY (tmf, 2/26/07)
- 18 Jan 2011 R. Yantosca Updated comments
- 20 Aug 2013 M. Sulprizio- Added ProTeX headers

8.2.31 soag_cloud

Subroutine SOAG_CLOUD produces SOAG from GLYX during a cloud event. Mimics the SO2 -; SO4 process from 'sulfate_mod.f'. (tmf, 2/26/07)

INTERFACE:

```
SUBROUTINE SOAG_CLOUD( State_Met, State_Chm )
```

USES:

USE CHEMGRID_MOD, ONLY : ITS_IN_THE_NOCHEMGRID
USE CMN_DIAG_MOD
USE CMN_SIZE_MOD
USE DAO_MOD, ONLY : IS_LAND
USE DIAG_MOD, ONLY : ADO7_SOAGM
USE State_Met_Mod, ONLY : MetState
USE State_Chm_Mod, ONLY : ChmState
USE TIME_MOD, ONLY : GET_TS_CHEM

INPUT PARAMETERS:

! Arguments

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

REVISION HISTORY:

- (1) SOAG (SOA product of GLYX is produced at existing hydrophilic aerosol surface. (tmf, 2/26/07)
- (2) Assume marine and continental cloud droplet size (tmf, 2/26/07)
- 14 Jan 2011 R. Yantosca Now compute cloud fraction and liquid water content directly from GEOS-5 & MERRA met fields
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 20 Aug 2013 M. Sulprizio- Added ProTeX headers
- 26 Sep 2013 R. Yantosca Renamed GEOS_57 Cpp switch to GEOS_FP
- 06 Nov 2014 R. Yantosca Now use State_Met%AIRDEN(I,J,L)
- 06 Nov 2014 R. Yantosca Now use State_Met%CLDF(I,J,L)
- 11 Aug 2015 R. Yantosca MERRA2 behaves the same way as GEOS-FP
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

8.2.32 soam_cloud

USE CMN_SIZE_MOD

Subroutine SOAM_CLOUD produces SOAM from MGLY during a cloud event. Mimics the SO2 -; SO4 process from 'sulfate_mod.f'. (tmf, 2/26/07)

INTERFACE:

SUBROUTINE SOAM_CLOUD(State_Met, State_Chm)

USES:

USE CHEMGRID_MOD, ONLY : ITS_IN_THE_NOCHEMGRID USE CMN_DIAG_MOD

```
USE DAO_MOD, ONLY: IS_LAND

USE DIAG_MOD, ONLY: ADO7_SOAGM

USE State_Met_Mod, ONLY: MetState

USE State_Chm_Mod, ONLY: ChmState

USE TIME_MOD, ONLY: GET_TS_CHEM
```

```
TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

REVISION HISTORY:

```
(1 ) SOAM (SOA product of MGLY is produced at existing hydrophilic aerosol surface. (tmf, 2/26/07)
```

(2) Assume typical marine and continental cloud droplet size (tmf, 2/26/07)

```
09 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met derived type object
```

20 Aug 2013 - M. Sulprizio- Added ProTeX headers

06 Nov 2014 - R. Yantosca - Now use State_Met%AIRDEN(I,J,L)

06 Nov 2014 - R. Yantosca - Now use State_Met%CLDF(I,J,L)

11 Aug 2015 - R. Yantosca - MERRA2 behaves the same way as GEOS-FP

30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

8.2.33 check_eqlb

Subroutine CHECK_EQLB makes sure aerosols are at equilibrium (checks SOA=SOG*KOM*Mo). Called inside SOA_SVPOA_CHEMISTRY I, J, L loop after SOA_SVPOA_LUMP. Created by Havala Pye (5/18/10).

INTERFACE:

```
SUBROUTINE CHECK_EQLB( I, J, L, KOMIJL, CONVFAC, MSOACHEM, & LOW, TOL, ASOANGAS, ASOANAER, OCPIOCPO, & State_Chm )
```

USES:

USE State_Chm_Mod, ONLY : ChmState

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I ! Longitude index
INTEGER, INTENT(IN) :: J ! Latitude index
INTEGER, INTENT(IN) :: L ! Altitude index
REAL(fp), INTENT(IN) :: KOMIJL(MPROD, MSV) ! KOM at grid box (adj T)
```

```
REAL(fp),
                                           ! Conversion factor kg to ug/m3
                INTENT(IN) :: CONVFAC
REAL(fp),
                INTENT(IN) :: OCPIOCPO
                                           ! POA mass [ug/m3]
! Arguments for debugging
REAL(fp),
               INTENT(IN) :: MSOACHEM
                                           ! MNEW from calling prog
REAL(fp),
               INTENT(IN) :: LOW
                                           ! Lower bound on soln
REAL(fp),
                                           ! Tolerance on soln
               INTENT(IN) :: TOL
REAL(fp),
               INTENT(IN) :: ASOANGAS
                                           ! Gas phase ASOAN (should =0)
                                           ! Aer phase ASOAN [ug/m3]
REAL(fp),
               INTENT(IN) :: ASOANAER
TYPE(ChmState), INTENT(IN) :: State_Chm
                                           ! Chemistry State object
```

REMARKS:

Note: There are some deviations from equilibrium due to the fact that ASOAN is supposed to be nonvolatile, but is modeled with a KOM of 10^6. An adjustment is made in SOA_CHEMISTRY to force all ASOAN to the aerosol phase. This was found to lead to error up to 1e-5 ug/m3 in Mo. This error is small, but the effects can be investigated here if you're interested!

As of 6/2010, KOM for ASOAN was increased and the error in Mo reduced.

REVISION HISTORY:

- (1) Updated for TSOA and ISOA (hotp 5/24/10)
- (2) Add OCPIOCPO and remove NOX (hotp 6/9/10)
- (3) Add TSOAO (hotp 6/12/10)
- 20 Aug 2013 M. Sulprizio- Added ProTeX headers
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

8.2.34 save_oaginit

Subroutine SAVE_OAGINIT saves total SOA+SOG before partitioning for diagnostic purposes. Units are the same as the STT array ([kg] or [kgC per box]). created hotp 5/17/10

INTERFACE:

```
SUBROUTINE SAVE_OAGINIT( State_Chm )
```

USES:

```
USE CMN_SIZE_MOD
USE State_Chm_Mod, ONLY : ChmState
```

INPUT PARAMETERS:

```
TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object
```

REVISION HISTORY:

- (1) added TSOA and ISOA (hotp 5/24/10)
- (2) OAGINITSAVE dimensions changes from (I,J,L,NOx,NPROD,JSV) to (I,J,L,NPROD,JSV)
- (3) Add compatability with non-vol sim (hotp 6/7/10)
- 20 Aug 2013 M. Sulprizio- Added ProTeX headers
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

8.2.35 check_mb

Subroutine CHECK_MB checks total SOA+SOG mass balance for diagnostic/debugging purposes. Units are the same as the STT array ([kg] or [kgC per box]). Routine also prints helpful budget info. Created by Havala Pye (5/18/10).

INTERFACE:

```
SUBROUTINE CHECK_MB( am_I_Root, Input_Opt, State_Met, State_Chm )
```

USES:

```
USE CHEMGRID_MOD, ONLY : ITS_IN_THE_STRAT

USE CMN_SIZE_MOD

USE Input_Opt_Mod, ONLY : OptInput

USE State_Met_Mod, ONLY : MetState

USE State_Chm_Mod, ONLY : ChmState
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object
```

- (1) added monoterpene, sesq, isoprene SOA (hotp 5/24/10)
- (2) updated OAGINITSAVE dimensions (hotp 5/24/10)
- (3) keeps track and prints to screen amount of parent HC reacted with each oxidant cumulative (hotp 5/24/10)
- (4) Add non-volatile compatability (hotp 6/9/10)
- 20 Aug 2013 M. Sulprizio- Added ProTeX headers
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

8.2.36 get_no

Function GET_NO returns NO from State_Chm(for coupled runs). (hotp 5/7/2010)

INTERFACE:

```
FUNCTION GET_NO( I, J, L, Input_Opt, State_Chm, State_Met )
& RESULT( NO_MOLEC_CM3 )
```

USES:

```
USE CHEMGRID_MOD, ONLY : ITS_IN_THE_CHEMGRID
```

USE CMN_SIZE_MOD

USE ERROR_MOD, ONLY : ERROR_STOP
USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I     ! Longitude index
INTEGER, INTENT(IN) :: J     ! Latitude index
INTEGER, INTENT(IN) :: L     ! Altitude index
```

!RETURN VALUE

REAL(fp) :: NO_MOLEC_CM3 ! NO conc [molec/cm3]

REVISION HISTORY:

- (1) We assume SETTRACE has been called to define IDNO (bmy, 11/1/02)
- (3) Now reference inquiry functions from "tracer_mod.f" (bmy, 7/20/04)
- (4) Based on GET_OH (hotp 5/7/2010)
- 20 Aug 2013 M. Sulprizio- Added ProTeX headers
- 25 Jun 2014 R. Yantosca Now accept Input_Opt via the arg list
- 25 Jun 2014 R. Yantosca Remove references to tracer_mod.F
- 22 Dec 2015 M. Sulprizio- Replace CSPEC with State_Chm%Species
- 28 Jul 2016 R. Yantosca Now convert NO from kg to molec/cm3
- 07 Sep 2016 M. Sulprizio- Get MolecRatio and NO3_MW_kg from species DB

8.2.37 get_ho2

Function GET_HO2 returns HO2 from State_Chm(for coupled runs). Created by Havala Pye (5/7/2010).

INTERFACE:

```
FUNCTION GET_HO2( I, J, L, Input_Opt, State_Chm, State_Met )
& RESULT( HO2_MOLEC_CM3 )
```

USES:

USE CHEMGRID_MOD, ONLY: ITS_IN_THE_CHEMGRID
USE CMN_SIZE_MOD

USE ERROR_MOD, ONLY: ERROR_STOP

USE Input_Opt_Mod, ONLY: OptInput

USE State_Chm_Mod, ONLY: ChmState

USE State_Met_Mod, ONLY: MetState

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: I ! Longitude index INTEGER, INTENT(IN) :: J ! Latitude index INTEGER, INTENT(IN) :: L ! Altitude index TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object !RETURN VALUE REAL(fp) :: HO2_MOLEC_CM3 ! HO2 conc [molec/cm3]

REVISION HISTORY:

- (1) We assume SETTRACE has been called to define IDHO2 (bmy, 11/1/02)
- (3) Now reference inquiry functions from "tracer_mod.f" (bmy, 7/20/04)
- (4) Based on GET_OH (hotp 5/6/2010)
- 20 Aug 2013 M. Sulprizio- Added ProTeX headers
- 25 Jun 2014 R. Yantosca Now accept Input_Opt via the arg list
- 25 Jun 2014 R. Yantosca Remove references to tracer_mod.F
- 22 Dec 2015 M. Sulprizio- Replace CSPEC with State_Chm%Species

8.2.38 get_isopno3

Modification of GET_DOH that returns the amount of isoprene [kgC] that has reacted with NO3 during the last chemistry time step. (hotp 5/22/10)

INTERFACE:

```
FUNCTION GET_ISOPNO3( I, J, L, Input_Opt, State_Chm, State_Met )
& RESULT( ISOPNO3 )
```

USES:

USE CHEMGRID_MOD, ONLY : ITS_IN_THE_CHEMGRID
USE CMN_SIZE_MOD

USE ERROR_MOD, ONLY : ERROR_STOP

USE Input_Opt_Mod, ONLY : OptInput

USE PhysConstants, ONLY : AVO

USE State_Chm_Mod, ONLY : ChmState

USE State_Met_Mod, ONLY : MetState

```
INTEGER,
                 INTENT(IN) :: I
                                         ! Longitude index
   INTEGER,
                 INTENT(IN) :: J
                                         ! Latitude index
                  INTENT(IN) :: L
   INTEGER,
                                         ! Altitude index
   TYPE(OptInput), INTENT(IN) :: Input_Opt   ! Input Options object
   TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object
   TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
!RETURN VALUE
   REAL(fp)
                         :: ISOPNO3
                                           ! ISOP replaced w/ NO3 [kg C]
```

REVISION HISTORY:

(1) IDLISOPNO3 is declared in tracerid_mod.f and initialized by SETTRACE in tracerid_mod (called in chemdr). Before each chemistry call, CSPEC(JLOOP,IDLISOPNO3) is zeroed so that the CSPEC array only stores the parent HC reacted during that timestep. (hotp 6/1/10)

```
20 Aug 2013 - M. Sulprizio- Added ProTeX headers
```

25 Jun 2014 - R. Yantosca - Now accept Input_Opt via the arg list

25 Jun 2014 - R. Yantosca - Remove references to tracer_mod.F

21 Dec 2015 - M. Sulprizio- Get grid box volume directly from State_Met

22 Dec 2015 - M. Sulprizio- Replace CSPEC with State_Met%Species

17 May 2016 - R. Yantosca - Now get MolecRatio from species database

31 May 2016 - E. Lundgren - Now get molecular weight from species database

07 Sep 2016 - M. Sulprizio- Bug fix: Convert State_Chm%Species from kg ISOPOH to kg ISOP

8.2.39 init_carbon

Subroutine INIT_CARBON initializes all module arrays. (rjp, bmy, 4/1/04, 12/19/09)

INTERFACE:

```
SUBROUTINE INIT_CARBON( am_I_Root, Input_Opt, RC )
```

USES:

```
USE CMN_SIZE_MOD

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ALLOC_ERR, ERROR_STOP
```

USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : Ind_

USE TIME_MOD, ONLY: GET_NYMDb, GET_NHMSb, GET_TAUb

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure

REVISION HISTORY:

- (1) Also added arrays for secondary organic aerosols (rjp, bmy, 7/8/04)
- (2) Remove reference to CMN, it's obsolete (bmy, 7/20/04)
- (3) Now reference LSOA from "logical_mod.f" not CMN_SETUP. Now call GET_BOUNDING_BOX from "grid_mod.f" to compute the indices I1_NA, I2_NA, J1_NA, J2_NA which define the N. America region. (bmy, 12/1/04)
- (4) Now call READ_GPROD_APROD to read GPROD & APROD from disk. (tmf, havala, bmy, 2/6/07)
- (5) Now set I1_NA, I2_NA, J1_NA, J2_NA appropriately for both 1 x 1 and 0.5 x 0.666 nested grids (yxw, dan, bmy, 11/6/08)
- (6) Now set parameters for NESTED_EU grid (amv, bmy, 12/19/09)
- 14 Jan 2011 R. Yantosca If we are using GEOS-5 or MERRA met, then get the cloud fraction directly from the met fields.
- 01 Mar 2012 R. Yantosca Now use GET_BOUNDING_BOX from grid_mod.F90
- 04 Mar 2013 R. Yantosca Now take am_I_Root, Input_Opt, RC as arguments
- 04 Mar 2013 R. Yantosca Now search for drydep flags here
- 05 Mar 2013 R. Yantosca Now use Input_Opt%LSOA
- 13 Aug 2013 M. Sulprizio- Add modifications for updated SOA and SOA + semivolatile POA simulations (H. Pye)
- 20 Aug 2013 M. Sulprizio- Added ProTeX headers
- 26 Sep 2013 R. Yantosca Removed SEAC4RS Cpp switch, this is supplanted by NESTED_NA
- 26 Sep 2013 R. Yantosca Renamed GEOS_57 Cpp switch to GEOS_FP
- 11 Aug 2015 R. Yantosca Add support for MERRA2 data
- 23 Sep 2015 R. Yantosca Remove reference to DRY* flags, they're obsolete

8.2.40 cleanup_carbon

Subroutine CLEANUP_CARBON deallocates all module arrays (rjp, bmy, 4/1/04, 7/8/04)

INTERFACE:

SUBROUTINE CLEANUP_CARBON

REVISION HISTORY:

- (1) Now deallocate arrays for secondary organic aerosols (rjp, bmy, 7/8/04)
- 13 Aug 2013 M. Sulprizio- Add modifications for updated SOA and SOA + semivolatile POA simulations (H. Pye)
- 20 Aug 2013 M. Sulprizio- Added ProTeX headers

8.3 Fortran: Module Interface dust_mod.F

Module DUST_MOD contains routines for computing dust aerosol emissions, chemistry, and optical depths.

INTERFACE:

MODULE DUST_MOD

USES:

USE inquireMod, ONLY : findFreeLUN

USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

IMPLICIT NONE

PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: CHEMDUST

#if defined(TOMAS)

PUBLIC :: SETTLEDUST

#endif

PUBLIC :: RDUST_ONLINE
PUBLIC :: RDUST_OFFLINE
PUBLIC :: GET_DUST_ALK
PUBLIC :: INIT_DUST
PUBLIC :: CLEANUP_DUST

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: DRY_SETTLING

- 30 Mar 2004 T. D. Fairlie Initial version
- (1) Bug fix in SRC_DUST_DEAD (bmy, 4/14/04)
- (2) Now references "logical_mod.f", "directory_mod.f", and "tracer_mod.f" Added comments. (bmy, 7/2/04)
- (3) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (4) Now references XNUMOL from "tracer_mod.f" (bmy, 10/25/05)
- (5) Bug fix in snow height computation (bmy, 11/18/05)
- (6) Now only do drydep if LDRYD=T (bmy, 5/23/06)
- (7) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (8) Updated output print statement in SRC_DUST_DEAD (bmy, 1/23/07)
- (9) Modifications for GEOS-5 (bmy, 1/24/07)
- (10) Modified to archive only hydrophilic aerosol/aqueous dust surface area (excluding BCPO and OCPO) for aqueous chemistry calculations

 Dust surfaces are considered aqueous only when RH > 35% (tmf, 3/6/09)
- (11) Add AOD output for all dust size bins (clh, 5/7/10)
- (12) Modify AOD output to wavelength specified in jv_spec_aod.dat (clh. 05/07/10)
- 25 Aug 2010 R. Yantosca Added ProTeX headers
- 03 Sep 2010 R. Yantosca Bug fix in SRC_DUST_DEAD

```
08 Feb 2012 - R. Yantosca - Add modifications for GEOS-5.7.x
01 Mar 2012 - R. Yantosca - Now reference the new grid_mod.F90
01 Aug 2012 - R. Yantosca - Add reference to findFreeLUN from inqure_mod.F90
03 Aug 2012 - R. Yantosca - Move calls to findFreeLUN out of DEVEL block
14 Nov 2012 - R. Yantosca - Add modifications for GIGC
04 Mar 2013 - R. Yantosca - Now call INIT_DUST from the init stage
                            which facilitates connection to GEOS-5 GCM
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
12 Sep 2013 - M. Sulprizio- Add modifications for acid uptake on dust
                            aerosols (T.D. Fairlie)
20 Jun 2014 - R. Yantosca - Remove obsolete emissions code; we now use HEMCO
13 Nov 2014 - M. Yannetti - Added PRECISION_MOD
01 Apr 2015 - R. Yantosca - Remove obsolete DUSTMIX, DRY_DEPOSITION routines
16 Jun 2016 - J. Kaiser - Move tracerIDs into variable names
20 Jun 2016 - R. Yantosca - Rename IDT* species ID's to id_*
20 Jun 2016 - R. Yantosca - Now only define species ID's in the INIT phase
29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90
```

8.3.1 chemdust

Subroutine CHEMDUST is the interface between the GEOS-Chem main program and the dust chemistry routines that mostly calculates dust dry deposition.

INTERFACE:

```
SUBROUTINE CHEMDUST( am_I_Root, Input_Opt, & State_Met, State_Chm, RC )
```

USES:

```
USE ErrCode_Mod

USE ERROR_MOD, ONLY : DEBUG_MSG

USE ERROR_MOD, ONLY : ERROR_STOP

USE Input_Opt_Mod, ONLY : OptInput

USE State_Met_Mod, ONLY : MetState

USE State_Chm_Mod, ONLY : ChmState
```

INPUT PARAMETERS:

USE CMN_SIZE_MOD

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

```
30 Mar 2004 - T. D. Fairlie - Initial version
(1 ) Now references STT from "tracer_mod.f" and LDUST from "logical_mod.f"
      (bmy, 7/20/04)
(5) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
(6) Now only do dry deposition if LDRYD = T (bmy, 5/23/06)
25 Aug 2010 - R. Yantosca - Added ProTeX headers
30 Jul 2012 - R. Yantosca - Now accept am_I_Root as an argument when
                            running with the traditional driver main.F
14 Nov 2012 - R. Yantosca - Add am_I_Root, Input_Opt, RC as arguments
15 Nov 2012 - M. Payer
                         - Now pass State_Met as an argument
05 Mar 2013 - R. Yantosca - Add ND70 debug print output
25 Mar 2013 - M. Payer
                         - Now pass State_Chm object via the arg list
12 Sep 2013 - M. Sulprizio- Add modifications for acid uptake on dust
                            aerosols (T.D. Fairlie)
01 Apr 2015 - R. Yantosca - Remove call to DRY_DEPOSITION, this is now
                            done in mixing_mod.F90.
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected
                            species ID from State_Chm%Map_Advect.
10 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code
```

8.3.2 settledust

Subroutine SETTLEDUST is the interface between the size-resolved dry deposition subroutine AERO_DRYDEP and the dust module. This is to call only gravitational settling and deals with removal of aerosol number with the dust mass. (win, 7/17/09)

INTERFACE:

```
SUBROUTINE SETTLEDUST( am_I_Root, Input_Opt,
                             State_Met, State_Chm, RC )
USES:
      USE CMN_SIZE_MOD
                                   ! Size parameters
      USE CMN_DIAG_MOD
                                   ! ND44
 #if defined( BPCH_DIAG )
      USE DIAG_MOD,
                             ONLY: AD44
 #endif
      USE ErrCode_Mod
      USE ERROR_MOD
      USE GC_GRID_MOD,
                             ONLY : GET_AREA_CM2
      USE Input_Opt_Mod,
                            ONLY : OptInput
      USE PhysConstants, ONLY: AVO
```

```
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState
USE TIME_MOD, ONLY : GET_TS_CHEM
```

USE TOMAS_MOD, ONLY : IBINS, Xk, SRTDUST

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REVISION HISTORY:

```
17 Jul 2009 - W. Trivitayanurak - Initial version

01 Mar 2012 - R. Yantosca - Now use GET_AREA_CM2(I,J,L) from grid_mod.F90

13 Dec 2012 - M. Payer - Add am_I_Root, Input_Opt, RC as arguments

31 May 2013 - R. Yantosca - Now pass State_Chm via the arg list

16 Jul 2015 - R. Yantosca - Now pass INDEX and IDISP to DRY_SETTLING

31 May 2016 - E. Lundgren - Replace Input_Opt%XNUMOL with AVO/(emMw_g*1e-3)

where emMw_g is from species database

30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

10 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code
```

8.3.3 emissdust

Subroutine EMISSDUST is the driver routine for the dust emission module. You may call either the GINOUX or the DEAD dust source function.

INTERFACE:

```
SUBROUTINE EMISSDUST( am_I_Root, Input_Opt, State_Met, State_Chm, RC )
```

USES:

```
USE CMN_DIAG_MOD ! ND59

USE CMN_SIZE_MOD ! Size parameters

USE DIAG_MOD, ONLY : AD59_DUST, AD59_NUMB !(win, 7/17/09)

USE ErrCode_Mod

USE ERROR_MOD, ONLY : DEBUG_MSG

USE ERROR_MOD, ONLY : ERROR_STOP
```

```
USE Input_Opt_Mod,
                       ONLY : OptInput
USE State_Chm_Mod,
                      ONLY : ChmState
USE State_Met_Mod,
                      ONLY : MetState
USE State_Met_Mod,
                    ONLY : MetState
USE TIME_MOD,
                      ONLY : GET_TS_EMIS
USE TOMAS_MOD,
                      ONLY : IBINS, XK
                                                  !(win, 7/17/09)
```

```
LOGICAL,
               INTENT(IN)
                            :: am_I_Root ! Are we on the root CPU?
                             :: Input_Opt    ! Input Options object
TYPE(OptInput), INTENT(IN)
TYPE(MetState), INTENT(IN) :: State_Met
                                           ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

INTENT(OUT) :: RC ! Success or failure? INTEGER.

REVISION HISTORY:

```
30 Mar 2004 - T. D. Fairlie - Initial version
```

- (1) Now reference LDEAD, LDUST, LPRT from "logical_mod.f". Now reference! STT from "tracer_mod.f" (bmy, 7/20/04)
- (2) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (3) Add if condition for selecting between emitting 4-bin or 30-bin dust. Add emission diagnostic calculation for 30bin dust(win, 7/17/09)
- 25 Aug 2010 R. Yantosca Added ProTeX headers
- 26 Nov 2012 R. Yantosca Now pass am_I_Root, Input_Opt, State_Met as args
- 26 Feb 2013 R. Yantosca Now pass Input_Opt to SRC_DUST_GINOUX
- 26 Feb 2013 R. Yantosca Changed INPUT_OPT to INTENT(IN), since we are now no longer calling INIT_DUST from here,

it is now called in the init stage

- 29 Apr 2016 R. Yantosca Don't initialize pointers in declaration stmts
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.
- 11 Aug 2016 R. Yantosca Remove temporary tracer-removal code

8.3.4 dry_settling

Subroutine DRY_SETTLING computes the dry settling of dust species.

INTERFACE:

```
SUBROUTINE DRY_SETTLING( am_I_Root, Input_Opt, State_Met,
                          State_Chm, TC, RC, INDEX, IDISP )
&
```

USES:

USE CMN_DIAG_MOD
USE CMN_SIZE_MOD
#if defined(BPCH_DIAG)

USE DIAG_MOD, ONLY: AD44

#endif

USE ErrCode_Mod

USE GC_GRID_MOD, ONLY : GET_AREA_CM2
USE Input_Opt_Mod, ONLY : OptInput

USE PhysConstants

USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState
USE TIME_MOD, ONLY : GET_TS_CHEM
USE Species_Mod, ONLY : Species

#if defined(NC_DIAG)

USE ERROR_MOD, ONLY : ERROR_STOP
USE HCO_INTERFACE_MOD, ONLY : HcoState
USE HCO_ERROR_MOD, ONLY : HCO_SUCCESS
USE HCO_DIAGN_MOD, ONLY : Diagn_Update

#endif

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

INTEGER, INTENT(IN) :: INDEX ! Species index

INTEGER, INTENT(IN) :: IDISP ! Displacement index for IIDEP

!INPUT/OUTPUT PARAMETERS

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object REAL(fp), INTENT(INOUT) :: TC(IIPAR,JJPAR,LLPAR,NDSTBIN) ! Dust [kg]

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

- 30 Mar 2004 T. D. Fairlie Initial version
- (1) Updated comments, cosmetic changes (bmy, 3/30/04)
- (2) Remove reference to CMN, it's not needed (bmy, 7/20/04)
- (3) Now references XNUMOL from "tracer_mod.f" (bmy, 10/25/05)
- 25 Aug 2010 R. Yantosca Added ProTeX headers
- 01 Mar 2012 R. Yantosca Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
- 14 Nov 2012 R. Yantosca Add am_I_Root, Input_Opt, RC as arguments
- 15 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object

```
19 Mar 2013 - R. Yantosca - Now copy Input_Opt%XNUMOL(1:N_TRACERS)

12 Sep 2013 - M. Sulprizio- Add modifications for acid uptake on dust aerosols (T.D. Fairlie)

26 Feb 2015 - E. Lundgren - Replace GET_PCENTER with State_Met%PMID and remove dependency on pressure_mod

25 Jan 2016 - E. Lundgren - Update netcdf drydep flux diagnostic

29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts

31 May 2016 - E. Lundgren - Use TCVV instead of XNUMOL for molecular weights

22 Jun 2016 - M. Yannetti - Replace TCVV with species db MW and phys constant
```

8.3.5 rdust_online

Subroutine RDUST_ONLINE reads global mineral dust concentrations as determined by P. Ginoux. Calculates dust optical depth at each level for the FAST-J routine "set_prof.f".

INTERFACE:

```
SUBROUTINE RDUST_ONLINE( am_I_Root, Input_Opt, State_Met, & State_Chm, DUST, ODSWITCH, & RC )
```

USES:

```
USE CMN_FJX_MOD
USE CMN_SIZE_MOD
USE CMN_DIAG_MOD
USE CHEMGRID_MOD,
                       ONLY : ITS_IN_THE_NOCHEMGRID
USE DIAG_MOD,
                       ONLY: AD21
USE ErrCode_Mod
USE ERROR_MOD,
                      ONLY : ERROR_STOP
                    ONLY : OptInput
USE Input_Opt_Mod,
USE State_Chm_Mod,
                       ONLY : ChmState
USE State_Met_Mod,
                       ONLY : MetState
USE TRANSFER_MOD,
                       ONLY: TRANSFER_3D
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

REAL(fp), INTENT(IN) :: DUST(IIPAR, JJPAR, LLPAR, NDUST) ! Dust [kg/m3]

INTEGER, INTENT(IN) :: ODSWITCH
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REVISION HISTORY:

```
01 Apr 2004 - R. Martin, R. Park - Initial version
(1) Bundled into "dust_mod.f" (bmy, 4/1/04)
(2 ) Now references DATA_DIR from "directory_mod.f". Now parallelize over
      the L-dimension for ND21 diagnostics. (bmy, 7/20/04)
(3) Archive only hydrophilic aerosol/aqueous dust surface area
     (excluding BCPO and OCPO), WTAREA and WERADIUS. (tmf, 3/6/09)
25 Aug 2010 - R. Yantosca - Added ProTeX headers
03 Feb 2011 - S. Kim.
                          - Include wavelength argument to determine the
                            wavelength at which the AOD should be computed.
                            This will set the optical properties that are
                            used for the calculation of the AOD. The ND21
                            diagnostic should only be updated when
                            WAVELENGTH = 1. (skim, 02/03/11)
                          - WAVELENGTH now ODSWITCH for clarity now
04 Sep 2012 - D. Ridley
                            that multiple wavelengths can be
                            calculated at once.
                          - Replaced all met field arrays with State_Met
09 Nov 2012 - M. Payer
                            derived type object
23 Jun 2014 - R. Yantosca - Now accept am_I_Root, Input_Opt, RC
12 May 2016 - M. Sulprizio- Remove 1D arrays that depend on JLOOP. ERADIUS,
                            TAREA, WERADIUS, WTAREA are now pointers that
                            point to 3D fields in State_Chm.
```

16 May 2016 - M. Sulprizio- Remove JLOOP entirely and loop over LLPAR, JJPAR,

IIPAR instead.

8.3.6 rdust_offline

Subroutine RDUST_OFFLINE reads global mineral dust concentrations as determined by P. Ginoux. Calculates dust optical depth at each level for the FAST-J routine "set_prof.f".

INTERFACE:

```
SUBROUTINE RDUST_OFFLINE( am_I_Root, Input_Opt, State_Met, & State_Chm, THISMONTH, THISYEAR, & ODSWITCH, RC)
```

USES:

USE	BPCH2_MOD,	ONLY	:	<pre>GET_NAME_EXT,</pre>	GET_RES_EXT
USE	BPCH2_MOD,	ONLY	:	GET_TAUO,	READ_BPCH2
USE	CHEMGRID_MOD,	ONLY	:	ITS_IN_THE_NOCHEMGRID	
USE	CMN_FJX_MOD				
USE	CMN_DIAG_MOD				
USE	DIAG_MOD,	ONLY	:	AD21	
USE	ErrCode_Mod				
USE	ERROR_MOD,	ONLY	:	ERROR_STOP	

```
USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState
USE TRANSFER_MOD, ONLY : TRANSFER_3D
```

IMPLICIT NONE

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

INTEGER, INTENT(IN) :: THISMONTH ! Current month (1-12)

INTEGER, INTENT(IN) :: THISYEAR ! Current year (YYYY format)

INTEGER, INTENT(IN) :: ODSWITCH ! Determine which wavelength to

! use for optical properties
```

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

- (1) RDUST was patterned after rdaerosol.f (rvm, 9/30/00)
- (2) Don't worry about rewinding the binary file...reading from binary files is pretty fast. And it's only done once a month.
- (3) Now references punch file utility routines from F90 module "bpch2_mod.f". Also reference variable DATA_DIR from the header file "CMN_SETUP". (bmy, 9/30/00)
- (4) Now selects proper GEOS-STRAT dust field for 1996 or 1997.

 Also need to pass THISYEAR thru the arg list. (rvm, bmy, 11/21/00)
- (5) CONC is now declared as REAL(fp) (rvm, bmy, 12/15/00)
- (6) Removed obsolete code from 12/15/00 (bmy, 12/21/00)
- (7) CONC(IIPAR, JJPAR, LGLOB, NDUST) is now CONC(IIPAR, JJPAR, LLPAR, NDUST).

 Now use routine TRANSFER_3D from "transfer_mod.f" to cast from REAL*4

 to REAL(fp) and also to convert from {IJL}GLOB to IIPAR, JJPAR, LLPAR

 space. Use 3 arguments in call to GET_TAUO. Updated comments.

 (bmy, 9/26/01)
- (8) Removed obsolete code from 9/01 (bmy, 10/24/01)
- (9) Now reference ERADIUS, IXSAVE, IYSAVE, IZSAVE, TAREA from

- "comode_mod.f". Compute ERADIUS and TAREA for the NDUST dust size bins from FAST-J. Renamed CONC to DUST to avoid conflicts. Also reference NTTLOOP from "comode.h". Also added parallel DO-loops. Also renamed MONTH and YEAR to THISMONTH and THISYEAR to avoid conflicts w/ other variables. (bmy, 11/15/01)
- (10) Bug fix: Make sure to use 1996 dust data for Dec 1995 for the GEOS-STRAT met field dataset. Set off CASE statement with an #if defined(GEOS_STRAT) block. (rvm, bmy, 1/2/02)
- (11) Eliminate obsolete code from 1/02 (bmy, 2/27/02)
- (12) Now report dust optical depths in ND21 diagnostic at 400 nm. Now report dust optical depths as one combined diagnostic field instead of 7 separate fields. Now reference JLOP from "comode_mod.f". Now save aerosol surface areas as tracer #5 of the ND21 diagnostic. (rvm, bmy, 2/28/02)
- (13) Remove declaration for TIME, since that is also defined in the header file "comode.h" (bmy, 3/20/02)
- (14) Now read mineral dust files directly from the DATA_DIR/dust_200203/ subdirectory (bmy, 4/2/02)
- (15) Now reference BXHEIGHT from "dao_mod.f". Also reference ERROR_STOP from "error_mod.f". (bmy, 10/15/02)
- (16) Now call READ_BPCH2 with QUIET=TRUE to suppress extra informational output from being printed. Added cosmetic changes. (bmy, 3/14/03)
- (17) Since December 1997 dust data does not exist, use November 1997 dust data as a proxy. (bnd, bmy, 6/30/03)
- (18) Bundled into "dust_mod.f" and renamed to RDUST_OFFLINE. (bmy, 4/1/04)
- (19) Now references DATA_DIR from "directory_mod.f". Now parallelize over the L-dimension for ND21 diagnostic. (bmy, 7/20/04)
- (20) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (21) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (22) Archive only hydrophilic aerosol/aqueous dust surface area (excluding BCPO and OCPO), WTAREA and WERADIUS. (tmf, 3/6/09)
- 25 Aug 2010 R. Yantosca Added ProTeX headers
- O3 Feb 2011 S. Kim Include third input argument to determine the wavelength at which the AOD should be computed. This will set the optical properties that are used for the calculation of the AOD. The ND21 diagnostic should only be updated when WAVELENGTH = 1.
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 04 Sep 2012 D. Ridley WAVELENGTH now ODSWITCH for clarity now that multiple wavelengths can be calculated at once.
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 17 Dec 2014 R. Yantosca Leave time/date variables as 8-byte
- 05 Mar 2015 R. Yantosca Add Input_Opt%RES_DIR to data path

```
23 Oct 2015 - E. Lundgren - Fix index for dust in ODAER/LUT arrays if UCX on 12 May 2016 - M. Sulprizio- Remove 1D arrays that depend on JLOOP. ERADIUS, TAREA, WERADIUS, WTAREA are now pointers that point to 3D fields in State_Chm.

16 May 2016 - M. Sulprizio- Remove JLOOP entirely and loop over LLPAR, JJPAR, IIPAR instead.
```

8.3.7 get_dust_alk

Subroutine GET_DUST_ALK returns: (1) dust alkalinity, ALK_d(NDSTBIN) [v/v], (2) rate coefficients, KTS(NDSTBIN), KTN(NDSTBIN), for uptake of SO2 and HNO3 on dust for use in sulfate_mod.f for chemistry on dust aerosols, (3) fraction, KTH(NDSTBIN), of the size-weighted total area of aerosols in the grid box. GET_DUST_ALK is analogous to GET_ALK for seasalt (bec, 12/7/04; tdf 04/08/08)

INTERFACE:

```
SUBROUTINE GET_DUST_ALK( I, J, L, ALK_d, KTS, KTN, KTH, & Input_Opt, State_Met, State_Chm)
```

USES:

```
USE CMN_SIZE_MOD ! Size parameters
USE ERROR_MOD, ONLY : IT_IS_NAN
USE Input_Opt_Mod, ONLY : OptInput
USE PhysConstants, ONLY : PI, AIRMW
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

INPUT/OUTPUT PARAMETERS:

OUTPUT PARAMETERS:

```
REAL(fp),
                INTENT(OUT)
                              :: ALK_d(NDSTBIN) ! Dust alkalinity [v/v]
REAL(fp),
                INTENT(OUT)
                              :: KTS (NDSTBIN) ! Rate coef for uptake of
                                                 ! SO2 on dust [s-1]
                                       (NDSTBIN) ! Rate coef for uptake of
REAL(fp),
                INTENT(OUT)
                              :: KTN
                                                 ! HNO3 on dust [s-1]
REAL(fp),
                INTENT(OUT)
                              :: KTH (NDSTBIN) ! Fraction of the size-
                                                 ! weighted total area
                                                 ! of aerosols in grid box
```

8.3.8 init_dust

Subroutine INIT_DUST allocates all module arrays.

INTERFACE:

```
SUBROUTINE INIT_DUST( am_I_Root, Input_Opt, State_Chm, RC )
```

USES:

```
USE CMN_SIZE_MOD
      USE ErrCode_Mod
      USE ERROR MOD.
                              ONLY : ALLOC_ERR
                            ONLY : ERROR_STOP
ONLY : OptInput
ONLY : PI, AIRMW
      USE ERROR_MOD,
      USE Input_Opt_Mod,
      USE PhysConstants,
      USE Species_Mod,
                              ONLY : Species
      USE State_Chm_Mod,
                              ONLY : ChmState
      USE State_Chm_Mod,
                               ONLY : Ind_
      defined( TOMAS )
#if
      USE TOMAS_MOD,
                          ONLY : IBINS, Xk
#endif
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
30 Mar 2004 - R. Yantosca - Initial version
(1) Now references LDEAD from "logical_mod.f" (bmy, 7/20/04)
(2) Modify to work with 30bin dust. Reference to IBINS from tomas_mod
     for number of total bin = 30 bins. (win, 7/17/09)
25 Aug 2010 - R. Yantosca - Added ProTeX headers
14 Nov 2012 - R. Yantosca - Add am_I_Root, Input_Opt, RC as arguments
26 Feb 2013 - M. Long
                         - Now use fields from Input_Opt
12 Sep 2013 - M. Sulprizio- Add modifications for acid uptake on dust
                           aerosols (T.D. Fairlie)
23 Sep 2015 - R. Yantosca - Now accept State_Chm as an argument so that
                           we can use the species database
30 Sep 2015 - R. Yantosca - DD_A_Density is now renamed to Density
30 Sep 2015 - R. Yantosca - DD_A_Radius is now renamed to Radius
05 Jan 2016 - E. Lundgren - Use global parameter PI
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
16 Jun 2016 - J. Kaiser - Now define species ID's with Ind_() function
20 Jun 2016 - R. Yantosca - Only define species ID's in the INIT phase
24 Jun 2016 - R. Yantosca - Add error checks for dust uptake species
```

8.3.9 cleanup_dust

Subroutine CLEANUP_DUST deallocates all module arrays.

INTERFACE:

SUBROUTINE CLEANUP_DUST

REVISION HISTORY:

```
30 Mar 2004 - R. Yantosca - Initial version
25 Aug 2010 - R. Yantosca - Added ProTeX headers
26 Feb 2013 - R. Yantosca - Now use Input_Opt instead of local arrays
```

8.4 Fortran: Module Interface seasalt_mod.F

Module SEASALT_MOD contains arrays and routines for performing either a coupled chemistry/aerosol run or an offline seasalt aerosol simulation. Original code taken from Mian Chin's GOCART model and modified accordingly. (bec, rjp, bmy, 6/22/00, 11/23/09)

INTERFACE:

MODULE SEASALT_MOD

USES:

USE HCO_ERROR_MOD

USE PRECISION_MOD ! For GEOS-Chem Precision (fp)
USE PHYSCONSTANTS

IMPLICIT NONE PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: CHEMSEASALT
PUBLIC :: CLEANUP_SEASALT
PUBLIC :: INIT_SEASALT

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: WET_SETTLING
PRIVATE :: CHEM_MOPO
PRIVATE :: CHEM_MOPI

PUBLIC DATA MEMBERS:

PUBLIC :: SALT_V PUBLIC :: DMID

REMARKS:

Seasalt aerosol species: (1) Accumulation mode (usually 0.1 - 0.5 um)
(2) Coarse mode (usually 0.5 - 10.0 um)

NOTE: You can change the bin sizes for accumulation mode and coarse mode seasalt in the "input.geos" file in v7-yy-zz and higher. References:

- (1) Chin, M., P. Ginoux, S. Kinne, B. Holben, B. Duncan, R. Martin, J. Logan, A. Higurashi, and T. Nakajima, "Tropospheric aerosol optical thickness from the GOCART model and comparisons with satellite and sunphotometers measurements", J. Atmos Sci., 2001.
- (2) Gong, S., L. Barrie, and J.-P. Blanchet, "Modeling sea-salt aerosols in the atmosphere. 1. Model development", J. Geophys. Res., v. 102, 3805-3818, 1997.

- (1) Now references "logical_mod.f" and "tracer_mod.f". Comment out SS_SIZE, this has been replaced by SALA_REDGE_um and SALC_REDGE_um from "tracer_mod.f". Increased NR_MAX to 200. (bmy, 7/20/04)
- (2) Added error check in EMISSSEASALT (bmy, 1/20/05)
- (3) Now references "pbl_mix_mod.f" (bmy, 2/22/05)
- (4) Added routine GET_ALK to account for alkalinity. (bec, bmy, 4/13/05)
- (5) Now references XNUMOL from "tracer_mod.f" (bmy, 10/25/05)
- (6) Now only call dry deposition routine if LDRYD=T (bec, bmy, 5/23/06)
- (7) Remove unused variables from GET_ALK. Also fixed variable declaration bug in WET_SETTLING. (bec, bmy, 9/5/06)

```
(8) Extra error check for low RH in WET_SETTLING (phs, 6/11/08)
(9) Bug fix to remove a double-substitution in GET_ALK (bec, bmy, 7/18/08)
(10) Save surface emissions separately (emis_save) for non-local scheme.
      (ccc, 5/14/09)
(11) Bug fixes in GET_ALK and SRCSALT (bec, lyj, bmy, 11/23/09)
(12) Add size-resolved emission subroutine SRCSALT30 and reference to
      tomas_mod.f. (win, 7/17/09)
22 Dec 2011 - M. Payer
                         - Added ProTeX headers
16 Feb 2012 - R. Yantosca - Moved SRCSALT30 to end of module
01 Mar 2012 - R. Yantosca - Now reference new grid_mod.F90
04 Mar 2013 - R. Yantosca - Now call INIT_SULFATE from the init stage
                            which facilitates connection to GEOS-5 GCM
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
23 Jun 2014 - R. Yantosca - Remove code now made obsolete by HEMCO
03 Nov 2014 - C. Keller - Moved GET_ALK to sulfate_mod.F.
20 Nov 2014 - M. Yannetti - Added PRECISION_MOD
12 Jun 2015 - R. Yantosca - Removed DRY_DEPOSITION routine, because we
                           now apply drydep in mixing_mod.F90
16 Jun 2016 - C. Miller - Now define species ID's with Ind_ function
17 Jun 2016 - R. Yantosca - Add species ID's as module variables
29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90
```

8.4.1 chemseasalt

Subroutine CHEMSEASALT is the interface between the GEOS-CHEM main program and the seasalt chemistry routines that mostly calculates seasalt dry deposition (rjp, bmy, 1/24/02, 5/23/06)

INTERFACE:

USES:

```
USE CMN_SIZE_MOD

USE ErrCode_Mod

USE ERROR_MOD, ONLY : DEBUG_MSG

USE Input_Opt_Mod, ONLY : OptInput

USE State_Chm_Mod, ONLY : ChmState

USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

Dry deposition is now handled in mixing_mod.F90. We have removed the calls to the DRY_DEPOSITION routine here. (bmy, 6/12/15)

REVISION HISTORY:

```
    (1 ) Now reference STT from "tracer_mod.f". Now references LPRT from "logical_mod.f" (bmy, 7/20/04)
    (2 ) Now only call DRY_DEPOSITION if LDRYD=T (bec, bmy, 5/23/06)
    22 Dec 2011 - M. Payer - Added ProTeX headers
```

30 Jul 2012 - R. Yantosca - Now accept am_I_Root as an argument when running with the traditional driver main.F

13 Nov 2012 - R. Yantosca - Now add Input_Opt, RC arguments for GIGC

15 Nov 2012 - M. Payer - Now pass met fields via State_Met object

25 Mar 2013 - M. Payer $\,$ - Now pass State_Chm object via the arg list

12 Jun 2015 - R. Yantosca - Drydep is now handled in mixing_mod.F90, so we can greatly collapse this code

17 Jun 2016 - R. Yantosca - Add error checks before calling routines

30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

10 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code

20 Sep 2016 - R. Yantosca - Bug fix: rewrite invalid (LMPOA > 0) test

8.4.2 wet_settling

Subroutine WET_SETTLING performs wet settling of sea salt. (bec, rjp, bmy, 4/20/04, 6/11/08)

INTERFACE:

```
SUBROUTINE WET_SETTLING( am_I_Root, Input_Opt, State_Met, & State_Chm, TC, N, & RC )
```

USES:

```
USE CMN_DIAG_MOD

USE CMN_SIZE_MOD

#if defined( BPCH_DIAG )

USE DIAG_MOD, ONLY : AD44

#endif
```

USE ErrCode_Mod USE ERROR_MOD, ONLY : DEBUG_MSG USE ERROR_MOD, ONLY : ERROR_STOP USE GC_GRID_MOD, ONLY : GET_AREA_CM2 USE Input_Opt_Mod, ONLY : OptInput USE PhysConstants USE State_Chm_Mod, ONLY : ChmState USE State_Met_Mod, ONLY : MetState USE TIME_MOD, ONLY : GET_TS_CHEM #if defined(NC_DIAG) USE HCO_INTERFACE_MOD, ONLY : HcoState USE ERROR_MOD, ONLY : ERROR_STOP USE HCO_ERROR_MOD, ONLY : HCO_SUCCESS USE HCO_DIAGN_MOD, ONLY : Diagn_Update

#endif

INPUT PARAMETERS:

:: N INTEGER, INTENT(IN) ! 1=accum mode; ! 2=coarse mode LOGICAL, INTENT(IN) :: am_I_Root ! Root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options TYPE(MetState), INTENT(IN) :: State_Met ! MeteorologyState TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object

INPUT/OUTPUT PARAMETERS:

REAL(fp), INTENT(INOUT) :: TC(IIPAR, JJPAR, LLPAR) ! Sea salt [kg]

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success/failure

- (1) Now references SALA_REDGE_um and SALC_REDGE_um from "tracer_mod.f" (bmy, 7/20/04)
- (2) Now references XNUMOL from "tracer_mod.f" (bmy, 10/25/05)
- (3) Bug fix: DTCHEM has to be REAL(fp), not integer. (bmy, 9/7/06)
- (4) Now limit relative humidity to [tiny(real(fp)),0.99] range for DLOG argument (phs, 5/1/08)
- (5) Update sea salt density calculation using Tang et al. (1997) (bec, jaegle 5/11/11)
- (6) Update hygroscopic growth for sea salt using Lewis and Schwartz (2006) and and density calculation based on Tang et al. (1997) (bec, jaegle 5/11/11)
- (7) Itegrate settling velocity over entire size distribution (jaegle 5/11/11)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 01 Mar 2012 R. Yantosca Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
- 14 Nov 2012 R. Yantosca Add am_I_Root, Input_Opt, RC as arguments

```
15 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met
derived type object

19 Mar 2013 - R. Yantosca - Now copy Input_Opt%XNUMOL(1:N_TRACERS)

12 Jun 2013 - R. Yantosca - Bug fix: SALT_MASS needs to be !OMP PRIVATE

12 Jun 2013 - R. Yantosca - Reformatted some comments for clarity

26 Feb 2015 - E. Lundgren - Replace GET_PCENTER with State_Met%PMID.
Remove dependency on pressure_mod.

25 Jan 2016 - E. Lundgren - Update netcdf drydep flux diagnostic

29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts

31 May 2016 - E. Lundgren - Remove usage of Input_Opt%XNUMOL

22 Jun 2016 - M. Yannetti - Replaced TCVV with spec db and phys constant
```

8.4.3 chem_mopo

Subroutine CHEM_MOPO modifies hydrophobic marine organic aerosol concentrations based on the conversion to hydrophilic marine organic aerosols.

INTERFACE:

```
SUBROUTINE CHEM_MOPO( am_I_Root, Input_Opt, State_Chm, RC )
```

USES:

```
USE CMN_DIAG_MOD
USE CMN_SIZE_MOD
USE ErrCode_Mod
USE Input_Opt_Mod,
```

USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE TIME_MOD, ONLY : GET_TS_CHEM

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success?
```

REMARKS:

```
10 Jul 2015 - E. Lundgren - Initial version (based on routine Chem_OCPO)
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.
```

8.4.4 chem_mopi

Subroutine CHEM_MOPI modifies hydrophilic marine organic aerosol concentrations based on the conversion from hydrophobic marine organic aerosols.

INTERFACE:

```
SUBROUTINE CHEM_MOPI( am_I_Root, Input_Opt, State_Chm, RC )
```

USES:

```
USE CMN_DIAG_MOD
USE CMN_SIZE_MOD
USE ErrCode_Mod
```

USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE TIME_MOD, ONLY : GET_TS_CHEM

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success?
```

REMARKS:

REVISION HISTORY:

```
10 Jul 2015 - E. Lundgren - Initial version (based on routine Chem_OCPI)
```

8.4.5 init_seasalt

Subroutine INIT_SEASALT initializes and zeroes all module arrays (bmy, 4/26/04, 4/13/05)

INTERFACE:

```
SUBROUTINE INIT_SEASALT( am_I_Root, Input_Opt, State_Chm, RC )
```

USES:

```
USE CMN_SIZE_MOD
USE ErrCode_Mod
```

```
USE ERROR_MOD, ONLY : ALLOC_ERR
USE Input_Opt_Mod, ONLY : OptInput
USE Species_Mod, ONLY : Species
USE State_Chm_Mod, ONLY : ChmState
USE State_Chm_Mod, ONLY : Ind_
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root
TYPE(OptInput), INTENT(IN) :: Input_Opt
TYPE(ChmState), INTENT(IN) :: State_Chm
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC

REVISION HISTORY:

13 Oct 2016 - R. Yantosca - Now allocate OCCONV for marine-POA simulations

8.4.6 cleanup_seasalt

Subroutine CLEANUP_SEASALT deallocates all module arrays (bmy, 4/26/04, 4/13/05)

INTERFACE:

SUBROUTINE CLEANUP_SEASALT

REVISION HISTORY:

```
(1) Now deallocates ALK_EMIS, N_DENS, SRC_N (bec, bmy, 4/13/05)
```

- (2) Deallocated SALT_V and DMID (jaegle 5/11/11)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 13 Oct 2016 R. Yantosca Bug fix: now deallocate OCCONV array

8.4.7 srcsalt30

Subroutine SRCSALT30 emits sea-salt into the 30-bin sea-salt mass and aerosol number arrays. Sea-salt emission parameterization of Clarke et al. [2006] (win, 7/17/09)

INTERFACE:

```
SUBROUTINE SRCSALT30( TC1, TC2, State_Met )
```

USES:

USE TOMAS_MOD,

USE TIME_MOD,

INPUT PARAMETERS:

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

ONLY : GET_TS_EMIS

ONLY : IBINS, Xk

INPUT/OUTPUT PARAMETERS:

```
! TC1 : Aerosol number tracer array [no.]
! TC2 (REAL(fp) ) : Sea salt tracer array [kg]
REAL(fp), INTENT(INOUT) :: TC1(IIPAR, JJPAR, LLPAR, IBINS)
REAL(fp), INTENT(INOUT) :: TC2(IIPAR, JJPAR, LLPAR, IBINS)
```

AUTHOR:

```
Contact: Win Trivitayanurak (win@cmu.edu)
```

Arguments as Input/Output:

REMARKS:

References:

(1) Clarke, A.D., Owens, S., Zhou, J. " An ultrafine sea-salt flux from breaking waves: Implications for CCN in the remote marine atmosphere" JGR, 2006

- (1) Originally from emisnaN3clarke.f in GISS GCM-II' (win, 7/18/07)
- (2) Now partition emission throughout the PBL (win, 7/18/07)
- (3) Add COEF to adjust emission in a 1x1 nested-grid (win, 4/27/08)
- 16 Feb 2012 R. Yantosca Added ProTeX headers
- 01 Mar 2012 R. Yantosca Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
- 01 Mar 2012 R. Yantosca A_M2 is now a scalar
- 10 Mar 2014 J. Pierce Avoid sea salt emissions over ice
- 25 Jul 2014 R. Yantosca Remove reference to function SFCWINDSQR

8.5 Fortran: Module Interface sulfate_mod.F

Module SULFATE_MOD contains arrays and routines for performing either a coupled chemistry/aerosol run or an offline sulfate aerosol simulation. Original code taken from Mian Chin's GOCART model and modified accordingly. (rjp, bdf, bmy, 6/22/00, 8/26/10)

INTERFACE:

MODULE SULFATE_MOD

USES:

```
USE HCO_ERROR_MOD ! For HEMCO error handling
USE PhysConstants ! Physical constants
USE PRECISION_MOD ! For GEOS-Chem Precision (fp, f4, f8)

IMPLICIT NONE
```

PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: CHEMSULFATE
PUBLIC :: CLEANUP_SULFATE
PUBLIC :: INIT_SULFATE
```

#if defined(TOMAS)

PRIVATE

PUBLIC :: EMISSSULFATETOMAS ! JKodros (6/2/15 - this is to connect TOMAS to HEMCO) #endif

REMARKS:

References:

- (1) Andreae, M.O. & P. Merlet, "Emission of trace gases and aerosols from biomass burning", Global Biogeochem. Cycles, 15, 955-966, 2001.
- (2) Nightingale et al [2000a], J. Geophys. Res, 14, 373-387
- (3) Nightingale et al [2000b], Geophys. Res. Lett, 27, 2117-2120
- (4) Wanninkhof, R., "Relation between wind speed and gas exchange over the ocean", J. Geophys. Res, 97, 7373-7382, 1992.

- (1) All module variables are declared PRIVATE (i.e., they can only be seen from within this module (bmy, 6/2/00)
- (2) The routines in "sulfate_mod.f" assume that we are doing chemistry over the global region (e.g. IIPAR=IIPAR, JJPAR=JJPAR). (bmy, 6/8/00)
- (3) Removed obsolete code from DRYDEP_SULFATE (bmy, 12/21/00)
- (4) Removed obsolete commented-out code from module routines (bmy, 4/23/01)
- (5) Now read data files from DATA_DIR/sulfate_sim_200106/ (bmy, 6/19/01)
- (6) Updated comments (bmy, 9/4/01)
- (7) XTRA2(IREF, JREF, 5) is now XTRA2(I, J). Now reference COSSZA from

- "dao_mod.f". (bmy, 9/27/01)
- (8) Removed obsolete commented out code from 9/01 (bmy, 10/24/01)
- (9) Minor fixes to facilitate compilation on ALPHA (bmy, 11/15/01)
- (11) Now divide module header into MODULE PRIVATE, MODULE VARIABLES, and MODULE ROUTINES sections. Updated comments (bmy, 5/28/02)
- (12) Replaced all instances of IM with IIPAR and JM with JJPAR, in order to prevent namespace confusion for the new TPCORE (bmy, 6/25/02)
- (13) Now reference "file_mod.f" (bmy, 6/27/02)
- (14) Now references GET_PEDGE from "pressure_mod.f", which computes P at the bottom edge of grid box (I,J,L). Also deleted obsolete, commented-out code. (dsa, bdf, bmy, 8/21/02)
- (15) Added updated code from Rokjin Park and Brendan Field, in order to perform coupled chemistry-aerosol simulations. Also added parallel DO-loops in several subroutines. Updated comments, cosmetic changes. Now reference "error_mod.f" and "wetscav_mod.f". Now only do chemistry below the tropopause. (rjp, bdf, bmy, 12/6/02)
- (16) Added ENH3_na array to hold natural source NH3 emissions. Also now facilitate passing DMS, SO2, SO4, NH3 to SMVGEAR for fullchem simulations. Added subroutine READ_NATURAL_NH3. (rjp, bmy, 3/23/03)
- (17) Now references "grid_mod.f" and "time_mod.f". Also made other minor cosmetic changes. (bmy, 3/27/03)
- (18) Updated chemistry routines to apply drydep losses throughout the entire PBL. (rjp, bmy, 8/1/03)
- (19) Now accounts for GEOS-4 PBL being in meters (bmy, 1/15/04)
- (20) Fix ND44 diag so that we get same results for sp or mp (bmy, 3/24/04)
- (21) Added COSZM array. Now use diurnal varying JH202 in CHEM_H202. (rjp, bmy, 3/39/04)
- (22) Added more parallel DO-loops (bmy, 4/14/04)
- (23) Now add SO2 from ships (bec, bmy, 5/20/04)
- (24) Now references "directory_mod.f", "logical_mod.f" and "tracer_mod.f". Now removed IJSURF. (bmy, 7/20/04)
- (25) Can overwrite USA with EPA/NEI99 emissions (rjp, rch, bmy, 11/16/04)
- (26) Modified for AS, AHS, LET, SO4aq, NH4aq (cas, bmy, 1/11/05)
- (27) Now also references "pbl_mix_mod.f". NOTE: Comment out phase transition code for now since it is still under development and will take a while to be rewritten. (bmy, 3/15/05)
- (28) Modified for SO4s, NITs chemistry (bec, 4/13/05)
- (29) Now reads updated files for SST and offline chemistry. Now read data for both GCAP and GEOS grids. Now references "tropopause_mod.f". (bmy, 8/22/05)
- (30) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (31) Now references XNUMOL & XNUMOLAIR from "tracer_mod.f" (bmy, 10/25/05)
- (32) Now read int'annual SST data on GEOS 1x1 grid (bmy, 11/17/05)
- (33) Bug fix for offline aerosol sim in SEASALT_CHEM (bec, bmy, 3/29/06)
- (34) Bug fix in INIT_DRYDEP (bmy, 5/23/06)
- (35) Now references "bravo_mod.f" (rjp, kfb, bmy, 6/26/06)
- (36) Now references "streets_anthro_mod.f" (yxw, bmy, 8/17/06)
- (37) Now references "biomass_mod.f" (bmy, 9/27/06)

- (38) Now prevent seg fault error in READ_BIOFUEL_SO2 (bmy, 11/3/06)
- (39) Bug fix in SEASALT_CHEM (havala, bec, bmy, 12/8/06)
- (40) Extra error check for low RH in GRAV_SETTLING (phs, 6/11/08)
- (41) Now references "cac_anthro_mod.f". And apply SO2 yearly scale factor to SO2 from GEIA (amv, phs, 3/11/08)
- (41) Bug fixes in reading EDGAR data w/ the right tracer number, when we are doing offline or nonstd simulations (dkh, 10/31/08)
- (42) Bug fix for AD13_SO2_sh in SRCSO2 (phs, 2/27/09)
- (43) Bug fix: need to add CAC_AN to PRIVATE statements (bmy, 5/27/09)
- (44) Constrain surface emissions to the first level and save them into emis_save (lin, 5/29/09)
- (45) Last year of SST data is now 2008 (see READ_SST) (bmy, 7/13/09)
- (46) Updated rxns in CHEM_DMS and CHEM_SO2 to JPL 2006 (jaf, bmy, 10/15/09)
- (47) Added new volcanic emissions of SO2 (jaf, bmy, 10/15/09)
- (48) Now accounts for NEI 2005 emissions, and multilevels S0xan emissions (amv, phs, 10/15/2009)
- (49) Fixes in SRCSO2 for SunStudio compiler (bmy, 12/3/09)
- (50) Add new subroutine SRCSF30 for emission to 30bin sulfate (win, 1/25/10)
- (51) Add new array PSO4_SO2AQ for SO4 produced via aqueous chemistry of SO2 excluding that from heterogeous reaction on sea-salt. (win, 1/25/10)
- (52) Standardized patch in READ_ANTHRO_NH3 (dkh, bmy, 3/5/10)
- (53) Use LWC from GEOS-5 met fields (jaf, bmy, 6/30/10)
- (54) Add module parameters MNYEAR_VOLC and MXYEAR_VOLC to define the 1st and last year with data for volcanic emissions. (ccc, 9/30/10)
- (55) Use updated volcanic emissions from 1979 to 2009
- 26 Aug 2010 R. Yantosca Add modifications for MERRA
- 12 Nov 2010 R. Yantosca Avoid div-by-zero when computing L2S, L3S
- 07 Sep 2011 P. Kasibathla Modified to include GFED3
- 22 Dec 2011 M. Payer Added ProTeX headers
- 08 Feb 2012 R. Yantosca Add modifications for GEOS-5.7.2 met
- 01 Mar 2012 R. Yantosca Now reference new grid_mod.F90
- 13 Mar 2012 M. Cooper Changed regrid algorithm to map_a2a
- 28 Nov 2012 R. Yantosca Use SUNCOS fields from the State_Met object
- 04 Mar 2013 R. Yantosca Now call INIT_SULFATE from the init stage which facilitates connection to GEOS-5 GCM
- 05 Mar 2013 R. Yantosca Now use Input_Opt%LNLPBL instead of LNLPBL from logical_mod.F
- 13 Mar 2013 R. Yantosca Bug fix: make sure we pass values to the SOIL_DRYDEP routine even when ND44 is off
- 30 May 2013 S. Farina Merged TOMAS code into sulfate_mod.F
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 12 Sep 2013 M. Sulprizio Add modifications for acid uptake on dust aerosol (T.D. Fairlie)
- 18 Sep 2014 M. Sulprizio Get oxidant fields for offline aerosol simulation from HEMCO
- 03 Nov 2014 C. Keller Incorporated GET_ALK from seasalt_mod.F
- 20 Nov 2014 M. Yannetti Added PRECISION_MOD
- 04 Mar 2015 R. Yantosca Remove obsolete, commented-out code

```
04 Mar 2015 - R. Yantosca - Use REAL(f4) for pointer args to HCO_GetPtr

22 May 2015 - R. Yantosca - Remove variables made obsolete by HEMCO

12 Jun 2015 - R. Yantosca - Now remove orphaned ND44 variables

12 Jun 2015 - R. Yantosca - Remove CHEM_NH3 and CHEM_NH4 routines

because drydep is now done in mixing_mod.F90

23 Sep 2015 - R. Yantosca - Remove DRY* flags for most species except

for those used in GRAV_SETTLING

05 Jan 2016 - E. Lundgren - Use global physical parameters

04 Aug 2016 - M. Yannetti - Replace TCVV with spc db MW and phys constant

29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90
```

8.5.1 get_vcldf

Subroutine GET_VCLDF computes the volume cloud fraction for SO2 chemistry. (rjp, bdf, bmy, 9/23/02)

INTERFACE:

```
SUBROUTINE GET_VCLDF( am_I_Root, State_Met, RC )
```

USES:

```
USE CMN_SIZE_MOD
USE ErrCode_Mod
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

OUTPUT PARAMETERS:

REMARKS:

References:

(1) Sundqvist et al. [1989]

```
14 Jan 2011 - R. Yantosca - Return if VCLDF is not allocated
22 Dec 2011 - M. Payer - Added ProTeX headers
14 Nov 2012 - R. Yantosca - Added am_I_Root, RC arguments
15 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met derived type object
26 Feb 2015 - E. Lundgren - Replace GET_PCENTER and GET_PEDGE with State_Met%PMID and State_Met%PEDGE.

Remove dependency on pressure_mod.
```

8.5.2 get_lwc

Function GET_LWC returns the cloud liquid water content [m3 H2O/m3 air] at a GEOS-CHEM grid box as a function of temperature. (rjp, bmy, 10/31/02, 1/14/03)

INTERFACE:

```
FUNCTION GET_LWC( T ) RESULT( LWC )
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: T ! Temperature value at a GEOS-CHEM grid box [K]
```

RETURN VALUE:

```
REAL(fp) :: LWC
```

REVISION HISTORY:

```
18 Jan 2011 - R. Yantosca - Updated comments
22 Dec 2011 - M. Payer - Added ProTeX header
```

8.5.3 chemsulfate

Subroutine CHEMSULFATE is the interface between the GEOS-CHEM main program and the sulfate chemistry routines. The user has the option of running a coupled chemistry-aerosols simulation or an offline aerosol simulation. (rjp, bdf, bmy, 5/31/00, 3/16/06)

INTERFACE:

```
SUBROUTINE CHEMSULFATE( am_I_Root, Input_Opt,
& State_Met, State_Chm, RC )
```

USES:

```
USE CMN_SIZE_MOD
USE ErrCode_Mod
USE ERROR_MOD
USE HCO_EMISLIST_MOD,
                        ONLY : HCO_GetPtr
USE HCO_INTERFACE_MOD,
                        ONLY : HcoState
USE Input_Opt_Mod,
                        ONLY : OptInput
USE State_Chm_Mod,
                        ONLY : ChmState
USE State_Chm_Mod,
                        ONLY : Ind_
USE State_Met_Mod,
                        ONLY : MetState
USE TIME_MOD,
                        ONLY : GET_MONTH
USE TIME_MOD,
                        ONLY : GET_TS_CHEM
USE TIME_MOD,
                        ONLY : GET_ELAPSED_SEC
USE TIME_MOD,
                        ONLY : ITS_A_NEW_MONTH
USE UCX_MOD,
                        ONLY : SETTLE_STRAT_AER
USE UnitConv_Mod
```

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

- (1) Now reference all arguments except FIRSTCHEM and RH from either F90 modules or from common block header files. Updated comments, cosmetic changes. Added NH3, NH4, NITRATE chemistry routines. Also call MAKE_RH and CONVERT_UNITS from "dao_mod.f". Now references IDTDMS, IDTSO2 etc. from "tracerid_mod.f". Now make FIRSTCHEM a local SAVEd variable. Now reference DEPSAV from "drydep_mod.f". Also get rid of extraneous dimensions of DEPSAV. Added NTIME, NHMSb arrays for OHNO3TIME. (rjp, bdf, bmy, 12/16/02)
- (2) CHEM_DMS is now only called for offline sulfate simulations. (rjp, bmy, 3/23/03)
- (3) Now remove NTIME, NHMSb from the arg list and call to OHNO3TIME.

 Now references functions GET_MONTH, GET_TS_CHEM, and GET_ELAPSED_SEC from the new "time_mod.f". (bmy, 3/27/03)
- (4) Now reference STT, TCVV, N_TRACERS, ITS_AN_AEROSOL_SIM from "tracer_mod.f". Now reference ITS_A_NEW_MONTH from "time_mod.f". Now references LPRT from "logical_mod.f". (bmy, 7/20/04)
- (5) Updated for AS, AHS, LET, SO4aq, NH4aq. Now references LCRYST from logical_mod.f. Now locate species in the DEPSAV array w/in INIT_SULFATE. (bmy, 12/21/04)
- (6) Now handle gravitational settling of SO4s, NITs (bec, bmy, 4/13/05)
- (7) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (8) Remove reference to MAKE_RH, it's not needed here (bmy, 3/16/06)
- (9) Reference to LTOMAS and add call CHEM_SO4_AQ using aqueous oxidation which is one of the TOMAS microphysics subroutine (win, 1/25/10)
- 05 Oct 2011 R. Yantosca SUNCOS is no longer needed here
- 22 Dec 2011 M. Payer Added ProTeX headers
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 14 Nov 2012 R. Yantosca Add Input_Opt, RC as arguments
- 15 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 04 Mar 2013 R. Yantosca Remove call to INIT_SULFATE
- 19 Mar 2013 R. Yantosca Now copy Input_Opt%TCVV(1:N_TRACERS)
- 25 Mar 2013 M. Payer Now pass State_Chm object via the arg list
- 23 Apr 2013 R. Yantosca Remove LTOMAS logical, since we now invoke TOMAS

```
with either TOMAS=yes or TOMAS40=yes
31 May 2013 - R. Yantosca - Now pass am_I_root, Input_Opt, State_Chm
                            and RC to TOMAS routine CHEM_SO4_AQ
12 Sep 2013 - M. Sulprizio- Include gravitational settling of dust_sulfate
                            and dust_nitrate. Changes made to CHEM_SO2 and
                            CHEM_SO4 (tdf, 04/07/08)
23 Oct 2013 - R. Yantosca - Now pass objects to GET_GLOBAL_OH routine
18 Sep 2014 - M. Sulprizio- Get oxidant fields for offline aerosol
                            simulation from HEMCO
30 Sep 2015 - E. Lundgren - Now use UNITCONV_MOD conversion routines
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
                          - Remove references to TRACERID_MOD and replace
16 Jun 2016 - M. Long
                            with STATE_CHM_MOD::Ind_()
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected
                            species ID from State_Chm%Map_Advect.
11 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code
```

8.5.4 emisssulfatetomas

Subroutine EMISSSULFATETOMAS connects HEMCO bulk emissions to the TOMAS tracers. Only use this for TOMAS sims. This should be quite similar to the TOMAS relevant parts of 'emisssulfate' in v9 (Jkodros 6/2/15)

INTERFACE:

```
SUBROUTINE EMISSSULFATETOMAS( am_I_Root, Input_Opt, & State_Met, State_Chm, RC )
```

USES:

```
USE CMN_DIAG_MOD
USE CMN_SIZE_MOD
USE ErrCode_Mod
USE ERROR_MOD
USE Input_Opt_Mod,
                        ONLY : OptInput
USE State_Chm_Mod,
                        ONLY : ChmState
USE State_Met_Mod,
                        ONLY : MetState
USE TOMAS_MOD,
                        ONLY : IBINS,
                                                    IDIAG
                                           ICOMP,
USE TOMAS_MOD,
                        ONLY: NH4BULKTOBIN
USE TOMAS_MOD,
                        ONLY: SRTNH4
USE UnitConv_Mod
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State objectt
OUTPUT PARAMETERS:
      INTEGER,
                     INTENT(OUT) :: RC ! Success or failure?
  Local variables
      ! Fields for TOMAS simulation
                 :: BINMASS(IIPAR, JJPAR, LLPAR, IBINS*ICOMP)
                  :: tempnh4(ibins)
      REAL*8
                 :: TID, I, J, L
      INTEGER
                  :: MK_TEMP(IBINS)
      REAL*8
      INTEGER
                 :: ii=53, jj=29, ll=1
      ! SAVEd scalars
      LOGICAL, SAVE :: FIRST = .TRUE.
      ! Pointers
      REAL*8, POINTER :: Spc(:,:,:,:)
      !-----
      ! EMISSSULFATETOMAS begins here!
      ! First-time setup
      IF (FIRST ) THEN
         ! Reset first-time flag
         FIRST = .FALSE.
      ENDIF
      ! Convert species from [kg/kg dry air] to [kg] for TOMAS.
      ! This will be removed once TOMAS uses mixing ratio instead of mass
      ! as tracer units (ewl, 9/11/15)
      CALL ConvertSpc_KgKgDry_to_Kg( am_I_Root, State_Met,
                                   State_Chm, RC
      IF ( RC /= GC_SUCCESS ) THEN
         CALL GC_Error('Unit conversion error', RC,
     &
                     'Routine EMISSSULFATETOMAS in sulfate_mod.F')
         R.F.TUR.N
      ENDIF
      ! Point to chemical species array [kg]
      Spc => State_Chm%Species
      IF (id_SF1 > 0 .and. id_NK1 > 0) THEN
```

```
!!! Get NH4 and aerosol water into the same array
        BINMASS(:,:,:,1:IBINS*(ICOMP-IDIAG)) =
    &
             Spc(:,:,:,id_SF1:id_SF1+IBINS*(ICOMP-IDIAG) - 1)
        IF (SRTNH4 > 0) THEN
           TID = IBINS*(ICOMP-IDIAG) + 1
%%%OMP PARALLEL DO
%%%OMP+DEFAULT( SHARED )
%%%OMP+PRIVATE( I, J, L, TMPNH4, MKTEMP )
%%%OMP+SCHEDULE( DYNAMIC )
           DO L=1,LLPAR
           DO J=1, JJPAR
           DO I=1, IIPAR
              ! Take a slice of size IBINS from Spc
              MK_TEMP = Spc(I,J,L,id_SF1:id_SF1-1+IBINS)
              ! Avoid array tmeporaries in subroutine call (bmy, 1/29/14)
              CALL NH4BULKTOBIN( MK_TEMP, Spc(I,J,L,id_NH4), TEMPNH4 )
              BINMASS(I,J,L,TID:TID+IBINS-1) = TEMPNH4(1:IBINS)
           Enddo
           ENDDO
           ENDDO
%%%OMP END PARALLEL DO
        ENDIF
        TID = IBINS*(ICOMP-1) +1
        BINMASS(:,:,:,TID:TID+IBINS-1) =
                Spc(:,:,:,id_AW1:id_AW1+IBINS-1)
    &
     !IF ( id_SF1 > 0 ) THEN
        CALL SRCSF30( Spc(:,:,:,id_NK1:id_NK1+IBINS-1),
              BINMASS(:,:,:,:), am_I_Root, Input_Opt, State_Met, RC )
    &
        ! Return the aerosol mass after emission subroutine to Spc
        ! excluding the NH4 aerosol and aerosol water (win, 9/27/08)
        Spc(:,:,:,id_SF1:id_SF1+IBINS*(ICOMP-IDIAG)-1) =
             BINMASS(:,:,:,1:IBINS*(ICOMP-IDIAG))
    &
     ENDIF
     ! Free pointer
     NULLIFY( Spc )
     ! Convert species back to kg (ewl, 9/11/15)
```

```
CALL ConvertSpc_Kg_to_KgKgDry( am_I_Root, State_Met,
       &
                                              State_Chm, RC
        IF ( RC /= GC_SUCCESS ) THEN
            CALL GC_Error('Unit conversion error', RC,
       &
                            'Routine EMISSSULFATETOMAS in sulfate_mod.F')
            RETURN
        ENDIF
        END SUBROUTINE EMISSSULFATETOMAS
  EOC
 #endif
                       Jack Kodros re-writing this
 #if defined( TOMAS )
        SUBROUTINE SRCSF30( TC1, TC2,
              am_I_Root, Input_Opt, State_Met, RC )
USES:
        USE CMN_SIZE_MOD
                                           ! Size parameters
       USE CMN_DIAG_MOD ! Size parameters

USE CMN_DIAG_MOD ! ND13 (for now)

USE DIAG_MOD, ONLY : AD59_SULF, AD59_NUMB

USE ERROR_MOD, ONLY : ERROR_STOP, IT_IS_NAN

USE Input_Opt_Mod, ONLY : OptInput

USE PBL_MIX_MOD, ONLY : GET_FRAC_OF_PBL, GET_PBL_TOP_L

USE State_Met_Mod, ONLY : MetState

USE TOMAS_MOD, ONLY : IBINS, AVGMASS, ICOMP
        USE TOMAS_MOD, ONLY: Xk, SUBGRIDCOAG, MNFIX
USE TOMAS_MOD, ONLY: SRTSO4, SRTNH4, DEBUGPRINT
        USE HCO_INTERFACE_MOD, ONLY : HcoState, GetHcoDiagn
INPUT PARAMETERS:
        LOGICAL.
                          INTENT(IN) :: am_I_Root ! Are we on the root CPU?
        TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
        TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
INPUT/OUTPUT PARAMETERS:
        REAL*8, INTENT(INOUT) :: TC1(IIPAR, JJPAR, LLPAR, IBINS)
        REAL*8, INTENT(INOUT) :: TC2(IIPAR, JJPAR, LLPAR, IBINS*ICOMP)
OUTPUT PARAMETERS:
                           INTENT(OUT) :: RC ! Success or failure?
        INTEGER,
   Local variables
        INTEGER
                                   :: I, J, K, L, DOW_LT, NTOP, C
                                    :: SO4(LLPAR), DTSRCE , EFRAC(LLPAR)
        REAL*8
        REAL*8
                                   :: TSO4. FEMIS
```

```
REAL*8
                             :: AREA_CM2
      REAL*8
                             :: SO4an(IIPAR, JJPAR, 2)
     REAL*8
                             :: SO4bf(IIPAR,JJPAR)
     REAL*8
                             :: SO4anbf(IIPAR, JJPAR, 2)
      REAL*8 BFRAC(IBINS)
                             ! Mass fraction emitted to each bin
#if defined( TOMAS12) || defined( TOMAS15)
      DATA BFRAC/
# if defined( TOMAS15)
                 0.0d0
                           , 0.0d0
                                       , 0.0d0,
# endif
                 4.3760E-02, 6.2140E-02, 3.6990E-02, 1.8270E-02,
     &
                 4.2720E-02, 1.1251E-01, 1.9552E-01, 2.2060E-01,
     &
                 1.6158E-01, 7.6810E-02, 2.8884E-02, 2.0027E-04/
     &
#else
     DATA BFRAC/
# if defined( TOMAS40)
                 0.000d00 , 0.000d00 , 0.000d00 , 0.000d00 , 0.000d00 ,
     &
                 0.000d00 , 0.000d00 , 0.000d00 , 0.000d00 , 0.000d00 ,
     &
# endif
     &
                 1.728d-02, 2.648d-02, 3.190d-02, 3.024d-02, 2.277d-02,
                 1.422d-02, 9.029d-03, 9.241d-03, 1.531d-02, 2.741d-02,
     &
                 4.529d-02, 6.722d-02, 8.932d-02, 1.062d-01, 1.130d-01,
     &
                 1.076d-01, 9.168d-02, 6.990d-02, 4.769d-02, 2.912d-02,
     &
                 1.591d-02, 7.776d-03, 3.401d-03, 1.331d-03, 4.664d-04,
     &
     &
                 1.462d-04, 4.100d-05, 1.029d-05, 2.311d-06, 4.645d-07/
#endif
      REAL*8
                             :: NDISTINIT(IBINS)
     REAL*8
                             :: NDISTFINAL(IBINS)
     REAL*8
                             :: MADDFINAL(IBINS)
     REAL*8
                             :: NDIST(IBINS), MDIST(IBINS,ICOMP)
     REAL*8
                             :: NDIST2(IBINS), MDIST2(IBINS,ICOMP)
     REAL*4
                             :: TSCALE, BOXVOL, TEMP, PRES
     REAL*8
                             :: NO(LLPAR, IBINS), MO(LLPAR, IBINS)
                             :: AREA(IIPAR, JJPAR)
      REAL(fp)
      REAL(fp)
                             :: AREA3D(IIPAR, JJPAR,2)
      ! Pointers
      REAL(f4),
                       POINTER :: Ptr2D(:,: )
                       POINTER :: Ptr3D(:,:,:)
      REAL(f4),
      INTEGER
                               :: N_TRACERS
```

```
LOGICAL
                    :: ERRORSWITCH, SGCOAG = .TRUE.
INTEGER
                   :: FLAG, ERR
                   :: pdbug !(temporary) win, 10/24/07
logical
!integer
                    :: ii, jj, ll
!data ii, jj, ll / 61, 1, 7 /
INTEGER
                    :: ii=53, jj=29, ll=1
! Ratio of molecular weights: S/S04
REAL*8, PARAMETER :: S_SO4 = 32d0 / 96d0
! debugging
real*8 dummy
! For fields from Input_Opt
LOGICAL :: LPRT, LNLPBL
LOGICAL
                    :: jkdbg=.true.
! Strings
CHARACTER(LEN= 63) :: DgnName
CHARACTER(LEN=255)
                     :: MSG
CHARACTER (LEN=255)
                    :: LOC='srcsf30 (sulfate_mod.F)'
|-----
! SRCSF30 begins here!
!-----
! Free pointers
Ptr2D => NULL()
Ptr3D => NULL()
! COpy values from Input_Opt
       = Input_Opt%LPRT
LNLPBL = Input_Opt%LNLPBL
! Import emissions from HEMCO (through HEMCO state)
IF ( .NOT. ASSOCIATED(HcoState) ) THEN
  CALL ERROR_STOP ( 'HcoState not defined!', LOC )
ENDIF
! Emission timestep [seconds]
DTSRCE = HcoState%TS_EMIS
! Grid box aarea
AREA = HcoState%Grid%AREA_M2%Val(:,:)
AREA3D(:,:,1) = AREA(:,:)
AREA3D(:,:,2) = AREA(:,:)
```

```
! READ IN HEMCO EMISSIONS
    DgnName = 'SO4_ANTH'
    CALL GetHcoDiagn( am_I_Root, DgnName, .FALSE., ERR,
   & Ptr3D=Ptr3D )
    IF ( .NOT. ASSOCIATED(Ptr3D) ) THEN
      CALL HCO_WARNING('Not found: '//TRIM(DgnName), ERR, THISLOC=LOC)
    ELSE
      SO4\_ANTH = Ptr3D(:,:,:)
    ENDIF
    Ptr3D => NULL()
    DgnName = 'SO4_BIOF'
    CALL GetHcoDiagn( am_I_Root, DgnName, .FALSE., ERR,
   & Ptr2D=Ptr2D )
    IF ( .NOT. ASSOCIATED(Ptr2D) ) THEN
      CALL HCO_WARNING('Not found: '//TRIM(DgnName), ERR, THISLOC=LOC)
    ELSE
      SO4_BIOF = Ptr2D(:,:)
    ENDIF
    Ptr2D => NULL()
    ! convert to kg/box/sec
    SO4an = SO4_ANTH(:,:,:) * AREA3d(:,:,:)
    SO4bf = SO4\_BIOF(:,:) * AREA(:,:)
    ! Compute SO4 emissions
    $OMP PARALLEL DO
$OMP+DEFAULT( SHARED )
$OMP+PRIVATE( I, J, NTOP, SO4, TSO4, L, FEMIS, EFRAC, NO, MO, K )
$OMP+PRIVATE( NDISTINIT, NDIST, MDIST, NDISTFINAL, MADDFINAL )
$OMP+PRIVATE( NDIST2, MDIST2, C )
$OMP+PRIVATE( BOXVOL, TEMP, PRES, TSCALE, pdbug )
$OMP+SCHEDULE( DYNAMIC )
    DO J = 1, JJPAR
    DO I = 1, IIPAR
       ! Top level of boundary layer at (I,J)
      NTOP = CEILING( GET_PBL_TOP_L( I, J ) )
       ! Zero SO4 array at all levels
      DO L = 1, LLPAR
         S04(L) = 0.0
      ENDDO
       ! Compute total anthro SO4 (surface + 100m) plus biofuel SO4
```

```
TSO4 = 0.d0
      TSO4 = SUM(SO4an(I,J,:)) + SO4bf(I,J)
      IF ( TSO4 == OdO ) CYCLE
            if(i==60.and.j==35) print *,'TSO4',TSO4
debug
       ! First calculate emission distribution vertically within PBL
       ! EFRAC(30) = fraction of total emission splitted for each
                   level until reaching PBL top.
      EFRAC = 0d0
       ! Partition the total anthro SO4 emissions thru the entire
       ! boundary layer (if PBL top is higher than level 2)
       ! Add option for non-local PBL (Lin, 03/31/09)
      IF (.NOT. LNLPBL) THEN
      IF ( NTOP > 2 ) THEN
         ! Loop thru boundary layer
         DO L = 1, NTOP
            ! Fraction of PBL spanned by grid box (I,J,L) [unitless]
            EFRAC(L) = GET_FRAC_OF_PBL( I, J, L )
         ENDDO
      ELSE
         EFRAC(1) = (SO4an(I,J,1) + SO4bf(I,J)) / TSO4
         EFRAC(2) = SO4an(I,J,2) / TSO4
      ENDIF
      IF ( ABS(SUM(EFRAC(:)) - 1.d0) > 1.D-5 ) THEN
         PRINT*, '### ERROR in SRCSF30!'
         PRINT*, '### I, J : ', I, J
         print*, 'EFRAC', EFRAC(:)
         PRINT*, '### SUM(EFRAC) : ', SUM( EFRAC(:) )
         PRINT*, '### This should exactly 1.00'
         CALL ERROR_STOP( 'Check SO4 redistribution',
                        'SRCSF30 (sulfate_mod.f)' )
   &
      ENDIF
      ELSE
         ! stop the program for now since I don't totally implement
         ! the subgrid coagulation option w/ Lin's new PBL scheme (win, 1/25/10)
         print *,'If the program stops here, that means you are ',
              'running TOMAS simulation with the new PBL scheme ',
   &
              'implemented since GEOS-Chem v.8-02-01.',
   &
```

```
&
               '----> Try not using the non-local PBL option'
          CALL ERROR_STOP( 'Code does not support new PBL scheme',
                          'SRCSF30 (sulfate_mod.f)')
   lг.
       ENDIF ! .not. LNLPBL
       ! Add the size-resolved SO4 emission to tracer array
       ! Having the options to do sub-grid coagulation or simply
       ! Sub-grid coagulation reduces the number being emitted
       ! and modifies the mass size distribution of existing particle
       ! as well as the size distribution being emitted.
       ! (win, 10/4/07)
       !-----
       IF ( SGCOAG ) THEN
          NO(:,:) = TC1(I,J,:,:)
          MO(:,:) = TC2(I,J,:,1:IBINS)
        DO L = 1, LLPAR
          SO4(L) = TSO4 * EFRAC(L) * DTSRCE
          IF (SO4(L) == 0.d0) CYCLE
          DO K = 1, IBINS
             NDISTINIT(K) = SO4(L) * BFRAC(K) /
                                  (SQRT(XK(K)*XK(K+1)))
   &
             NDIST(K) = TC1(I,J,L,K)
             DO C = 1, ICOMP
               MDIST(K,C) = TC2(I,J,L,K+(C-1)*IBINS)
               IF( IT_IS_NAN( MDIST(K,C) ) ) THEN
                  PRINT *,'++++++ Found NaN in SRCSF30 +++++++
                  PRINT *,'Location (I,J,L):',I,J,L,'Bin',K,'comp',C
                  CALL ERROR_STOP('SRCSF30 SGCCOAG', 'sulfate_mod.f')
               ENDIF
             ENDDO
             NDISTFINAL(K) = 0
             MADDFINAL(K) = 0
          ENDDO
          CALL MNFIX( NDIST, MDIST, ERRORSWITCH )
          IF( ERRORSWITCH ) PRINT *, 'SRCSF30: MNFIX found error ',
                 'before SUBGRIDCOAG at ',I,J,L
   &
          ERRORSWITCH = .FALSE.
          ! Overwrite number and mass before emission for diagnostic
          ! just in case there was any change by MNFIX (win, 10/27/08)
          NO(L,:) = NDIST(:)
          MO(L,:) = MDIST(:,SRTSO4)
               if (I== ii .and. J==jj .and. L==ll)
debug
```

```
&
                  CALL DEBUGPRINT(NDIST, MDIST, I, J, L,
                  'SRCSF30 Before SUBGRIDCOAG')
      ! Define subgrid coagulation timescale (win, 10/28/08)
#if
      defined( GRID4x5
            TSCALE = 10.*3600.
                                ! 10 hours
#elif defined( GRID2x25 )
            TSCALE = 5.*3600.
#elif defined( GRID1x125 )
            TSCALE = 2.*3600.
#elif defined( GRID1x1 )
            TSCALE = 2.*3600.
#elif defined( GRID05x0625 )
            TSCALE = 1.*3600. ! Placeholder: the 0.5 x 0.666 value
#elif defined( GRID05x0666 )
            TSCALE = 1.*3600.
#elif defined( GRID025x03125 )
            !\%\% KLUDGE, just copied the 0.5 x 0.666 value
            1\%\% Someone needs to add the right value (bmy, 2/16/12)
            TSCALE = 1.*3600.
#endif
            !Prior to 10/28/08 (win)
            !TSCALE = 10.*3600.
            BOXVOL = State_Met%AIRVOL(I,J,L) * 1.e6 !convert from m3 -> cm3
                    = State_Met%T(I,J,L)
            TEMP
            PRES
                    = State_Met%PMID(i,j,l)*100.0 ! in Pa
             print *, 'Now doing subgrid coag with timescale ',
                  TSCALE/3600., 'hr'
            pdbug=.false.
                  if (I.eq.II.and.J.eq.JJ .and. L==LL) pdbug=.true.
 debug
            CALL SUBGRIDCOAG( NDISTINIT, NDIST, MDIST, BOXVOL, TEMP,
                              PRES, TSCALE, NDISTFINAL, MADDFINAL, pdbug)
     &
            DO K = 1, IBINS
               NDIST(K) = NDIST(K) + NDISTFINAL(K)
               MDIST(K,SRTSO4) = MDIST(K,SRTSO4) +
                                 NDISTFINAL(K) * (SQRT(XK(K)*XK(K+1)))+
     &
                                 MADDFINAL(K)
                     if (I.eq.II.and.J.eq.JJ .and. L==11) then
 debug
                   print *,(NDISTFINAL(K) * (SQRT(XK(K)*XK(K+1)))+
                        MADDFINAL(K) )
                endif
 debug---
            ENDDO
            DO K= 1, IBINS
               NDIST2(K) = NDIST(K)
```

```
DO C = 1, ICOMP
                MDIST2(K,C) = MDIST(K,C)
             ENDDO
          ENDDO
                if(i==ii.and.j==jj.and.l==ll )
debug
               CALL DEBUGPRINT(NDIST2, MDIST2, I, J, L,
                               'SRCSF30 : After SUBGRIDCOAG')
          ERRORSWITCH = .FALSE.
                 if(i==ii.and.j==ii.and.l==ll) errorswitch=.true.
debug
     print *, 'mnfix in sulfate_mod:6430'
          CALL MNFIX( NDIST2, MDIST2, ERRORSWITCH )
           IF( ERRORSWITCH ) PRINT *, 'SRCSF30: MNFIX found error ',
                'after SUBGRIDCOAG at ',I,J,L
    &
debug
                if(i==ii .and.j==jj .and.l==11)
               CALL DEBUGPRINT(NDIST2, MDIST2, I, J, L,
                               'SRCSF30 : After MNFIX')
     &
          DO K = 1, IBINS
             TC1(I,J,L,K) = NDIST2(K)
             DO C=1,ICOMP
                TC2(I,J,L,K+(C-1)*IBINS) = MDIST2(K,C)
             ENDDO
          ENDDO
       ENDDO ! L loop
          !-----
          ! ND59 Diagnostic: Size-resolved primary sulfate emission in
                            [kg S/box/timestep] and the corresponding
                            number emission [no./box/timestep]
          ļ
          IF ( ND59 > 0 ) THEN
              !print*, 'JACK IN ND59 SULFATE'
             DO L = 1, LLPAR
             DO K = 1, IBINS
                if(TC2(I,J,L,K)-MO(L,K) < Od0)
    &
                  print *,'Negative SF emis ',TC2(I,J,L,K)-MO(L,K),
    &
                      'at', I, J, L, K
                if(TC1(I,J,L,K)-NO(L,K) < Od0)
                  print *,'Negative NK emis ',TC1(I,J,L,K)-NO(L,K),
    &
                      'at', I, J, L, K
                 if(I==ii .and. J==jj) then
              !
                    print*, 'TC2: ', TC2(ii,jj,0,:)
              !
                    print*, 'MO: ', MO(0,:)
                    print*, 'S_SO4: ', S_SO4
```

```
!
           ENDIF
          AD59\_SULF(I,J,1,K) = AD59\_SULF(I,J,1,K) +
&
                             (TC2(I,J,L,K)-MO(L,K))*S_S04
          AD59_NUMB(I,J,1,K) = AD59_NUMB(I,J,1,K) +
&
                             TC1(I,J,L,K)-NO(L,K)
        ENDDO
        ENDDO
     ENDIF
   ELSE
   ! Distributing primary emission without sub-grid coagulation
   ! Add SO4 emissions to tracer array
   ! For SF: Convert from [kg SO4/box/s] -> [kg SO4/box/timestep]
   ! For NK: Convert from [kg SO4/box/s] -> [No. /box/timestep]
   !-----
     DO L = 1, LLPAR
        SO4(L) = TSO4 * EFRAC(L)
        DO K = 1, IBINS
          TC1(I,J,L,K) = TC1(I,J,L,K) +
                 ( SO4(L) * DTSRCE * BFRAC(K) / AVGMASS(K) )
&
          TC2(I,J,L,K) = TC2(I,J,L,K) +
&
                 ( SO4(L) * DTSRCE * BFRAC(K)
                                                     )
        ENDDO
     ENDDO
     ! ND59 Diagnostic: Size-resolved primary sulfate emission in
                    [kg S/box/timestep] and the corresponding
                    number emission [no./box/timestep]
     IF ( ND59 > 0 ) THEN
        SO4anbf(:,:,1) = SO4an(:,:,1) + SO4bf(:,:)
        SO4anbf(:,:,2) = SO4an(:,:,2)
        DO L = 1, 2
        DO K = 1, IBINS
          AD59\_SULF(I,J,L,K) = AD59\_SULF(I,J,L,K) +
&
                           ( SO4anbf(I,J,L) * BFRAC(K)
                              * S_SO4 * DTSRCE
&
                                                   )
          AD59_NUMB(I,J,L,K) = AD59_NUMB(I,J,L,K) +
                           ( SO4anbf(I,J,L) * BFRAC(K)
&
                               / AVGMASS(K) * DTSRCE
&
        ENDDO
        ENDDO
     ENDIF
```

```
ENDIF !SGCOAG
      F.NDD0
      ENDDO
 $OMP END PARALLEL DO
      IF ( LPRT ) print *,' ### Finish SRCSF30'
      END SUBROUTINE SRCSF30
#endif
 EOC
                  GEOS-Chem Global Chemical Transport Model
\mbox{}\hrulefill\
 \subsubsection [grav\_settling] {grav\_settling}
 Subroutine GRAV\_SETTLING performs gravitational settling of
   sulfate and nitrate in coarse sea salt (SO4S and NITS).
   (bec, rjp, bmy, 4/20/04, 7/20/04, 10/25/05)
 \\{\bf INTERFACE:}
\begin{verbatim}
                     SUBROUTINE GRAV_SETTLING( am_I_Root, Input_Opt, State_Met,
     &
                               State_Chm,
     &
                               TC,
                                                   RC
                                                              )
                                         N,
USES:
      USE CMN_DIAG_MOD
      USE CMN_SIZE_MOD
#if defined( BPCH_DIAG )
      USE DIAG_MOD,
                             ONLY: AD44
#endif
      USE ErrCode_Mod
      USE GC_GRID_MOD,
                             ONLY : GET_AREA_CM2
      USE Input_Opt_Mod,
                            ONLY: OptInput
      USE State_Chm_Mod,
                            ONLY : ChmState
      USE State_Met_Mod,
                             ONLY : MetState
      USE TIME_MOD,
                             ONLY : GET_ELAPSED_SEC
      USE TIME_MOD,
                             ONLY : GET_TS_CHEM
#if defined( NC_DIAG )
      USE HCO_INTERFACE_MOD, ONLY : HcoState
      USE ERROR_MOD,
                             ONLY : ERROR_STOP
      USE HCO_ERROR_MOD, ONLY : HCO_SUCCESS
```

USE HCO_DIAGN_MOD, ONLY : Diagn_Update

#endif

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

INTEGER, INTENT(IN) :: N ! N=1 is SO4S; N=2 is NITS
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

INPUT/OUTPUT PARAMETERS:

N=1 is SO4S; N=2 is NITS

```
REAL(fp), INTENT(INOUT) :: TC(IIPAR, JJPAR, LLPAR) ! Tracer [kg]
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

REMARKS:

```
tdf Include Coarse Mode DUST size bins
N=3 is S04d2; N=4 is NIT_d1
N=5 is S04d3; N=6 is NIT_d2
N=7 is S04d4; N=8 is NIT_d3
N=9 is S04d4; N=10 is NIT_d4
tdf Treat these coated DUSTs as DRY for now
```

- (1) Now references SALA_REDGE_um and SALC_REDGE_um from "tracer_mod.f" (bmy, 7/20/04)
- (2) Now references XNUMOL from "tracer_mod.f" (bmy, 10/25/05)
- (3) Now limit relative humidity to [tiny(real(fp)),0.99] range for DLOG argument (phs, 5/1/08)
- (4) Bug fixes to the Gerber hygroscopic growth for sea salt aerosols (jaegle, 5/5/11)
- (5) Update hygroscopic growth to Lewis and Schwartz formulation (2006) and density calculation based on Tang et al. (1997) (bec, jaegle 5/5/11)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 01 Mar 2012 R. Yantosca Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
- 14 Nov 2012 R. Yantosca Now pass am_I_Root, Input_Opt, RC as arguments
- 15 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 12 Sep 2013 M. Sulprizio- Include Coarse Mode DUST size bins (T.D. Fairlie)
- 06 Jan 2015 M. Yannetti Changed some variables to f8 as needed
- 26 Feb 2015 E. Lundgren Replace GET_PCENTER with State_Met%PMID and remove dependency on pressure_mod.
- 22 Jan 2016 E. Lundgren Update netcdf drydep flux diagnostics

```
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
31 May 2016 - E. Lundgren - Remove usage of Input_Opt%XNUMOL
24 Jun 2016 - R. Yantosca - Now return if id_S04d1<0 or id_NITd1<0 (not ==0)
```

8.5.5 chem_dms

Subroutine CHEM_DMS is the DMS chemistry subroutine from Mian Chin's GOCART model, modified for use with the GEOS-CHEM model. (rjp, bdf, bmy, 5/31/00, 10/15/09)

INTERFACE:

```
SUBROUTINE CHEM_DMS( am_I_Root, Input_Opt, State_Met, State_Chm, RC )
```

USES:

```
USE CHEMGRID_MOD, ONLY : ITS_IN_THE_NOCHEMGRID USE CMN_DIAG_MOD
```

USE CMN_SIZE_MOD

USE DIAG_MOD, ONLY : ADO5

USE ErrCode_Mod

USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState
USE TIME_MOD, ONLY : GET_TS_CHEM

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REMARKS:

```
Reaction List (by Mian Chin, chin@rondo.gsfc.nasa.gov)
```

```
R1: DMS + OH -> a*SO2 + b*MSA OH addition channel k1 = { 1.7e-42*exp(7810/T)*[02] / (1+5.5e-31*exp(7460/T)*[02] } a = 0.75, b = 0.25

R2: DMS + OH -> SO2 + ... OH abstraction channel
```

```
k2 = 1.2e-11*exp(-260/T)

DMS_OH = DMSO * exp(-(r1+r2)* NDT1)
where DMSO is the DMS concentration at the beginning,
r1 = k1*[OH], r2 = k2*[OH].

R3: DMS + NO3 -> SO2 + ...
k3 = 1.9e-13*exp(500/T)

DMS = DMS_OH * exp(-r3*NDT1)
where r3 = k3*[NO3].

R4: DMS + X -> SO2 + ...
assume to be at the rate of DMS+OH and DMS+NO3 combined.
```

The production of SO2 and MSA here, PSO2_DMS and PMSA_DMS, are saved for use in CHEM_SO2 and CHEM_MSA subroutines as a source term. They are in unit of [v/v/timestep].

- (1) Now reference AD, AIRDEN, and SUNCOS from "dao_mod.f". Added parallel DO-loops. Also now extract OH and NO3 from SMVGEAR for coupled chemistry-aerosol runs. (rjp, bdf, bmy, 9/16/02)
- (2) Bug fix: remove duplicate definition of RK3 (bmy, 3/23/03)
- (3) Now use function GET_TS_CHEM from "time_mod.f". (bmy, 3/27/03)
- (4) Now reference STT and ITS_A_FULLCHEM_SIM from "tracer_mod.f"

 Now replace IJSURF w/ an analytic function. (bmy, 7/20/04)
- (5) Shift rows 8,9 in AD05 to 9,10 in to make room for P(SO4) from O3 oxidation in sea-salt aerosols (bec, bmy, 4/13/05)
- (6) Now remove reference to CMN, it's obsolete. Now reference ITS_IN_THE_STRAT from "tropopause_mod.f". (bmy, 8/22/05)
- (7) Now references XNUMOL from "tracer_mod.f" (bmy, 10/25/05)
- (8) Now correctly records P(SO2) from OH in ADO5 (pjh)
- (9) Update reaction rate to match JPL06 and full chem (jaf, bmy, 10/15/09)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 31 Jul 2012 R. Yantosca Now loop from 1..LLPAR for GIGC compatibility
- 14 Nov 2012 R. Yantosca Add am_I_Root, Input_Opt, RC as arguments
- 15 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 28 Nov 2012 R. Yantosca Replace SUNCOS with State_Met%SUNCOS
- 24 Jul 2014 R. Yantosca Now compute BOXVL internally
- 06 Nov 2014 R. Yantosca Now use State_Met%AIRDEN(I,J,L)
- 24 Jun 2016 R. Yantosca Now Return if id_DMS < 0 (not == 0)
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

8.5.6 chem_h2o2

Subroutine CHEM_H2O2 is the H2O2 chemistry subroutine for offline sulfate simulations. For coupled runs, H2O2 chemistry is already computed by the SMVGEAR module. (rjp, bmy, 11/26/02, 10/25/05)

INTERFACE:

```
SUBROUTINE CHEM_H2O2( am_I_Root, Input_Opt, & State_Met, State_Chm, RC )
```

USES:

```
USE CHEMGRID_MOD, ONLY : ITS_IN_THE_NOCHEMGRID
USE CMN_SIZE_MOD

USE CMN_DIAG_MOD

#if defined( BPCH_DIAG )
USE DIAG_MOD, ONLY : AD44
```

#endif

USE ErrCode_Mod

USE PBL_MIX_MOD, ONLY : GET_FRAC_UNDER_PBLTOP

USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState
USE TIME_MOD, ONLY : GET_MONTH
USE TIME_MOD, ONLY : GET_TS_CHEM
USE TIME_MOD, ONLY : ITS_A_NEW_MONTH

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

- (1) Bug fix: need to multiply DXYP by 1d4 for cm2 (bmy, 3/23/03)
- (2) Now replace DXYP(JREF)*1d4 with routine GET_AREA_CM2 of "grid_mod.f" Now use functions GET_MONTH and GET_TS_CHEM from "time_mod.f". (bmy, 3/27/03)
- (3) Now references PBLFRAC from "drydep_mod.f". Now apply dry deposition throughout the entire PBL. Added FREQ variable. (bmy, 8/1/03)
- (4) Now use ND44_TMP array to store vertical levels of drydep flux, then

```
sum into AD44 array. This preents numerical differences when using multiple processors. (bmy, 3/24/04)
```

- (5) Now use diurnally-varying JO1D. Now use new unit conversion for the ND44 diagnostic. (rjp, bmy, 3/30/04)
- (6) Now use parallel DO-loop to zero ND44_TMP. Now uses ITS_A_NEW_MONTH from time_mod.f. (bmy, 4/14/04)
- (7) Now reference STT & TCVV from "tracer_mod.f". Also replace IJSURF with an analytic function. Now references DATA_DIR from "directory_mod.f". (bmy, 7/20/04)
- (8) Now suppress output from READ_BPCH with QUIET keyword (bmy, 1/25/05)
- (9) Replace PBLFRAC from "drydep_mod.f" with GET_FRAC_UNDER_PBLTOP from "pbl_mix_mod.f" (bmy, 2/22/05)
- (10) Now read offline files from "sulfate_sim_200508/offline". Now remove reference to CMN, it's obsolete. Now reference ITS_IN_THE_STRAT from "tropopause_mod.f". (bmy, 8/22/05)
- (11) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (12) Now references XNUMOL from "tracer_mod.f" (bmy, 10/25/05)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 01 Mar 2012 R. Yantosca Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
- 30 Jul 2012 R. Yantosca Now accept am_I_Root as an argument when running with the traditional driver main.F
- 31 Jul 2012 R. Yantosca Now loop from 1..LLPAR for GIGC compatibility
- 31 Jul 2012 R. Yantosca Declare temp drydep arrays w/ LLPAR (not LLTROP)
- 14 Nov 2012 R. Yantosca Add am_I_Root, Input_Opt, RC as arguments
- 15 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 26 Nov 2012 R. Yantosca Dimension ND44_TMP array with LLPAR, not LLTROP
- 28 Nov 2012 R. Yantosca Replace SUNCOS with State_Met%SUNCOS
- 05 Mar 2013 R. Yantosca Now use Input_Opt%LNLPBL
- 19 Mar 2013 R. Yantosca Now copy Input_Opt%TCVV(1:N_TRACERS) and Input_Opt%XNUMOL(1:N_TRACERS) -- avoid OOB errs
- 25 Mar 2013 M. Payer Now pass State_Chm object via the arg list
- 18 Sep 2014 M. Sulprizio- Now get J(H2O2) and PH2O2m from HEMCO
- 06 Nov 2014 R. Yantosca Now use State_Met%AIRDEN(I,J,L)
- 12 Jun 2015 R. Yantosca Now remove orphaned ND44 variables
- 23 Sep 2015 R. Yantosca Remove reference to obsolete DRYH202 flag
- 24 Jun 2016 R. Yantosca Now return if id_H202 < 0 (not == 0)
- 30 Jun 2016 R. Yantosca Remove instances of Spc. Now get the advected species ID from State_Chm%Map_Advect.

EOC

BOC

DEFINED PARAMETERS:

REAL(fp), PARAMETER :: $A = 2.9e-12_{fp}$

LOCAL VARIABLES:

! SAVEd Scalars

```
LOGICAL
                 :: FIRST = .TRUE.
   INTEGER, SAVE
                :: LASTMONTH = -99
   ! Scalars
   INTEGER
                 :: I,
                         J,
                              L
                        Koh, DH2O2, M, F,
   REAL(fp)
                 :: DT,
   REAL(fp)
              :: H2O2O, H2O2, ALPHA, FREQ, PHOTJ
   ! Strings
   CHARACTER(LEN=255) :: FILENAME
   ! Arrays
   REAL*4
                 :: ARRAY(IIPAR, JJPAR, LLCHEM)
   ! Pointers
   REAL(fp), POINTER :: Spc(:,:,:):
   ! CHEM_H2O2 begins here!
   !-----
   IF ( id_H202 < 0 ) RETURN
   ! Assume success
   RC
         = GC_SUCCESS
   ! Point to chemical species array [v/v dry]
          => State_Chm%Species
   ! Chemistry timestep [s]
           = GET_TS_CHEM() * 60e+0_fp
   ! Factor to convert AIRDEN from kgair/m3 to molecules/cm3:
           = 1000.e+0_fp / AIRMW * AVO * 1.e-6_fp
   ! Loop over tropopsheric grid boxes and do chemistry
   $OMP PARALLEL DO
$OMP+DEFAULT( SHARED )
$OMP+PRIVATE( I, J, L, M, H2O2O, KOH, FREQ, ALPHA, DH2O2, H2O2 )
$OMP+PRIVATE( PHOTJ )
$OMP+SCHEDULE( DYNAMIC )
   DO L = 1, LLPAR
   DO J = 1, JJPAR
   DO I = 1, IIPAR
      ! Initialize for safety's sake
      FREQ = 0e+0_fp
```

```
! Skip non-chemistry boxes
        IF ( ITS_IN_THE_NOCHEMGRID( I, J, L, State_Met ) ) CYCLE
        ! Density of air [molec/cm3]
              = State_Met%AIRDEN(I,J,L) * f
        ! Initial H202 [v/v]
        H2020 = Spc(I,J,L,id_H202)
        ! Loss frequenty due to OH oxidation [s-1]
              = A * EXP( -160.e+0_{fp} / State_Met%T(I,J,L) ) *
                GET_OH( I, J, L, Input_Opt, State_Chm, State_Met )
    &
        ! Now do all dry deposition in mixing_mod.F90 (ckeller, 3/5/15)
        FREQ = 0.e+0_fp
        ! Impose a diurnal variation of jH202 by multiplying COS of
        ! solar zenith angle normalized by maximum solar zenith angle
        ! because the archived JH202 is for local noon time
        IF ( COSZM(I,J) > 0.e+0_fp ) THEN
          PHOTJ = JH202(I,J,L) * State_Met%SUNCOS(I,J) / COSZM(I,J)
          PHOTJ = MAX( PHOTJ, Oe+O_fp )
        ELSE
          PHOTJ = Oe+O_fp
        ENDIF
        ! Compute loss fraction from OH, photolysis, drydep [unitless].
        ALPHA = 1.e+0_fp + (KOH + PHOTJ + FREQ) * DT
        ! Delta H202 [v/v]
        ! PH202m is in kg/m3 (from HEMCO), convert to molec/cm3/s (mps,9/18/14)
        DH2O2 = (PH2O2m(I,J,L) / TS_EMIS * XNUMOL_H2O2 / CM3PERM3)
    &r.
                * DT / ( ALPHA * M )
        ! Final H202 [v/v]
        H202 = (H2020 / ALPHA + DH202)
        IF ( H202 < SMALLNUM ) H202 = Oe+O_fp
        ! Store final H2O2 in Spc
        Spc(I,J,L,id_{H202}) = H202
     ENDDO
     ENDDO
     ENDDO
$OMP END PARALLEL DO
     ! Free pointer
```

```
Spc => NULL()
        END SUBROUTINE CHEM_H2O2
  EOC
                       GEOS-Chem Global Chemical Transport Model
\mbox{}\hrulefill\
  \subsubsection [chem\_so2] {chem\_so2}
  Subroutine CHEM\_SO2 is the SO2 chemistry subroutine.
     (rjp, bmy, 11/26/02, 8/26/10)
  //
  \\{\bf INTERFACE:}
\begin{verbatim} SUBROUTINE CHEM_SO2( am_I_Root, Input_Opt,
       &
                                 State_Met, State_Chm, RC )
USES:
        USE CHEMGRID_MOD,
                                    ONLY : ITS_IN_THE_NOCHEMGRID
        USE CMN_DIAG_MOD
        USE CMN_SIZE_MOD
        USE DAO_MOD,
                                    ONLY : IS_WATER
        USE DIAG_MOD,
                                  ONLY : ADO5
        USE DUST_MOD,
                                   ONLY: GET_DUST_ALK ! tdf 04/08/08
       USE ERROR_MOD, ONLY: IS_SAFE_EXP

USE ERROR_MOD, ONLY: SAFE_DIV

USE ERROR_MOD, ONLY: ERROR_STOP

USE Input_Opt_Mod, ONLY: OptInput

USE PRESSURE_MOD, ONLY: GET_PCENTER

USE State_Chm_Mod, ONLY: ChmState

USE State_Met_Mod, ONLY: MetState

USE TIME_MOD, ONLY: GET_TS_CHEM, GET_MONTH

USE TIME_MOD, ONLY: ITS_A_NEW_MONTH

USE WETSCAY_MOD, ONLY: H202s
        USE ErrCode_Mod
                              ONLY : SO2s
        USE WETSCAV_MOD,
        USE HCO_INTERFACE_MOD, ONLY : GetHcoDiagn
INPUT PARAMETERS:
        LOGICAL,
                          INTENT(IN)
                                           :: am_I_Root ! Is this the root CPU?
        TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
        TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC ! Success or failure?

REMARKS:

Reaction List (by Rokjin Park, rjp@io.harvard.edu)

(1) SO2 production:

DMS + OH, DMS + NO3 (saved in CHEM_DMS)

(2) SO2 loss:

- (a) SO2 + OH -> SO4
- (b) SO2 -> drydep
- (c) S02 + H202 or O3 (aq) -> S04
- $(3) SO2 = SO2_0 * exp(-bt) + PSO2_DMS/bt * [1-exp(-bt)]$

where b is the sum of the reaction rate of SO2 + OH and the dry deposition rate of SO2, $PSO2_DMS$ is SO2 production from DMS in MixingRatio/timestep.

If there is cloud in the gridbox (fraction = fc), then the aqueous phase chemistry also takes place in cloud. The amount of SO2 oxidized by H2O2 in cloud is limited by the available H2O2; the rest may be oxidized due to additional chemistry, e.g, reaction with O3 or O2 (catalyzed by trace metal).

- (1) Removed duplicate definition of Ki (bmy, 11/15/01)
- (2) Eliminate duplicate HPLUS definition. Make adjustments to facilitate SMVGEAR chemistry for fullchem runs (rjp, bmy, 3/23/03)
- (3) Now replace DXYP(J+J0)*1d4 with routine GET_AREA_CM2 of "grid_mod.f" Now use function GET_TS_CHEM from "time_mod.f".
- (4) Now apply dry deposition to entire PBL. Now references PBLFRAC array from "drydep_mod.f". (bmy, 8/1/03)
- (5) Now use ND44_TMP array to store vertical levels of drydep flux, then sum into AD44 array. This preents numerical differences when using multiple processors. (bmy, 3/24/04)
- (6) Now use parallel DO-loop to zero ND44_TMP (bmy, 4/14/04)
- (7) Now reference STT, TCVV, & ITS_AN_AEROSOL_SIM from "tracer_mod.f". Now reference DATA_DIR from "directory_mod.f" (bmy, 7/20/04)
- (8) Replace PBLFRAC from "drydep_mod.f" with GET_FRAC_UNDER_PBLTOP from "pbl_mix_mod.f" (bmy, 2/22/05)
- (9) Modified for SO4s, NITs. Also modified for alkalinity w/in the

```
seasalt chemistry. (bec, bmy, 4/13/05)
(10) Now remove reference to CMN, it's obsolete. Now reference
      ITS_IN_THE_STRAT from "tropopause_mod.f" (bmy, 8/22/05)
(11) Now references XNUMOL from "tracer_mod.f" (bmy, 10/25/05)
(12) Updated to match JPL 2006 + full chem (jaf, bmy, 10/15/09)
(13) Now prevent floating-point exceptions when taking the exponential
      terms. (win, bmy, 1/4/10)
(14) Save aqueous production rate to PSO4_SO2AQ for TOMAS microphyics
      (win, 1/25/10)
(15) Added extra error checks to prevent negative L2S, L3S (bmy, 4/28/10)
(16) Use liq. water content from met fields in GEOS-5 (jaf, bmy, 6/30/10)
26 Aug 2010 - R. Yantosca - Use liquid water content from MERRA
12 Nov 2010 - R. Yantosca - Prevent div-by-zero when computing L2S and L3S
                          - Divide LWC by cloud fraction for GEOS/MERRA
27 May 2011 - L. Zhang
                            and adjust the L2S and L3S rates accordingly
                          - Added ProTeX headers
22 Dec 2011 - M. Payer
08 Feb 2012 - R. Yantosca - Treat GEOS-5.7.2 in the same way as MERRA
01 Mar 2012 - R. Yantosca - Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
31 Jul 2012 - R. Yantosca - Now loop over 1..LLPAR for GIGC compatibility
31 Jul 2012 - R. Yantosca - Declare temp drydep arrays w/ LLPAR (not LLTROP)
14 Nov 2012 - R. Yantosca - Add am_I_Root, Input_Opt, RC as arguments
                          - Replaced all met field arrays with State_Met
15 Nov 2012 - M. Payer
                            derived type object
05 Mar 2013 - R. Yantosca - Now use Input_Opt%LNLPBL
19 Mar 2013 - R. Yantosca - Now copy Input_Opt%TCVV(1:N_TRACERS) and
                            Input_Opt%XNUMOL(1:N_TRACERS) -- avoid OOB errs
                          - Now pass State_Chm object via the arg list
25 Mar 2013 - M. Payer
05 Sep 2013 - M. Sulprizio- Add modifications for cloud pH (B. Alexander)
06 Sep 2013 - M. Sulprizio- Bug fix: Prevent divide-by-zero if LWC=0. Only
                            do aqueous SO2 chemistry when LWC>0.
12 Sep 2013 - M. Sulprizio- Modified for SO4d, NITd. Also modified for
                            alkalinity w/in the dust chemistry. (tdf 4/07/08)
26 Sep 2013 - R. Yantosca - Renamed GEOS_57 Cpp switch to GEOS_FP
28 Jan 2014 - R. Yantosca - Bug fix for TOMAS. Set ALKdst=0 since TOMAS
                            carries its own dust tracers instead of DST1-4.
25 Jun 2014 - R. Yantosca - Now pass Input_Opt to GET_ALK
18 Sep 2014 - M. Sulprizio- Now get HNO3 for offline aerosol sim from HEMCO
06 Nov 2014 - R. Yantosca - Now use State_Met%AIRDEN(I,J,L)
06 Nov 2014 - R. Yantosca - Now use State_Met%CLDF(I,J,L)
12 Jan 2015 - C. Keller - Now allow NDENS_SALA and NDENS_SALC to be empty.
```

26 Feb 2015 - E. Lundgren - Replace GET_PCENTER with State_Met%PMID_DRY.

24 Jun 2016 - R. Yantosca - Now return id_H2O2 < 0 or id_SO2 < 0 (not == 0)

23 Sep 2015 - R. Yantosca - Remove reference to obsolete DRYSO2 flag

12 Aug 2015 - R. Yantosca - Add support for MERRA2 meteorology

Remove dependency on pressure_mod.

8.5.7 seasalt_chem

Subroutine SEASALT_CHEM computes SO4 formed from S(IV) + O3 on seasalt aerosols as a function of seasalt alkalinity. (bec, bmy, 4/13/05, 10/7/08)

INTERFACE:

```
SUBROUTINE SEASALT_CHEM ( I,
                                         J,
                                                  L,
                              ALK1,
                                         ALK2,
                                                   SO2_cd,
                              Kt1,
                                        Kt2,
                                                   Kt1N,
     &
     &
                              Kt2N,
                                        SO2_ss,
                                                   PSO4E,
                                        am_I_Root, Input_Opt,
     &
                              PSO4F,
                              State_Met, State_Chm, RC )
     &
USES:
      ! DIAGNOSTICS -- leave commented out for now (bec, bmy, 4/13/05)
      !USE CMN_DIAG_MOD
                               ! ND19
      !USE DIAG_MOD,
                          ONLY: ADO9
      !-----
      USE CMN_DIAG_MOD
                                 ! NDO5, LDO5
      USE CMN_SIZE_MOD
      USE DIAG_MOD,
                            ONLY: ADO5
      USE ErrCode_Mod
      USE ERROR_MOD,
                            ONLY : GEOS_CHEM_STOP
      USE ERROR_MOD,
                            ONLY : IT_IS_NAN
                        ONLY : IT_IS_NAMONLY : OptInput
      USE Input_Opt_Mod,
      USE State_Chm_Mod,
                          ONLY : ChmState
      USE State_Met_Mod,
                            ONLY : MetState
      USE TIME_MOD,
                            ONLY : GET_TS_CHEM
                          ONLY : GET_ELAPSED_SEC
      USE TIME_MOD,
      USE TIME_MOD,
                            ONLY : GET_MONTH
      USE TIME_MOD,
                            ONLY : ITS_A_NEW_MONTH
```

INPUT PARAMETERS:

INTEGER,	INTENT(IN)	::	I, J, L	!	Grid box indices
REAL(fp),	INTENT(IN)	::	S02_cd	!	SO2 mixing ratio [v/v] after
				!	gas phase chemistry and
				!	dry deposition
REAL(fp),	INTENT(IN)	::	Kt1, Kt2	!	Rate constant [s-1] for
				!	sulfate formation on sea
				!	salt aerosols from GET_ALK
				!	(1=fine; 2=coarse)
REAL(fp),	INTENT(IN)	::	Kt1N, Kt2N		
REAL(fp),	INTENT(IN)	::	ALK1, ALK2	!	Alkalinity [kg] from
				!	seasalt_mod
<pre>TYPE(MetState),</pre>	INTENT(IN)	::	State_Met	!	Meteorology State object
<pre>TYPE(OptInput),</pre>	INTENT(IN)	::	Input_Opt	!	Input Options object
LOGICAL,	INTENT(IN)	::	am_I_Root	!	Are we on the root CPU?

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

REAL(fp), INTENT(OUT) :: SO2_ss ! SO2 mixing ratio [v/v] ! after sea salt chemistry

REAL(fp), INTENT(OUT) :: PSO4E ! SO4E (sulfate produced by ! S(IV)+03 on fine seasalt) ! mixing ratio [v/v]

REAL(fp), INTENT(OUT) :: PSO4F ! SO4F (sulfate produced by

REAL(ip), INTENT(UUT) :: PSU4F ! SU4F (sulfate produced by ! S(IV)+03 on coarse seasalt)

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

Chemical reactions:

(R1) SO2 + O3 + ALK => SO4 + O2
Modeled after Chamedies and Stelson, 1992?

- (1) Now references XNUMOLAIR from "tracer_mod.f" (bmy, 10/25/05)
- (2) Bug fix: now avoid seg fault error if IDTHNO3 is zero, as it would be for an offline aerosol simulation. (bmy, 3/29/06)
- (3) Fixed typo in FALK_A_SO2 equation: C_FLUX_C should be C_FLUX_A. (havala, bec, bmy, 12/8/06)
- (4) Bug fix for mass balance, replace TITR_HN03 w/ HN03_SSC in the expression for HN03_ss. Bug fix: now do equivalent computation for GET_GN03, which is now no longer called because it's in "isoropia_mod.f". (bec, bmy, 7/30/08)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 25 Mar 2013 M. Payer Now pass State_Chm object via the arg list
- 12 Sep 2013 M. Sulprizio- Added loss of HNO3 on sea salt diagnostic (T.D. Fairlie)
- 18 Sep 2014 M. Sulprizio- Now get HNO3 for offline aerosol sim from HEMCO
- 24 Mar 2015 E. Lundgren Remove dependency on tracer_mod since XNUMOLAIR now defined in CMN_GTCM_MOD
- 06 Jan 2016 E. Lundgren Use global physical parameters
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.
- 11 Oct 2016 R. Yantosca Bug fix: make sure that MW_HNO3 is defined for aerosol-only sims (where id_HNO3 < 0)

8.5.8 dust_chem

Subroutine DUST_CHEM computes SO4 formed from S(IV) + O3 on dust aerosols as a function of dust alkalinity (tdf 3/28/2K8) Based on routine SEASALT_CHEM (bec, bmy, 4/13/05, 10/25/05)

INTERFACE:

SUBROUTINE	DUST_CHEM	(I,	J,	L,		
&			ALK,	SO2_cd,	H2SO4_cd,		
&			KTS,	KTN,	KTH,		
&			SO2_gas,	$H2SO4_gas$,	PSO4d,		
&			PH2SO4d,	PNITd,	ALKA,		
&			<pre>Input_Opt,</pre>	State_Met,	State_Chm,	RC)

USES:

```
USE CMN_SIZE_MOD
                             ! Size parameters
USE ErrCode_Mod
USE ERROR_MOD,
                        ONLY : GEOS_CHEM_STOP
USE ERROR_MOD,
                        ONLY : IT_IS_NAN
USE Input_Opt_Mod,
                        ONLY : OptInput
USE State_Chm_Mod,
                        ONLY : ChmState
USE State_Met_Mod,
                        ONLY : MetState
USE TIME_MOD,
                        ONLY : GET_TS_CHEM,
                                                    GET_ELAPSED_SEC
USE TIME_MOD,
                        ONLY : GET_ELAPSED_SEC,
                                                    GET_MONTH
                        ONLY : ITS_A_NEW_MONTH
USE TIME_MOD,
```

INPUT PARAMETERS:

INTEGER,	INTENT(IN)	:: I, J, L	! Grid box indices
REAL(fp),	INTENT(IN)	:: SO2_cd	! SO2 mixing ratio after
			! gas phase chemistry and
			! dry deposition $[v/v]$
REAL(fp),	INTENT(IN)	:: H2SO4_cd	! H2SO4 mixing ratio after
			! gas phase chemistry and
			! dry deposition $[v/v]$
REAL(fp),	INTENT(IN)	:: ALK(NDSTBIN)	! Dust Alkalinity $[v/v]$
REAL(fp),	INTENT(IN)	:: KTS(NDSTBIN)	! Rate constant for uptake
			! of SO2 on dust [s-1]
REAL(fp),	INTENT(IN)	:: KTN(NDSTBIN)	! Rate constant for uptake
			! of HNO3 on dust [s-1]
REAL(fp),	INTENT(IN)	:: KTH(NDSTBIN)	! Size- and area-weighted
			! FRACTION for uptake of
			! H2SO4 on dust
TYPE(MetState),	INTENT(IN)	:: State_Met	! Meteorology State object
TYPE(OptInput),	INTENT(IN)	:: Input_Opt	! Input Options object

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

REAL(fp),	INTENT(OUT)	:: S02_gas	! SO2 mixing ratio after
			! dust chem [v/v]
REAL(fp),	INTENT(OUT)	:: PSO4d(NDSTBIN)	! Sulfate produced by
			! $S(IV)+03$ on dust in
			! each size bin
REAL(fp),	INTENT(OUT)	:: H2SO4_gas	! H2SO4 mixing ratio
			! after dust chem [v/v]
REAL(fp),	INTENT(OUT)	:: PNITd (NDSTBIN)	! Nitrate produced by
			! HNO3 uptake on dust
			! in each size bin
REAL(fp),	INTENT(OUT)	:: PH2SO4d(NDSTBIN)! Sulfate produced by
			! uptake of H2SO4 on
			! dust in each size bin
REAL(fp),	INTENT(OUT)	:: ALKA(NDSTBIN)	! Dust Alkalinity after
			! dust chemistry [v/v]
INTEGER,	INTENT(OUT)	:: RC	! Success or failure?

REMARKS:

Chemical reactions:

```
(R1) SO2 + O3 + CaCO3 => CaSO4 + O2 + CO2
```

(R2) 2(HNO3) + CaCO3 => Ca(NO3)2 + CO2 + H2O

Added sulfate production due to ${\tt H2SO4}$ adsorption tdf ${\tt 2/13/2K9}$

(R3) H2S04 + CaC03 => CaS04 + H20 + C02

REVISION HISTORY:

```
28 Mar 2008 - T.D. Fairlie- Initial version
```

16 Sep 2013 - M. Sulprizio- Added ProTeX headers

17 Sep 2013 - M. Sulprizio- Now pass Input_Opt, State_Met, State_Chm, and RC as arguments

30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

8.5.9 get_hplus

Subroutine GET_HPLUS computes H+ concentrations in cloud liquid water for pH dependent cloud chemistry. (bec, 4/11/11)

INTERFACE:

```
SUBROUTINE GET_HPLUS( SO4nss, TNH3, TNO3, SO2, & T, PRES, LWC, iHPLUS, HPLUS)
```

USES:

USE ERROR_MOD, ONLY : IT_IS_NAN, GEOS_CHEM_STOP

INPUT PARAMETERS:

OUTPUT PARAMETERS:

REAL(fp), INTENT(OUT) :: HPLUS ! Calculated [H+] [M]

REMARKS:

Calculation:

```
Solve the following electroneutrality equation:
```

```
[H+] = 2[S04]nss + [C1] + [OH] + [HC03] + 2[C03] + [HS03] + 2[S03] + [N03] - [Na] - 2[Ca] - [K] - 2[Mg] - [NH4]
```

Aqueous concentrations of [Cl], [Na], [Ca], [K], and [Mg] come from ISORROPIA II

Let concentrations of [HCO3], [CO3], [HSO3], [SO3], [NO3] and [NH4] evolve according to Henry's law equilibrium.

Assume [S(VI)] = [SO4] nss (this applies for pH > 3)

REVISION HISTORY:

```
25 Jan 2012 - M. Payer - Added ProTeX headers
06 Jan 2015 - M. Yannetti - Set some variables to f8 that required it
28 Apr 2015 - E. Lundgren - Input pressure is now dry air partial pressure
```

8.5.10 kCO21

Function kCO21

INTERFACE:

```
FUNCTION kCO21 ( P, T, LWC, HPLUS ) RESULT ( KCO2p )
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: T, P, LWC, HPLUS
```

OUTPUT PARAMETERS:

REAL(fp) :: KCO2p, KCO2p2

REVISION HISTORY:

```
25 Jan 2012 - M. Payer - Added ProTeX headers
```

28 Apr 2015 - E. Lundgren - Input pressure is now dry air partial pressure

8.5.11 kCO22

Function kCO22

INTERFACE:

```
FUNCTION kCO22 ( P, T, LWC, HPLUS ) RESULT ( KCO2p2 )
```

INPUT PARAMETERS:

REAL(fp), INTENT(IN) :: T, P, LWC, HPLUS

OUTPUT PARAMETERS:

REAL(fp) :: KCO2p, KCO2p2

REVISION HISTORY:

```
25 Jan 2012 - M. Payer - Added ProTeX headers
```

28 Apr 2015 - E. Lundgren - Input pressure is now dry air partial pressure

8.5.12 kSO21

Function kSO21

INTERFACE:

FUNCTION kSO21 (P, T, LWC, HPLUS, SO2) RESULT (KSO2p)

INPUT PARAMETERS:

REAL(fp), INTENT(IN) :: T, P, LWC, HPLUS, SO2

OUTPUT PARAMETERS:

REAL(fp) :: KSO2p, KSO2p2

REVISION HISTORY:

25 Jan 2012 - M. Payer - Added ProTeX headers

28 Apr 2015 - E. Lundgren - Input pressure is now dry air partial pressure

8.5.13 kSO22

Function kSO22

INTERFACE:

FUNCTION kSO22 (P, T, LWC, HPLUS, SO2) RESULT (KSO2p2)

INPUT PARAMETERS:

REAL(fp), INTENT(IN) :: T, P, LWC, HPLUS, SO2

OUTPUT PARAMETERS:

REAL(fp) :: KSO2p, KSO2p2

REVISION HISTORY:

25 Jan 2012 - M. Payer - Added ProTeX headers

28 Apr 2015 - E. Lundgren - Input pressure is now dry air partial pressure

8.5.14 kHNO3

Function kNO3

INTERFACE:

FUNCTION kHNO3 (P, T, LWC, HPLUS, HNO3) RESULT (KHNO3p)

INPUT PARAMETERS:

REAL(fp), INTENT(IN) :: T, P, LWC, HPLUS, HNO3

OUTPUT PARAMETERS:

REAL(fp) :: KHNO3p

REVISION HISTORY:

25 Jan 2012 - M. Payer - Added ProTeX headers

28 Apr 2015 - E. Lundgren - Input pressure is now dry air partial pressure

8.5.15 kHCl

Function kHCl

INTERFACE:

FUNCTION kHCl (P, T, LWC, HPLUS, Cl) RESULT (KHClp)

INPUT PARAMETERS:

REAL(fp), INTENT(IN) :: T, P, LWC, HPLUS, Cl

OUTPUT PARAMETERS:

REAL(fp) :: KHClp

REVISION HISTORY:

25 Jan 2012 - M. Payer - Added ProTeX headers

28 Apr 2015 - E. Lundgren - Input pressure is now dry air partial pressure

8.5.16 kNH3

Function kNH3

INTERFACE:

FUNCTION kNH3 (P, T, LWC, HPLUS, NH3, Kw) RESULT (KNH3p)

INPUT PARAMETERS:

REAL(fp), INTENT(IN) :: T, P, LWC, HPLUS, NH3, Kw

OUTPUT PARAMETERS:

REAL(fp) :: KNH3p

REVISION HISTORY:

25 Jan 2012 - M. Payer - Added ProTeX headers

28 Apr 2015 - E. Lundgren - Input pressure is now dry air partial pressure

8.5.17 cubic

Subroutine CUBIC finds the roots of a cubic equation / 3rd order polynomial

INTERFACE:

SUBROUTINE CUBIC(A2, A1, A0, NR, CRUTES)

USES:

USE ERROR_MOD, ONLY : GEOS_CHEM_STOP !ERROR_STOP

INPUT PARAMETERS:

INTEGER :: NR

REAL(f8) :: A2, A1, A0 REAL(fp) :: CRUTES(3)

REMARKS:

```
Formulae can be found in numer. recip. on page 145
kiran developed this version on 25/4/1990
Dr. Francis S. Binkowski modified the routine on 6/24/91, 8/7/97
***

*** modified 2/23/98 by fsb to incorporate Dr. Ingmar Ackermann's recommendations for setting a0, a1,a2 as real(fp) variables.

Modified by Bob Yantosca (10/15/02)

- Now use upper case / white space

- force double precision with "D" exponents
```

- now call ERROR_STOP from "error_mod.f" to stop the run safely

REVISION HISTORY:

- updated comments / cosmetic changes

```
25 Jan 2012 - M. Payer - Added ProTeX headers
06 Jan 2015 - M. Yannetti - Manual changes of some variables to f8
```

8.5.18 agchem_so2

Subroutine AQCHEM_SO2 computes the reaction rates for aqueous SO2 chemistry. (rjp, bmy, 10/31/02, 12/12/02)

INTERFACE:

```
SUBROUTINE AQCHEM_SO2( LWC, T, P, SO2, H2O2, & O3, Hplus, KaqH2O2, KaqO3 )
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: LWC ! Liq water content [m3/m3]=1.E-6*L [g/m3] REAL(fp), INTENT(IN) :: T ! Temperature [K] REAL(fp), INTENT(IN) :: P ! Dry air partial pressure [atm] REAL(fp), INTENT(IN) :: SO2 ! SO2 mixing ratio [v/v] REAL(fp), INTENT(IN) :: H2O2 ! H2O2 mixing ratio [v/v] REAL(fp), INTENT(IN) :: O3 ! O3 mixing ratio [v/v] REAL(fp), INTENT(IN) :: HPLUS ! Concentration of H+ ion (i.e. pH) [v/v]
```

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT) :: KaqH2O2 ! Reaction rate for H2O2
REAL(fp), INTENT(OUT) :: KaqO3 ! Reaction rate for O3
```

REMARKS:

```
Chemical Reactions:
```

```
R1) HS03- + H202(aq) + H+ => S04-- + 2H+ + H20 [Jacob, 1986]

d[S(VI)]/dt = k[H+][H202(aq)][HS03-]/(1 + K[H+])
[Seinfeld and Pandis, 1998, page 366]
```

```
(R2) SO2(aq) + O3(aq) =>
        HS03-
                + 03(aq) =>
        S03-- + 03(aq) =>
         [Jacob, 1986; Jacobson, 1999]
        d[S(VI)]/dt = (k0[SO2(aq)] + k1[HSO3-] + K2[SO3--])[O3(aq)]
         [Seinfeld and Pandis, 1998, page 363]
   Reaction rates can be given as
               = k [H2O2(ag)] [S(IV)] [mole/liter*s] OR
        Krate = Ra LWC R T / P
                                        [1/s]
   Where:
        LWC = Liquid water content(g/m3)*10-6 [m3(water)/m3(gas)]
            = 0.08205 (atm L / mol-K), Universal gas const.
            = Temperature (K)
            = Pressure (atm)
   Procedure:
    (a) Given [SO2] which is assumed to be total SO2 (gas+liquid) in
          equilibrium between gas and liquid phase.
    (b) We can compute SO2(g) using Henry's law
            P(so2(g)) = Xg * [SO2]
           Xg = 1/(1 + Faq), Fraction of SO2 in gas
        where:
                 = Kheff * R * T * LWC,
           Fag
            KHeff = Effective Henry's constant
    (c ) Then Calculate Aquous phase, S[IV] concentrations
         S[IV] = Kheff * P(so2(g) in atm) [M]
    (d ) The exact same procedure is applied to calculate H2O2(aq)
REVISION HISTORY:
    (1) Updated by Rokjin Park (rjp, bmy, 12/12/02)
    22 Dec 2011 - M. Payer
                             - Added ProTeX headers
    28 Apr 2015 - E. Lundgren - Input pressure is now dry air partial pressure
```

8.5.19 het_drop_chem

Subroutine HET_DROP_CHEM estimates the in-cloud sulfate production rate in heterogeneous cloud droplets based on the Yuen et al., 1996 parameterization. (bec, 6/16/11)

INTERFACE:

```
SUBROUTINE HET_DROP_CHEM( I,
                                     J,
                                         L,
                                                  LSTOT, SSCvv,
                               aSO4, GNH3, SO2_sr, H2O2O, GNO3,
                                     Input_Opt,
                                                  State_Met,
     &
                               SR,
     &
                               State_Chm
                                                              )
USES:
      USE ERROR_MOD,
                             ONLY : IT_IS_FINITE, GEOS_CHEM_STOP
      USE Input_Opt_Mod,
                             ONLY : OptInput
      USE State_Chm_Mod,
                             ONLY : ChmState
      USE State_Met_Mod,
                            ONLY : MetState
      USE TIME_MOD,
                             ONLY : GET_TS_CHEM
INPUT PARAMETERS:
      INTEGER,
                     INTENT(IN) :: I, J, L
      REAL(fp),
                     INTENT(IN) :: LSTOT
                    INTENT(IN) :: SSCvv
      REAL(fp),
      REAL(fp),
                    INTENT(IN) :: aS04
      REAL(fp),
                     INTENT(IN) :: GNH3
      REAL(fp),
                     INTENT(IN) :: SO2_sr
      REAL(fp),
                     INTENT(IN) :: H2020
      REAL(fp),
                     INTENT(IN) :: GNO3
      TYPE(OptInput), INTENT(IN) :: Input_Opt
                                               ! Input Options object
      TYPE(MetState), INTENT(IN) :: State_Met
                                               ! Meteorology State object
INPUT/OUTPUT PARAMETERS:
      TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
OUTPUT PARAMETERS:
      REAL(fp),
                     INTENT(OUT) :: SR ! Sulfate production rate
REVISION HISTORY:
   25 Jan 2012 - M. Payer
                          - Added ProTeX headers
   05 Sep 2013 - M. Sulprizio- Now pass met fields using the State_Met object
```

```
06 Nov 2014 - R. Yantosca - Now use State_Met%AIRDEN(I,J,L)
22 Jun 2016 - M. Yannetti - Pass State_Chm as arg for spc db access
```

8.5.20 chem_so4

Subroutine CHEM_SO4 is the SO4 chemistry subroutine from Mian Chin's GOCART model, modified for the GEOS-CHEM model. Now also modified to account for production of crystalline and aqueous sulfur tracers. (rjp, bdf, cas, bmy, 5/31/00, 5/23/06)

INTERFACE:

```
SUBROUTINE CHEM_SO4( am_I_Root, Input_Opt,
                      State_Met, State_Chm, RC )
&
```

USES:

USE CHEMGRID_MOD, ONLY : ITS_IN_THE_NOCHEMGRID

USE CMN_SIZE_MOD

USE CMN_DIAG_MOD

USE ErrCode_Mod

USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState
USE TIME_MOD, ONLY : GET_TS_CHEM

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

The only production is from SO2 oxidation (save in CHEM_SO2). Dry deposition is now handled in mixing_mod.F90, so we can must add the production from SO2 into the SO4 tracers.

- (1) Now reference AD from "dao_mod.f". Added parallel DO-loops.

 Updated comments, cosmetic changes. (rjp, bdf, bmy, 9/16/02)
- (2) Now replace DXYP(JREF)*1d4 with routine GET_AREA_CM2 of "grid_mod.f"
 Now use function GET_TS_CHEM from "time_mod.f" (bmy, 3/27/03)
- (3) Now reference PBLFRAC from "drydep_mod.f". Now apply dry deposition to the entire PBL. (rjp, bmy, 8/1/03)
- (4) Now use ND44_TMP array to store vertical levels of drydep flux, then sum into AD44 array. This preents numerical differences when using multiple processors. (bmy, 3/24/04)
- (5) Now use parallel DO-loop to zero ND44_TMP (bmy, 4/14/04)
- (6) Now reference STT & TCVV from "tracer_mod.f" (bmy, 7/20/04)
- (7) Now references LCRYST from "logical_mod.f". Modified for crystalline and aqueous sulfate2 tracers: AS, AHS, LET, SO4aq. Also changed name of ND44_TMP to T44 to save space. (cas, bmy, 12/21/04)
- (8) Replace PBLFRAC from "drydep_mod.f" with GET_FRAC_UNDER_PBLTOP from "pbl_mix_mod.f" (bmy, 2/22/05)
- (9) Now remove reference to CMN, it's obsolete. Now reference

```
ITS_IN_THE_STRAT from "tropopause_mod.f" (bmy, 8/22/05)
(10) Now references XNUMOL from "tracer_mod.f" (bmy, 10/25/05)
(11) Rearrange error check to avoid SEG FAULTS (bmy, 5/23/06)
22 Dec 2011 - M. Payer
                          - Added ProTeX headers
01 Mar 2012 - R. Yantosca - Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
30 Jul 2012 - R. Yantosca - Now accept am_I_Root as an argument when
                            running with the traditional driver main.F
31 Jul 2012 - R. Yantosca - Now loop from 1..LLPAR for GIGC compatibility
31 Jul 2012 - R. Yantosca - Declare temp drydep arrays w/ LLPAR (not LLTROP)
14 Nov 2012 - R. Yantosca - Add am_I_Root, Input_Opt, RC as arguments
                          - Replaced all met field arrays with State_Met
15 Nov 2012 - M. Payer
                            derived type object
05 Mar 2013 - R. Yantosca - Now use Input_Opt%LNLPBL
19 Mar 2013 - R. Yantosca - Now copy Input_Opt%TCVV(1:N_TRACERS) and
                            Input_Opt%XNUMOL(1:N_TRACERS) -- avoid OOB errs
25 Mar 2013 - M. Payer
                          - Now pass State_Chm object via the arg list
12 Sep 2013 - M. Sulprizio- Now include references to dust-sulfate chemistry
                            (tdf 04/07/08)
12 Jun 2015 - R. Yantosca - Now remove orphaned ND44 variables
12 Jun 2015 - R. Yantosca - Drydep is now handled in mixing_mod.F90,
                            so we can greatly collapse this code
23 Sep 2015 - R. Yantosca - Remove references to DRYSO4 and DRYSO4s
24 Jun 2016 - R. Yantosca - Now return if id_S04<0 or id_S04s<0 (not == 0)
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected
                            species ID from State_Chm%Map_Advect.
```

8.5.21 chem_so4_aq

USE UnitConv_Mod

Subroutine CHEM_SO4_AQ takes the SO4 produced via aqueous chemistry of SO2 and distribute onto the size-resolved aerosol number and sulfate mass as a part of the TOMAS aerosol microphysics module (win, 1/25/10)

INTERFACE:

```
SUBROUTINE CHEM_SO4_AQ( am_I_Root, Input_Opt, & State_Met, State_Chm, RC )

USES:
```

```
USE CHEMGRID_MOD, ONLY : ITS_IN_THE_NOCHEMGRID
USE CMN_SIZE_MOD
USE ErrCode_Mod
USE ERROR_MOD
USE Input_Opt_Mod, ONLY : OptINput
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState
USE TOMAS_MOD, ONLY : AQOXID, GETACTBIN
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

NOTE: This subroutine is ignored unless we compile for TOMAS microphysics.

REVISION HISTORY:

- (1) As of now the SO4 produced via heterogeneous reaction on the 2-mode seasalt is not include in this treatment (win, 7/23/07)
- (2) Change a fixed kmin = 8 (corresponding to the assumed activation dia. of 55nm to be varying with current chemical composition. Take average of the activating bin for LS and CONV rains. (win, 9/25/07)
- 16 Feb 2012 R. Yantosca Added ProTeX headers
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 31 May 2013 R. Yantosca Now accept am_I_Root, Input_Opt, State_Chm and RC arguments
- 31 May 2013 R. Yantosca Now pass State_Chm to TOMAS routines
- 30 Sep 2015 E. Lundgren Now use UNITCONV_MOD conversion routine

8.5.22 chem_msa

USE ErrCode_Mod

Subroutine CHEM_MSA is the SO4 chemistry subroutine from Mian Chin's GOCART model, modified for the GEOS-CHEM model. (rjp, bdf, bmy, 5/31/00, 10/25/05)

INTERFACE:

```
SUBROUTINE CHEM_MSA( am_I_Root, Input_Opt, & State_Met, State_Chm, RC )
```

USES:

USE CHEMGRID_MOD, ONLY : ITS_IN_THE_NOCHEMGRID
USE CMN_DIAG_MOD
USE CMN_SIZE_MOD

USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState

USE TIME_MOD, ONLY : GET_TS_CHEM

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

The only production is from DMS oxidation (saved in CHEM_DMS). Dry deposition is now treaded in mixing_mod.F90.

REVISION HISTORY:

- (1) Now reference AD from "dao_mod.f". Added parallel DO-loops.

 Updated comments, cosmetic changes. (rjp, bmy, bdf, 9/16/02)
- (2) Now replace DXYP(JREF)*1d4 with routine GET_AREA_CM2 of "grid_mod.f" Now use function GET_TS_CHEM from "time_mod.f" (bmy, 3/27/03)
- (3) Now reference PBLFRAC from "drydep_mod.f". Now apply dry deposition to the entire PBL. (rjp, bmy, 8/1/03)
- (4) Now use ND44_TMP array to store vertical levels of drydep flux, then sum into AD44 array. This preents numerical differences when using multiple processors. (bmy, 3/24/04)
- (5) Now use parallel DO-loop to zero ND44_TMP (bmy, 4/14/04)
- (6) Now references STT & TCVV from "tracer_mod.f" (bmy, 7/20/04)
- (7) Replace PBLFRAC from "drydep_mod.f" with GET_FRAC_UNDER_PBLTOP from "pbl_mix_mod.f". Also reference GET_PBL_MAX_L from "pbl_mix_mod.f" Vertical DO-loops can run up to PBL_MAX and not LLTROP. Also remove reference to header file CMN. (bmy, 2/22/05)
- (8) Now references XNUMOL from "tracer_mod.f" (bmy, 10/25/05)
- (9) Change loop back to over entire troposphere to correctly add production of MSA (PMSA_dms) to the MSA tracer array.

Added reference USE_TROPOPAUSE_MOD, ONLY: ITS_IN_THE_STRAT as a precaution. (pjh, 8/19/2009)

- 22 Dec 2011 M. Payer Added ProTeX headers
- 01 Mar 2012 R. Yantosca Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
- 31 Jul 2012 R. Yantosca Now loop from 1..LLPAR for GIGC compatibility
- 31 Jul 2012 R. Yantosca Declare temp drydep arrays w/ LLPAR (not LLTROP)
- 14 Nov 2012 R. Yantosca Add am_I_Root, Input_Opt, RC as arguments
- 15 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 05 Mar 2013 R. Yantosca Now use Input_Opt%LNLPBL
- 19 Mar 2013 R. Yantosca Now copy Input_Opt%TCVV(1:N_TRACERS) and

```
Input_Opt%XNUMOL(1:N_TRACERS) -- avoid 00B errs

25 Mar 2013 - M. Payer - Now pass State_Chm object via the arg list

12 Jun 2015 - R. Yantosca - Now remove orphaned ND44 variables

12 Jun 2015 - R. Yantosca - Drydep is now handled in mixing_mod.F90,

so we can greatly collapse this code

23 Sep 2015 - R. Yantosca - Remove references to obsolete DRYMSA flag

24 Jun 2016 - R. Yantosca - Now return if id_MSA < 0 (not == 0)

30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.
```

8.5.23 chem_nit

Subroutine CHEM_NIT removes SULFUR NITRATES (NIT) from the surface via dry deposition. (rjp, bdf, bmy, 1/2/02, 5/23/06)

INTERFACE:

```
SUBROUTINE CHEM_NIT( am_I_Root, Input_Opt, & State_Met, State_Chm, RC )
```

USES:

```
USE CHEMGRID_MOD, ONLY : ITS_IN_THE_NOCHEMGRID

USE CMN_DIAG_MOD

USE CMN_SIZE_MOD

USE ErrCode_Mod

USE Input_Opt_Mod, ONLY : OptInput

USE State_Chm_Mod, ONLY : ChmState

USE State_Met_Mod, ONLY : MetState

USE PBL_MIX_MOD, ONLY : GET_FRAC_UNDER_PBLTOP
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REMARKS:

Dry deposition is now applied in mixing_mod.F90. Therefore we can

REMARKS:

Reaction List:

(1) NIT = NIT_0 * EXP(-dt) where d = dry deposition rate [s-1]

- (1) Now reference AD from "dao_mod.f". Added parallel DO-loops. Updated comments, cosmetic changes. (rjp, bmy, bdf, 9/20/02)
- (2) Now replace DXYP(J+J0)*1d4 with routine GET_AREA_CM2 from "grid_mod.f".

 Now use function GET_TS_CHEM from "time_mod.f" (bmy, 3/27/03)
- (3) Now reference PBLFRAC from "drydep_mod.f". Now apply dry deposition to the entire PBL. Added L and FREQ variables. Recode to avoid underflow from EXP(). (rjp, bmy, 8/1/03)
- (4) Now use ND44_TMP array to store vertical levels of drydep flux, then sum into AD44 array. This preents numerical differences when using multiple processors. (bmy, 3/24/04)
- (5) Now use parallel DO-loop to zero ND44_TMP (bmy, 4/14/04)
- (6) Now reference STT & TCVV from "tracer_mod.f". Also remove reference to CMN, it's not needed anymore. (bmy, 7/20/04)
- (7) Replace PBLFRAC from "drydep_mod.f" with GET_FRAC_UNDER_PBLTOP from "pbl_mix_mod.f". Also reference GET_PBL_MAX_L from "pbl_mix_mod.f" Vertical DO-loops can run up to PBL_MAX and not LLTROP. (bmy, 2/22/05)
- (8) Now references XNUMOL from "tracer_mod.f" (bmy, 10/25/05)
- (9) Rearrange error check to avoid SEG FAULTS (bmy, 5/23/06)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 01 Mar 2012 R. Yantosca Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
- 31 Jul 2012 R. Yantosca Now loop from 1..LLPAR for GIGC compatibility
- 31 Jul 2012 R. Yantosca Declare temp drydep arrays w/ LLPAR (not LLTROP)
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 05 Mar 2013 R. Yantosca Now use Input_Opt%LNLPBL
- 13 Mar 2013 R. Yantosca Bug fix: make sure we pass values to the SOIL_DRYDEP routine even when ND44 is off (this happens when LNLPBL = F)
- 19 Mar 2013 R. Yantosca Now copy Input_Opt%TCVV(1:N_TRACERS) and Input_Opt%XNUMOL(1:N_TRACERS) -- avoid OOB errs
- 25 Mar 2013 M. Payer Now pass State_Chm object via the arg list
- 12 Sep 2013 M. Sulprizio- Now include references to nitrate on dust (tdf, 04/07/08)
- 23 Sep 2013 M. Sulprizio- Bug fix: Skip stratospheric boxes to prevent out-of-bounds error in PNIT_DUST
- 12 Jun 2015 R. Yantosca Now remove orphaned ND44 variables
- 12 Jun 2015 R. Yantosca Drydep is now handled in mixing_mod.F90, so we can greatly collapse this code
- 23 Sep 2015 R. Yantosca Remove reference to DRYNIT, DRYNITs
- 24 Jun 2016 R. Yantosca Now return if id_NIT<0 or id_NITs<0 (not == 0)

30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

8.5.24 sulfate_pbl_mix

Subroutine SULFATE_PBL_MIX partitions the total anthro sulfate emissions thru the entire boundary layer. Emissions above the PBL are not used, and left in their level, regardless of the mixing scheme. For non-local mixing scheme, all emissions within the PBL are put in the first level.

INTERFACE:

```
SUBROUTINE SULFATE_PBL_MIX ( EMISS, SULFATE, FRAC_OF_PBL, $ PBL_TOP, IS_LOCAL )
```

USES:

```
USE ERROR_MOD, ONLY : ERROR_STOP IMPLICIT NONE
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: PBL_TOP ! Top level of boundary layer
LOGICAL, INTENT(IN) :: IS_LOCAL ! mixing scheme
REAL(fp), INTENT(IN) :: FRAC_OF_PBL(:) !
REAL(fp), INTENT(IN) :: EMISS(:)
```

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(INOUT) :: SULFATE(:) ! partitioned emissions
```

REVISION HISTORY:

```
27 Oct 2009 - P. Le Sager - initial
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
```

8.5.25 get_oh

Function GET_OH returns OH from State_Chmcoupled runs) or monthly mean OH (for offline runs). Imposes a diurnal variation on OH for offline simulations. (bmy, 12/16/02, 7/20/04)

INTERFACE:

```
FUNCTION GET_OH( I, J, L, Input_Opt, State_Chm, State_Met ) & RESULT( OH_MOLEC_CM3 )
```

USES:

```
USE CHEMGRID_MOD, ONLY : ITS_IN_THE_CHEMGRID
USE CMN_SIZE_MOD

USE ERROR_MOD, ONLY : ERROR_STOP

USE Input_Opt_Mod, ONLY : OptInput

USE State_Chm_Mod, ONLY : ChmState

USE State_Met_Mod, ONLY : MetState

USE TIME_MOD, ONLY : GET_TS_CHEM
```

INPUT PARAMETERS:

REVISION HISTORY:

- (1) We assume SETTRACE has been called to define IDOH (bmy, 11/1/02)
- (2) Now use function GET_TS_CHEM from "time_mod.f" (bmy, 3/27/03)
- (3) Now reference ITS_A_FULLCHEM_SIM, ITS_AN_AEROSOL_SIM from "tracer_mod.f". Also replace IJSURF w/ an analytic function. (bmy, 7/20/04)

```
22 Dec 2011 - M. Payer - Added ProTeX headers
```

- 28 Nov 2012 R. Yantosca Replace SUNCOS with State_Met%SUNCOS
- 28 Nov 2012 R. Yantosca Add State_Met to argument list
- 04 Mar 2013 R. Yantosca Now pass Input_Opt%ITS_A_FULLCHEM_SIM and Input_Opt%ITS_AN_AEROSOL_SIM
- 18 Sep 2014 M. Sulprizio- Now get OH for offline aerosol sim from HEMCO
- 22 Dec 2015 M. Sulprizio- Remove references to CSPEC and JLOOP. We now get species concentrations from State_Chm%Species.

8.5.26 get_no3

Function GET_NO3 returns NO3 from State_Chmcoupled runs) or monthly mean OH (for offline runs). For offline runs, the concentration of NO3 is set to zero during the day. (rjp, bmy, 12/16/02)

INTERFACE:

```
FUNCTION GET_NO3( I, J, L, Input_Opt, State_Chm, State_Met )
& RESULT( NO3_MOLEC_CM3 )
```

USES:

```
USE CHEMGRID_MOD, ONLY : ITS_IN_THE_CHEMGRID
USE CMN_SIZE_MOD

USE ERROR_MOD, ONLY : ERROR_STOP

USE Input_Opt_Mod, ONLY : OptInput

USE State_Chm_Mod, ONLY : ChmState

USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

REVISION HISTORY:

- (1) Now references ERROR_STOP from "error_mod.f". We also assume that SETTRACE has been called to define IDNO3. Now also set NO3 to zero during the day. (rjp, bmy, 12/16/02)
- (2) Now reference ITS_A_FULLCHEM_SIM and ITS_AN_AEROSOL_SIM from "tracer_mod.f". Also remove reference to CMN. Also replace IJSURF with an analytic function. (bmy, 7/20/04)

```
22 Dec 2011 - M. Payer - Added ProTeX headers
```

- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 28 Nov 2012 R. Yantosca Replace SUNCOS with State_Met%SUNCOS
- 04 Mar 2013 R. Yantosca Now pass Input_Opt%ITS_A_FULLCHEM_SIM and Input_Opt%ITS_AN_AEROSOL_SIM
- 24 Jul 2014 R. Yantosca Now compute BOXVL internally
- 18 Sep 2014 M. Sulprizio- Now get NO3 for offline aerosol sims from HEMCO
- 22 Dec 2015 M. Sulprizio- Remove references to CSPEC and JLOOP. We now get species concentrations from State_Chm%Species.

$8.5.27 \text{ get}_o3$

Function GET_O3 returns monthly mean O3 for offline sulfate aerosol simulations. (bmy, 12/16/02, 10/25/05)

INTERFACE:

```
FUNCTION GET_03( I, J, L, Input_Opt, State_Chm, State_Met )
& RESULT( 03_VV )
```

USES:

```
USE CHEMGRID_MOD, ONLY : ITS_IN_THE_CHEMGRID
```

USE CMN_SIZE_MOD

USE ERROR_MOD, ONLY : ERROR_STOP
USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

REVISION HISTORY:

- (1) We assume SETTRACE has been called to define IDO3. (bmy, 12/16/02)
- (2) Now reference inquiry functions from "tracer_mod.f" (bmy, 7/20/04)
- (3) Now remove reference to CMN, it's obsolete. (bmy, 8/22/05)
- (4) Now references XNUMOLAIR from "tracer_mod.f" (bmy, 10/25/05)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 04 Mar 2013 R. Yantosca Now pass Input_Opt%ITS_A_FULLCHEM_SIM and Input_Opt%ITS_AN_AEROSOL_SIM
- 06 Nov 2014 R. Yantosca Now use State_Met%AIRDEN(I,J,L)
- 24 Mar 2015 E. Lundgren Replace dependency on tracer_mod with CMN_GTCM_MOD to get XNUMOLAIR.
- 22 Dec 2015 M. Sulprizio- Remove references to CSPEC and JLOOP. We now get species concentrations from State_Chm%Species.

8.5.28 ohno3time

Subroutine OHNO3TIME computes the sum of cosine of the solar zenith angle over a 24 hour day, as well as the total length of daylight. This is needed to scale the offline OH and NO3 concentrations. (rjp, bmy, 12/16/02, 3/30/04)

INTERFACE:

SUBROUTINE OHNOSTIME

USES:

```
USE CMN_SIZE_MOD
```

USE GC_GRID_MOD, ONLY : GET_XMID, GET_YMID_R

USE TIME_MOD, ONLY: GET_NHMSb, GET_ELAPSED_SEC

USE TIME_MOD, ONLY: GET_TS_CHEM, GET_DAY_OF_YEAR, GET_GMT

- (1) Copy code from COSSZA directly for now, so that we don't get NaN values. Figure this out later (rjp, bmy, 1/10/03)
- (2) Now replace XMID(I) with routine GET_XMID from "grid_mod.f". Now replace RLAT(J) with routine GET_YMID_R from "grid_mod.f". Removed NTIME, NHMSb from the arg list. Now use GET_NHMSb, GET_ELAPSED_SEC, GET_TS_CHEM, GET_DAY_OF_YEAR, GET_GMT from "time_mod.f". (bmy, 3/27/03)
- (3) Now store the peak SUNCOS value for each surface grid box (I,J) in the COSZM array. (rjp, bmy, 3/30/04)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 16 May 2016 M. Sulprizio- Remove IJLOOP and change SUNTMP array dimensions from (MAXIJ) to (IIPAR, JJPAR)

8.5.29 get_alk

Subroutine GET_ALK returns the seasalt alkalinity emitted at each timestep to sulfate_mod.f for chemistry on seasalt aerosols. (bec, 12/7/04, 11/23/09)

INTERFACE:

```
SUBROUTINE GET_ALK( am_I_Root, I,J,L, ALK1, ALK2, Kt1, Kt2,
                     Kt1N, Kt2N, Input_Opt, State_Met, State_Chm,
&
                     RC)
&
```

USES:

```
USE CMN_SIZE_MOD,
                       ONLY: NDUST
```

USE ErrCode_Mod

USE ERROR_MOD, ONLY : IT_IS_NAN, ERROR_STOP

USE HCO_INTERFACE_MOD, ONLY : GetHcoVal

(jas, 8/4/15) calculate kt using sea salt surface area concentration

USE CMN_SIZE_MOD, ONLY : NDUST USE Input_Opt_Mod, ONLY : OptInput

USE PBL_MIX_MOD, ONLY : GET_FRAC_OF_PBL, GET_PBL_TOP_L

ONLY : ChmState USE State_Chm_Mod, USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

```
LOGICAL,
               INTENT(IN)
                            :: am_I_Root ! Root CPU?
```

INTEGER, INTENT(IN) :: I, J, L ! Lon-lat-alt indices
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

OUTPUT PARAMETERS:

```
REAL(fp),
               INTENT(OUT) :: ALK1, ALK2 ! [kg]
```

REAL(fp), INTENT(OUT) :: Kt1, Kt2, Kt1N, Kt2N ! [s-1]

INPUT/OUTPUT PARAMETERS:

```
INTENT(INOUT) :: RC
```

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

- (1) Becky Alexander says we can remove AREA1, AREA2 (bec, bmy, 9/5/06)
- (2) Bug fix to remove a double-substitution. Replace code lines for TERM{123}A, TERM{123}B, TERM{123}AN, TERM{123}BN. (bec, bmy, 7/18/08)
- (3) Updated hygroscopic growth parameters (bec, bmy, 11/23/09)
- (4) Fixed bug when calculating rate constants for uptake of SO2 and HNO3 (kt). The bug caused kt to be too small and prevented acidification of SSA. (jas, 8/4/15)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 09 Nov 2012 M. Payer - Replaced all met field arrays with State_Met

```
derived type object
```

```
25 Jun 2014 - R. Yantosca - Now accept Input_Opt via the arg list
25 Jun 2014 - R. Yantosca - Removed references to tracer_mod.F

02 Nov 2014 - C. Keller - Now get alkalinity and number density from HEMCO

04 Nov 2014 - C. Keller - Moved from seasalt_mod.F

12 Nov 2014 - C. Keller - Now weight # dens. and alk. by fraction of PBL

12 May 2016 - M. Sulprizio- Remove 1D arrays that depend on JLOOP. ERADIUS,

TAREA, are now pointers that point to 3D fields
fields in State_Chm.
```

8.5.30 init_sulfate

Subroutine INIT_SULFATE initializes and zeros all allocatable arrays declared in "sulfate_mod.f" (bmy, 6/2/00, 10/15/09)

INTERFACE:

```
SUBROUTINE INIT_SULFATE( am_I_Root, Input_Opt, State_Chm, RC )
```

USES:

```
USE ErrCode_Mod

USE ERROR_MOD, ONLY : Alloc_Err

USE ERROR_MOD, ONLY : Error_Stop

USE Input_Opt_Mod, ONLY : OptInput

USE State_Chm_Mod, ONLY : ChmState

USE State_Chm_Mod, ONLY : Ind_
```

INPUT PARAMETERS:

USE CMN_SIZE_MOD

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object
```

INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

- (1) Only allocate some arrays for the standalone simulation (NSRCX==10). Also reference NSRCX from "CMN". Now eferences routine ALLOC_ERR from "error_mod.f" ((rjp, bdf, bmy, 10/15/02)
- (2) Now also allocate the IJSURF array to keep the 1-D grid box indices for SUNCOS (for both coupled & offline runs). Now allocate PH2O2m and O3m for offline runs. Also allocate ESO2_bf (bmy, 1/16/03)
- (3) Now allocate ENH3_na array (rjp, bmy, 3/23/03)
- (4) Now allocate COSZM for offline runs (bmy, 3/30/04)
- (5) Now allocate ESO2_sh array (bec, bmy, 5/20/04)

- (6) Now allocates ITS_AN_AEROSOL_SIM from "tracer_mod.f". Now remove IJSURF (bmy, 7/20/04)
- (7) Now locate species in the DEPSAV array here instead of in CHEMSULFATE.

 Now reference LDRYD from "logical_mod.f". Updated for AS, AHS, LET,

 S04aq, NH4aq. (bmy, 1/6/06)
- (8) Now allocates PSO4_ss, PNITs (bec, bmy, 4/13/05)
- (9) Initialize drydep flags outside of IF block (bmy, 5/23/06)
- (10) Now redimension EEV & NEV arrays for new SO2 volcanic emissions inventory. Deleted obsolete arrays from older SO2 volcanic emissions inventory. (jaf, bmy, 10/15/09)
- (11) Now alllocate PSO4_SO2AQ (win, 1/25/10)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 04 Mar 2013 R. Yantosca Now accept am_I_Root, Input_Opt, RC arguments
- 05 Mar 2013 R. Yantosca Now use Input_Opt%ITS_AN_AEROSOL_SIM
- 30 May 2013 S. Farina Allocate PSO4_SO2AQ for TOMAS
- 12 Sep 2013 M. Sulprizio- Add PSO4_dust and PNIT_dust for acid update on dust aerosols (T.D. Fairlie)
- 26 Sep 2013 R. Yantosca Renamed GEOS_57 Cpp switch to GEOS_FP
- 22 May 2015 R. Yantosca Remove variables made obsolete by HEMCO
- 29 Apr 2016 R. Yantosca Don't initialize pointers in declaration stmts
- 21 Jun 2016 R. Yantosca Reorder the Ind_ declaration statements a bit
- 24 Jun 2016 R. Yantosca Add error checks for dust uptake species

8.5.31 cleanup_sulfate

Subroutine CLEANUP_SULFATE deallocates all previously allocated arrays for sulfate emissions – call at the end of the run (bmy, 6/1/00, 10/15/09)

INTERFACE:

SUBROUTINE CLEANUP_SULFATE()

- (1) Now also deallocates IJSURF. (bmy, 11/12/02)
- (2) Now also deallocates ENH3_na (rjp, bmy, 3/23/03)
- (3) Now also deallocates COSZM (rjp, bmy, 3/30/04)
- (4) Now also deallocates ESO4_sh (bec, bmy, 5/20/04)
- (5) Now remove IJSURF (bmy, 7/20/04)
- (6) Bug fix: now deallocate PSO4_ss, PNITs (bmy, 5/3/06)
- (7) Deleted obsolete arrays from older SO2 volcanic emissions inventory (jaf, bmy, 10/15/09)
- (8) Deallocate PSO4_SO2AQ (win, 1/25/10)
- 22 Dec 2011 M. Payer Added ProTeX headers
- 30 May 2013 S. Farina Deallocate PSO4_SO2AQ for TOMAS
- 04 Mar 2015 R. Yantosca Remove EEV, NEV. Volcano eruptions are now handled via HEMCO.

22 May 2015 - R. Yantosca - Remove variables made obsolete by HEMCO

8.6 Fortran: Module Interface isoropiaii_mod.F

Module ISOROPIAILMOD contains the routines that provide the interface between ISOR-ROPIA II and GEOS-Chem.

The actual ISORROPIA II code which performs Na-SO4-NH3-NO3-Cl-(Ca-K-Mg) aerosol thermodynamic equilibrium is in isoropialIcode.f.

INTERFACE:

MODULE ISOROPIAII_MOD

USES:

USE HCO_ERROR_MOD ! For real precisions (hp)
USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

IMPLICIT NONE PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: CLEANUP_ISOROPIAII

PUBLIC :: DO_ISOROPIAII
PUBLIC :: GET_GNO3
PUBLIC :: GET_ISRINFO

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: GET_HNO3

PRIVATE :: INIT_ISOROPIAII

PRIVATE :: SAFELOG10
PRIVATE :: SET_HNO3

REMARKS:

Original Author:

```
*** COPYRIGHT 1996-2006, UNIVERSITY OF MIAMI, CARNEGIE MELLON UNIVERSITY,
```

*** GEORGIA INSTITUTE OF TECHNOLOGY

*** WRITTEN BY ATHANASIOS NENES

*** UPDATED BY CHRISTOS FOUNTOUKIS

Original v1.3 isoropia implementation into GEOS-Chem by Becky Alexander and Bob Yantosca (bec, bmy, 4/12/05, 11/2/05)

For Ca,K,Mg = 0, ISOROPIA II performs exactly like ISOROPIAv1.7 Ca, K, Mg, Na from dust is not currently considered

To implement ISOROPIA II into GEOS-Chem:

- * cleanup_isoropiaII needs to be called from cleanup.f
- * DO_ISOROPIA needs to be replaced with DO_ISOROPIAII in chemistry_mod.f
- * Change ISOROPIA to ISOROPIAII in sulfate_mod.f
- * add isoropiaII_mod.f, isoropiaIIcode.f, and irspia.inc to Makefile

ISOROPIA II implementation notes by Havala O.T. Pye:

- (1) The original isoropia code from T.Nenes is left as unmodified as possible. Original isoropia code can be found in isoropiaIIcode.f and common blocks can be found in isrpia.inc. For future upgrades to isoropia, replace isrpia.inc and isoropiaIIcode.f with the new version of isoropia and modify the call to ISOROPIA in this module. Please let the original author know of any changes made to ISOROPIA.
- (2) As of Nov 2007, routines using non-zero Ca, K, and Mg do not always conserve mass. Ca, K, and Mg are set to zero.

NOTE: ISORROPIA is Greek for "equilibrium", in case you were wondering.

REVISION HISTORY:

```
06 Jul 2007 - H. O. T. Pye - Initial version
29 Jan 2010 - R. Yantosca - Added ProTeX headers
21 Apr 2010 - R. Yantosca - Bug fix in DO_ISOROPIAII for offline aerosol
16 Feb 2011 - R. Yantosca - Add modifications for APM from G. Luo
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
23 Sep 2014 - M. Sulprizio - Get global HNO3 for offline aerosol simulation from HEMCO
14 Nov 2014 - M. Yannetti - Added PRECISION_MOD
23 Jun 2016 - R. Yantosca - Remove references to APM code; it is no longer compatible with the FlexChem implementation
```

8.6.1 do_isoropiaii

Subroutine DO_ISOROPIAII is the interface between the GEOS-Chem model and the aerosol thermodynamical equilibrium routine ISORROPIA II.

INTERFACE:

USES:

```
USE CHEMGRID_MOD, ONLY : ITS_IN_THE_STRATMESO
USE CMN_SIZE_MOD
USE ErrCode_Mod
USE ERROR_MOD, ONLY : DEBUG_MSG
USE ERROR_MOD, ONLY : ERROR_STOP
```

```
USE ERROR_MOD,
                        ONLY : SAFE_DIV
USE HCO_INTERFACE_MOD, ONLY : HcoState
USE HCO_EMISLIST_MOD,
                       ONLY : HCO_GetPtr
USE Input_Opt_Mod,
                       ONLY : OptInput
USE State_Chm_Mod,
                       ONLY : ChmState
USE State_Chm_Mod,
                       ONLY : Ind_
USE State_Met_Mod,
                       ONLY : MetState
USE TIME_MOD,
                       ONLY : GET_MONTH
USE TIME_MOD,
                       ONLY : ITS_A_NEW_MONTH
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Is this the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

Original isoropia v1.3 implmentation: (rjp, bec, bmy, 12/17/01, 8/22/05)

```
24 Aug 2007 - H. O. T. Pye - Initial version, in ISORROPIA II
18 Dec 2009 - H. O. T. Pye - Added division checks
29 Jan 2010 - R. Yantosca - Added ProTeX headers
21 Apr 2010 - E. Sofen
                          - Prevent out-of-bounds errors for offline
                             aerosol simulations where HNO3 is undefined
23 Jul 2010 - R. Yantosca - Bug fix: corrected typo in ND42 diag section
30 Jul 2012 - R. Yantosca - Now accept am_I_Root as an argument when
                             running with the traditional driver main.F
31 Jul 2012 - R. Yantosca - Now loop from 1..LLPAR for GIGC compatibilit
14 Nov 2012 - R. Yantosca - Add am_I_Root, Input_Opt, RC as arguments
15 Nov 2012 - M. Payer
                           - Replaced all met field arrays with State_Met
                             derived type object
25 Mar 2013 - M. Payer
                           - Now pass State_Chm object via the arg list
23 Sep 2014 - M. Sulprizio - Now get HNO3 for offline aerosol sim from HEMCO
16 Jun 2016 - K. Travis
                           - Now define species ID's with the Ind_ function
17 Jun 2016 - R. Yantosca - Now only define species ID's on the first call;
                             we don't want to do it on each loop iteration
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected
                             species ID from State_Chm%Map_Advect.
10 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code
```

8.6.2 safelog10

Calculates the LOG (base 10) of a number X. Returns a minimum value if X is too small, in order to avoid NaN or Infinity problems.

INTERFACE:

```
FUNCTION SAFELOG10( X ) RESULT ( SAFLOG )
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: X ! Argument for LOG10 function
```

RETURN VALUE:

```
REAL(fp) :: SAFLOG ! LOG10 output --
```

REVISION HISTORY:

```
11 Aug 2009 - H. O. T. Pye - Initial version, in ISORROPIA II
29 Jan 2010 - R. Yantosca - Added ProTeX headers
```

8.6.3 get_isrinfo

Subroutine GET_ISRINFO returns information related to aerosol pH.

INTERFACE:

```
FUNCTION GET_ISRINFO( I, J, L, N ) RESULT ( RETURNVALUE )
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I   ! GEOS-Chem longitude index
INTEGER, INTENT(IN) :: J   ! GEOS-Chem latitude index
INTEGER, INTENT(IN) :: L   ! GEOS-Chem level index
INTEGER, INTENT(IN) :: N   ! Flag for which information is desired
```

RETURN VALUE:

```
REAL(fp) :: RETURNVALUE
```

```
11 Aug 2009 - H. O. T. Pye - Initial version
29 Jan 2010 - R. Yantosca - Added ProTeX headers
```

8.6.4 get_hno3

Subroutine GET_HNO3 allows the HNO3 concentrations to evolve with time, but relaxes back to the monthly mean concentrations every 3 hours.

INTERFACE:

```
FUNCTION GET_HNO3( I, J, L, State_Met ) RESULT ( HNO3_UGM3 )
```

USES:

```
USE Input_Opt_Mod, ONLY : OptInput
USE PhysConstants, ONLY : AIRMW
USE State_Met_Mod, ONLY : MetState
```

USE TIME_MOD, ONLY : GET_ELAPSED_MIN

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I ! GEOS-Chem longitude index
INTEGER, INTENT(IN) :: J ! GEOS-Chem latitude index
INTEGER, INTENT(IN) :: L ! GEOS-Chem level index
TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

REVISION HISTORY:

```
16 Dec 2002 - R. Yantosca - Initial version, in ISORROPIA I
24 Mar 2003 - R. Yantosca - Now use function GET_ELAPSED_MIN() from the
new "time_mod.f" to get the elapsed minutes
since the start of run.

06 Jul 2007 - H. O. T. Pye - Initial version, in ISORROPIA II
29 Jan 2010 - R. Yantosca - Added ProTeX headers
23 Sep 2014 - M. Sulprizio - Now get HNO3 for offline aerosol sims from HEMCO
06 Jan 2016 - E. Lundgren - Use global physical parameters
```

8.6.5 set_hno3

Subroutine SET_HNO3 stores the modified HNO3 value back into the HNO3_sav array for the next timestep.

INTERFACE:

```
SUBROUTINE SET_HNO3( I, J, L, HNO3_UGM3 )
```

INPUT PARAMETERS:

REVISION HISTORY:

```
16 Dec 2002 - R. Yantosca - Initial version, in ISORROPIA I
06 Jul 2007 - H. O. T. Pye - Initial version, in ISORROPIA II
29 Jan 2010 - R. Yantosca - Added ProTeX headers
11 Jan 2015 - M. Yannetti - Some precision edits, for safety.
19 Sep 2016 - R. Yantosca - Bug fix: #ifdef's should be lower case
19 Sep 2016 - R. Yantosca - Bug fix: elif should be else
```

$8.6.6 \quad \text{get_gno3}$

Function GET_GNO3 returns the gas-phase HNO3 [v/v] for calculation of sea-salt chemistry in sulfate_mod (SEASALT_CHEM).

INTERFACE:

```
SUBROUTINE GET_GNO3( I, J, L, HNO3_kg, State_Met )
```

USES:

```
USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I ! GEOS-Chem longitude index
INTEGER, INTENT(IN) :: J ! GEOS-Chem latitude index
INTEGER, INTENT(IN) :: L ! GEOS-Chem level index
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT) :: HNO3_kg ! Gas-phase HNO3 [kg]
```

REVISION HISTORY:

```
15 Apr 2005 - B. Alexander - Initial version, in ISORROPIA I
06 Jul 2007 - H. O. T. Pye - Initial version, in ISORROPIA II
29 Jan 2010 - R. Yantosca - Added ProTeX headers
09 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met derived type object
```

8.6.7 init_isoropiaII

Subroutine INIT_ISOROPIAII initializes all module arrays.

INTERFACE:

SUBROUTINE INIT_ISOROPIAII

USES:

```
USE CMN_SIZE_MOD ! Size parameters USE ERROR_MOD, ONLY : ALLOC_ERR
```

REVISION HISTORY:

```
06 Jul 2007 - H. O. T. Pye - Initial version
29 Jan 2010 - R. Yantosca - Added ProTeX headers
31 Jul 2012 - R. Yantosca - Declare diag arrays w/ LLPAR (not LLTROP)
```

8.6.8 cleanup_isoropiaII

Subroutine CLEANUP_ISOROPIAII deallocates all module arrays.

INTERFACE:

```
SUBROUTINE CLEANUP_ISOROPIAII
```

REVISION HISTORY:

```
06 Jul 2007 - H. O. T. Pye - Initial version
29 Jan 2010 - R. Yantosca - Added ProTeX headers
```

9 Meteorological field modules

These modules contain routines to read archived meteorology into GEOS-Chem.

9.1 Fortran: Module Interface dao_mod.F

Module DAO_MOD contains both arrays that hold DAO met fields, as well as subroutines that compute, interpolate, or otherwise process DAO met field data.

INTERFACE:

```
MODULE DAO_MOD
```

USES:

```
USE CMN_SIZE_MOD ! Size parameters
USE PhysConstants ! Physical constants
USE PRECISION_MOD ! For GEOS-Chem Precision (fp)
```

```
IMPLICIT NONE
```

PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: AVGPOLE
PUBLIC :: AIRQNT

PUBLIC :: COPY_I3_I6_FIELDS
PUBLIC :: GET_COSINE_SZA

PUBLIC :: GET_OBK
PUBLIC :: INTERP
PUBLIC :: IS_LAND
PUBLIC :: IS_WATER
PUBLIC :: IS_ICE
PUBLIC :: IS_NEAR

PUBLIC :: SET_DRY_SURFACE_PRESSURE

- 26 Jun 2010 R. Yantosca Initial version
- (1) Added sea level pressure (SLP) met field for GEOS-3 (bmy, 10/10/00)
- (2) Moved MAKE_QQ to "wetscav_mod.f" (bmy, 10/12/00)
- (3) Now get LWI from ALBEDO for GEOS-3 in routines IS_LAND and IS_WATER (bmy, 4/4/01)
- (4) Define OPTDEP allocatable array for GEOS-3 -- this is the grid box optical depth and is now stored as a met field (bmy, 8/15/01)
- (5) Updated comments (bmy, 9/4/01)
- (6) Now make AVGW an allocatable module array. Also replace obsolete parameters {IJL}GCMPAR with IIPAR,JJPAR,LLPAR. (bmy, 9/27/01)
- (7) Remove arguments LMAKEPW, PW, and LM from AIRQNT (bmy, 10/3/01)
- (8) Remove obsolete code from 9/01 (bmy, 10/23/01)
- (9) Bug fixes in IS_LAND and IS_WATER. Also cosmetic changes and updated some comments. (mje, bmy, 1/9/02)
- (10) Now add additional array PSC2 in order to pass to TPCORE, which will fix the mixing ratio bug. Compute PSC2 in subroutine INTERP. Now bundle "convert_units.f" into "dao_mod.f". Updated comments. (bmy, 3/27/02)
- (11) Updated comments (bmy, 5/28/02)
- (12) Replaced all instances of IM with IIPAR and JM with JJPAR, in order to prevent namespace confusion for the new TPCORE (bmy, 6/25/02)
- (13) Eliminated PS, PSC arrays. Now reference "pressure_mod.f". Also updated AIRQNT for hybrid grid. Added routine MAKE_RH to this module. (dsa, bdf, bmy, 8/27/02)
- (14) Added arrays AD, BXHEIGHT, and T to "dao_mod.f". Also removed obsolete code from 8/02 from several module routines. Now references "error_mod.f". Remove all references to QQ, it is now declared in "wetscav_mod.f". (bmy, 11/8/02)
- (15) Now references "grid_mod.f". Also added PHIS field, which was formerly stored as PALTD in "CMN". Added bug fix in routine AVGPOLE for 1x1 nested grid. (bmy, 3/11/03)
- (16) Added SUNCOSB array for SMVGEAR II. Also removed KZZ array, since that is now obsolete. (bmy, 4/28/03)

- (17) Now moved MAKE_CLDFRC into "a6_read_mod.f". Added HKBETA, HKETA, TSKIN, GWETTOP, ZMEU, ZMMD, ZMMU, PARDF, PARDR fields for GEOS-4/fvDAS. (bmy, 6/25/03)
- (18) Added CLDFRC, RADSWG, RADLWG, SNOW arrays (bmy, 12/9/03)
- (19) Added routine COPY_I6_FIELDS w/ parallel DO-loops (bmy, 4/13/04)
- (20) Now also allocate AVGW for offline aerosol simulation (bmy, 9/28/04)
- (21) AVGPOLE now uses NESTED_CH and NESTED_NA cpp switches (bmy, 12/1/04)
- (22) Now modified for GEOS-5 and GCAP met fields (swu, bmy, 5/25/05)
- (23) Now allocate SNOW and GWET for GCAP (bmy, 8/17/05)
- (24) Now also add TSKIN for GEOS-3 (tmf, bmy, 10/20/05)
- (25) Modifications for near-land formulation (ltm, bmy, 5/16/06)
- (26) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (27) Modified for variable tropopause (phs, bdf, 9/14/06)
- (28) Add in extra fields for GEOS-5. Updated COSSZA. Now cap var trop at 200hPa near poles in INTERP (bmy, phs, 9/18/07)
- (29) Bug fix in INIT_DAO for CMFMC array (bmy, jaf, 6/11/08)
- (30) Add heat flux EFLUX for GEOS5. (lin, ccc, 5/29/09)
- (31) Add fractions of land and water, FRLAND, FROCEAN, FRLANDIC, FRLAKE for methane (kjw, 8/18/09)
- (32) Bug fix in AVGPOLE (bmy, 12/18/09)
- (33) Remove obsolete SUNCOSB array (bmy, 4/28/10)
- 16 Aug 2010 R. Yantosca Added ProTeX headers
- 18 Aug 2010 R. Yantosca Added modifications for MERRA data
- 18 Aug 2010 R. Yantosca Move CMN_SIZE, CMN_DIAG to top of module
- 25 Aug 2010 R. Yantosca Now read LWI (land/water/ice) for MERRA met
- 05 Oct 2011 R. Yantosca Add SUNCOS_30 array to hold the cos(SZA) computed @ 30 mins after each GMT hour.
- 07 Oct 2011 R. Yantosca Rename SUNCOS30 to SUNCOS_MID, which is the cos(SZA) at the midpt of the chemistry timestep
- 06 Feb 2012 R. Yantosca Add modifications for GEOS-5.7.x met fields
- 06 Feb 2012 R. Yantosca Split up INIT_DAO into several routines
- 07 Feb 2012 M. Payer Add subroutine GET_COSINE_SZA to compute sun angles at the current time and 5 hours prior to the current time (for the PARANOX ship emissions plume model) (R. Yantosca)
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 01 Mar 2012 R. Yantosca Now references the new grid_mod.F90
- 06 Mar 2012 R. Yantosca Now allocate TO3 for all met fields
- 21 Nov 2012 R. Yantosca Removed met fields now contained in State_met
- 21 Nov 2012 R. Yantosca Remove functions INIT_DAO_GCAP, INIT_DAO_GEOS4, INIT_DAO_GEOS5, INIT_DAO_GEOS57, INIT_DAO_MERRA
- 27 Nov 2012 R. Yantosca Removed obsolete AIRQNT_FULLGRID routine and obsolete arrays AIRDEN_FULLGRID, T_FULLGRID
- 28 Nov 2012 R. Yantosca Removed SUNCOS, SUNCOS_MID, SUNCOS_MID_5hr
- 28 Nov 2012 R. Yantosca Removed routines INIT_DAO, INIT_DAO_DERIVED, and CLEANUP_DAO; we have no more allocatable arrays
- 14 Mar 2013 M. Payer Restored routines AIRQNT_FULLGRID, INIT_DAO, CLEANUP_DAO and arrays AIRDEN_FULLGRID and

T_FULLGRID. They are required to correct vertical regridding of OH for offline simulations.

20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete

07 Nov 2014 - M. Yannetti - Added PRECISION_MOD

23 Feb 2015 - E. Lundgren - Change AIRQNT and formulas to take into account the presence of water vapor

26 Feb 2015 - E. Lundgren - Move calculations of RH and AVGW from MAKE_RH and MAKE_AVGW to AIRQNT. Update algorithms to account for the presence of water vapor and to use [g water / kg moist air] for the definition of specific humidity (SPHU).

16 Apr 2015 - R. Yantosca - Removed AIRQNT_FULLGRID, this was used to regrid OH fields, but that is now done by HEMCO

16 Apr 2015 - R. Yantosca - Also remove INIT_DAO and CLEANUP_DAO, since these allocated/deallocated the FULLGRID arrays

29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90

9.1.1 avgpole

Subroutine AVGPOLE computes average quantity near polar caps, defined by $(J=1,\,2)$ and $(J=JJPAR-1,\,JJPAR)$.

INTERFACE:

SUBROUTINE AVGPOLE(Z)

USES:

USE GC_GRID_MOD, ONLY : GET_AREA_M2

INPUT/OUTPUT PARAMETERS:

```
REAL(fp), INTENT(INOUT) :: Z(IIPAR, JJPAR) ! Quantity to be averaged ! over the pole (usually PS)
```

- 30 Jan 1998 R. Yantosca Initial version
- (1) AVGPOLE is written in Fixed-Form Fortran 90. Use F90 syntax for declarations, etc (bmy, 4/14/99)
- (2) MAIN now passes the Harvard CTM variable for surface area of a gridbox, DXYP(JJPAR), to AVGPOLE. Use window offset J+JO when accessing DXYP. Add JJPAR to the parameter list.
- (3) Added this routine to "dao_mod.f" (bmy, 6/27/00)
- (4) Updated comments (bmy, 4/4/01)
- (5) Now replaced DXYP(J) with routine GET_AREA_M2 of "grid_mod.f"

 Now also return immediately if GRID1x1 is selected. (bmy, 3/11/03)
- (6) Now use cpp switches NESTED_CH and NESTED_NA to denote nested

9.1.2 airqnt

Subroutine AIRQNT sets several members of State_Met, the meteorology object of derived type MetState, and optionally updates the tracer concentrations to conserve tracer mass when air quantities change.

INTERFACE:

```
SUBROUTINE AIRQNT( am_I_Root, Input_Opt, State_Met, State_Chm,
& RC, update_mixing_ratio )
```

USES:

```
USE ERROR_MOD

USE GC_GRID_MOD, ONLY: GET_AREA_M2

USE Input_Opt_Mod, ONLY: OptInput

USE State_Met_Mod, ONLY: MetState

USE State_Chm_Mod, ONLY: ChmState

USE PRESSURE_MOD

! Temporary fix for calculating air density (mps, 12/23/15)

USE PhysConstants, ONLY: AIRMW, AVO
```

INPUT PARAMETERS:

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met   ! Obj for met fields
TYPE(ChmState), INTENT(INOUT) :: State_Chm   ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REMARKS:

DAO met fields updated by AIRQNT:

(1)	PEDGE	(REAL(fp))	:	Moist air pressure at grid box bottom	[hPa]
(2)	PEDGE_DRY	(REAL(fp))	:	Dry air partial pressure at box bottom	[hPa]
(3)	PMID	(REAL(fp))	:	Moist air pressure at grid box centroid	[hPa]
(4)	PMID_DRY	(REAL(fp))	:	Dry air partial pressure at box centroid	[hPa]
(5)	PMEAN	(REAL(fp))	:	Altitude-weighted mean moist air pressure	[hPa]
(6)	PMEAN_DRY	(REAL(fp))	:	Alt-weighted mean dry air partial pressure	e [hPa]
(7)	DELP	(REAL(fp))	:	Delta-P extent of grid box	[hPa]
				(Same for both moist and dry air since we	
				assume constant water vapor pressure	
				across box)	
(8)	AIRDEN	(REAL(fp))	:	Mean grid box dry air density	[kg/m^3]
				(defined as total dry air mass/box vol)	
(9)	MAIRDEN	(REAL(fp))	:	Mean grid box moist air density	[kg/m^3]
				<pre>(defined as total moist air mass/box vol)</pre>	
(10)	AD	(REAL(fp))	:	Total dry air mass in grid box	[kg]
(11)	ADMOIST	(REAL(fp))	:	Total moist air mass in grid box	[kg]
(12)	BXHEIGHT	(REAL(fp))	:	Vertical height of grid box	[m]
(13)	AIRVOL	(REAL(fp))	:	Volume of grid box	[m^3]
(14)	MOISTMW	(REAL(fp))	:	Molecular weight of moist air in box	[g/mol]
(15)	DELP_PREV	(REAL(fp))	:	Prev delta-P for trcr mixing ratio update	[hPa]

- 30 Jan 1998 R. Yantosca Initial version
- (1) AIRQNT is written in Fixed-Form Fortran 90. Use F90 syntax for declarations etc. (bmy, 4/14/99)
- (2) AIRQNT can now compute PW from PS (if LMAKEPW=T) or PS from PW.
- (3) AIRQNT should also be called after TPCORE, since TPCORE changes the PW values. AIRQNT must then be called to compute the post-TPCORE values of AD, BXHEIGHT, AIRVOL, and AIRDEN.
- (4) The AIRDEN and DELP arrays are now dimensioned as (LLPAR, IIPAR, JJPAR) for better efficiency when processing a whole (I,J) column layer by layer. In FORTRAN, the best efficiency is obtained when the leftmost array index corresponds to the innermost loop.
- (5) Remove PTOP from the arg list. PTOP is now a parameter in "CMN_SIZE". Also updated comments. (bmy, 2/22/00)
- (6) Replace IM, JM, LM with IIPAR, JJPAR, LLPAR as loop boundaries. This ensures that all quantities get defined up to the top of the atmosphere. (bmy, 6/15/00)
- (7) Added to "dao_mod.f" (bmy, 6/26/00)
- (8) Updated comments (bmy, 4/4/01)
- (9) P(IREF, JREF) is now P(I,J). T(IREF, JREF, L) is now T(I,J,L). Also removed LM from the arg list, it is obsolete. Also updated comments. (bmy, 9/26/01)
- (10) Remove PW -- it is now obsolete. Also make PW a local variable, we need to preserve the way it computes P so as to avoid numerical drift. (bmy, 10/4/01)

- (11) Removed obsolete code from 9/01 and 10/01 (bmy, 10/23/01)
- (12) Removed LMAKEPW from arg list. Added parallel DO loops (bmy, 11/15/01)
- (13) Removed obsolete code from 11/01 (bmy, 1/9/02)
- (14) Now rename G_SIGE to SIGE, and dimension it (1:LLPAR+1). Updated comments, cosmetic changes. (bmy, 4/4/02)
- (15) Removed obsolete, commented-out code (bmy, 6/25/02)
- (16) Removed PS, P, SIGE from the arg list for hybrid grid. Now reference routines GET_PEDGE and GET_BP from "pressure_mod.f". Removed obsolete, commented-out code. (dsa, bdf, bmy, 8/27/02)
- (17) Now only pass DXYP via the arg list -- the other arguments are actually are already contained within "dao_mod.f" (bmy, 11/15/02)
- (18) Now replace DXYP(JREF) with routine GET_AREA_M2 of "grid_mod.f". (bmy, 3/11/03)
- (19) Now move computation of DELP into main loop. Also remove P, LOGP,

 JREF, DSIG variables -- these are obsolete for fvDAS. (bmy, 6/19/03)
- 16 Aug 2010 R. Yantosca Added ProTeX headers
- 01 Mar 2012 R. Yantosca Now use GET_AREA_M2(I,J,L) from grid_mod.F90
- 22 Oct 2012 R. Yantosca Now reference gigc_state_met_mod.F90
- 22 Oct 2012 R. Yantosca Renamed LOCAL_MET argument to State_Met
- 09 Nov 2012 M. Payer Copy met field arrays to the State_Met derived type object
- 06 Nov 2014 R. Yantosca Now use State_Met%AIRDEN(I,J,L)
- 06 Nov 2014 R. Yantosca Now use State_Met%DELP(I,J,L)
- 07 Jan 2015 E. Lundgren Add new Met field MAIRDEN (moist air density)
- 13 Feb 2015 E. Lundgren Incorporate water vapor in calculations of densities. Calculate dry air pressures.
- 23 Feb 2015 E. Lundgren Change box height formula to include water vapor
- 24 Feb 2015 E. Lundgren Add calculation of RH to subroutine. Use new formulate for H2O saturation pressure.
- 03 Mar 2015 E. Lundgren Set State_Met%TV (virtual temperature)
- 16 Apr 2015 E. Lundgren Add new State_Met variables PMEAN, PMEAN_DRY, MOISTMW, and ADMOIST
- 28 Oct 2015 E. Lundgren Pass update_mixing_ratio flag, Input_Opt, and State_Chm to optionally update tracer units
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.
- 15 Aug 2016 E. Lundgren Update conc w/ RH for all species

9.1.3 interp

Subroutine INTERP linearly interpolates GEOS-Chem I6 and I3 fields (winds, surface pressure, temperature, surface albedo, specific humidity etc.) to the current dynamic timestep.

INTERFACE:

SUBROUTINE INTERP(NTIMEO, NTIME1, NTDT, Input_Opt, State_Met)

USES:

USE GC_GRID_MOD, ONLY : GET_YEDGE
USE Input_Opt_Mod, ONLY : OptInput
USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: NTIMEO ! Elapsed time [s] at

! start of outer time step

INTEGER, INTENT(IN) :: NTIME1 ! Elapsed time [s] at

! current time

INTEGER, INTENT(IN) :: NTDT ! Dynamic timestep [s]
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INPUT/OUTPUT PARAMETERS:

TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object

REMARKS:

Different met fields are archived at I6 (instantaneous 6-hr) and I3 (instantaneous 3-hr) time resolution depending on the specific product. For example, relative humidity is an instantaneous 6hr field in MERRA and a 6-hr time averaged field in GEOS-5.

- 30 Jan 1998 R. Yantosca Initial version
- (1) INTERP is written in Fixed-Form Fortran 90.
- (2) Subtract PINT from PSC since the only subroutine that uses PSC is TPCORE. This prevents having to subtract and add PINT to PSC before and after each call of TPCORE.
- (3) Pass the Harvard CTM temperature variable T(IGCMPAR, JGCMPAR, LGCMPAR) to INTERP via the argument list (instead of including file CMN). It is computationally inefficient to keep two large arrays for the same quantity. Use the proper window offsets with T.
- (4) Added to "dao_mod.f" (bmy, 6/26/00)
- (5) Updated comments (bmy, 4/4/01)
- (6) Replaced {IJL}GCMPAR w/ IIPAR, JJPAR, LLPAR. Also now use parallel DO-loop for interpolation. Updated comments. (bmy, 9/26/01)
- (7) Removed obsolete code from 9/01 (bmy, 10/23/01)
- (8) Add PSC2 as the surface pressure at the end of the dynamic timestep. This needs to be passed to TPCORE and AIRQNT so that the mixing ratio can be converted to mass properly. Removed PINT from the arg list, since we don't need it anymore. Also updated comments and made some cosmetic changes. (bmy, 3/27/02)
- (9) Removed obsolete, commented-out code (bmy, 6/25/02)
- (10) Eliminated PS, PSC from the arg list, for floating-pressure fix. (dsa, bdf, bmy, 8/27/02)
- (11) Met field arrays are module variables, so we don't need to pass them as arguments. (bmy, 11/20/02)

- (12) Removed NDT from the arg list since that is always 21600. For GEOS-4 met fields, only interpolate PSC2; the other fields are 6-h averages. Eliminate TC variable, it's obsolete. Now use double precision to compute TM and TC2 values. Renamed NTIME to NTIME1 and NTIME1 to NTIME0. Updated comments. (bmy, 6/19/03)
- (13) Now modified for GEOS-5 and GCAP met fields. (swu, bmy, 5/25/05)
- (14) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (15) Now interpolate TROPP, only if variable tropopause is used (phs, 9/12/06)
- (16) Don't interpolate TROPP for GEOS-5 (bmy, 1/17/07)
- (17) Now limit tropopause pressure to 200 mbar at latitudes above 60deg (phs, 9/18/07)
- 16 Aug 2010 R. Yantosca Added ProTeX headers
- 18 Aug 2010 R. Yantosca Rewrite #if block logic for clarity
- 06 Feb 2012 R. Yantosca Add modifications for GEOS-5.7.x met fields
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 01 Mar 2012 R. Yantosca Now use GET_YEDGE(I,J,L) from new grid_mod.F90
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 26 Sep 2013 R. Yantosca Renamed GEOS_57 Cpp switch to GEOS_FP
- 29 Oct 2013 R. Yantosca Now interpolate T_FULLGRID field for GEOS-FP met
- 12 May 2015 E. Lundgren Fix I3 interpolation bug where time fraction spans from 1 to 2, not 0 to 1, for hrs 3 to 6
- 11 Aug 2015 R. Yantosca MERRA2 behaves the same way as GEOS-FP
- 28 Oct 2015 E. Lundgren Set previous SPHU to current SPHU before update
- 04 May 2016 E. Lundgren Now also interpolate dry pressure calculated in SET_DRY_SURFACE_PRESSURE using GMAO wet P

9.1.4 set_dry_surface_pressure

Subroutine SET_DRY_SURFACE_PRESSURE sets the dry surface pressures PS1_DRY or PS2_DRY by removing the water vapor from the column constructed with MET pressure fields PS1_WET or PS2_WET.

INTERFACE:

SUBROUTINE SET_DRY_SURFACE_PRESSURE(State_Met, PS_ID)

USES:

USE CMN_SIZE_MOD

USE ERROR_MOD, ONLY : CHECK_VALUE USE State_Met_Mod, ONLY : MetState

USE PRESSURE_MOD, ONLY : GET_AP, GET_BP

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: PS_{ID} ! 1 = PS1, 2 = PS2

INPUT/OUTPUT PARAMETERS:

TYPE(MetState), INTENT(INOUT) :: State_Met ! Object for met fields

REVISION HISTORY:

03 May 2002 - E. Lundgren - Initial version (M. Lee, JPL)

REMARKS:

This subroutine is an adaptation of the GEOS-Chem moisture fix implemented by Meemong Lee (JPL) in the adjoint model. Like PS1_WET and PS2_WET, from which PS1_DRY and PS2_DRY are derived, these values are interpolated within routine INTERP to derive instantaneous PSC2_DRY. Note that PSC2_WET and PSC2_DRY are not used to fetch pressures and calculate air quantities until after advection. Also note that the dry surface pressure calculated in this routine may be used to calculate delta dry pressures across a level by utilitizing GMAO parameters Ap and Bp but should not be used to extract dry pressure edge values as a height proxy.

9.1.5 is land

Function IS_LAND returns TRUE if surface grid box (I,J) is a land box.

INTERFACE:

FUNCTION IS_LAND(I, J, State_Met) RESULT (LAND)

USES:

USE State_Met_Mod, ONLY : MetState USE TIME_MOD, ONLY : GET_YEAR

INPUT PARAMETERS:

RETURN VALUE:

LOGICAL :: LAND ! =T if it is a land box

- 26 Jun 2000 R. Yantosca Initial version
- (1) Now use ALBEDO field to determine land or land ice boxes for GEOS-3. (bmy, 4/4/01)
- (2) For 4x5 data, regridded albedo field can cause small inaccuracies

near the poles (bmy, 4/4/01)

- (3) Add references to CMN_SIZE and CMN, so that we can use the JYEAR variable to get the current year. Also, for 1998, we need to compute if is a land box or not from the surface albedo, since for this year the LWI/SURFTYPE field is not given. For other years than 1998, we use LWI(I,J) < 50 as our land box criterion. Deleted obsolete code and updated comments.(mje, bmy, 1/9/02)</p>
- (4) Deleted GEOS-2 #ifdef statement. GEOS-2 met fields never really materialized, we use GEOS-3 instead. (bmy, 9/18/02)
- (5) Now uses function GET_YEAR from "time_mod.f". Removed reference to CMN header file. (bmy, 3/11/03)
- (6) Added code to determine land boxes for GEOS-4 (bmy, 6/18/03)
- (7) Now modified for GEOS-5 and GCAP met fields (swu, bmy, 5/25/05)
- (8) Now return TRUE only for land boxes (w/ no ice) (bmy, 8/10/05)
- (9) Now use NINT to round LWI for GEOS-4/GEOS-5 (ltm, bmy, 5/9/06)
- (10) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- 16 Aug 2010 R. Yantosca Added ProTeX headers
- 25 Aug 2010 R. Yantosca Treat MERRA in the same way as GEOS-5
- 06 Feb 2012 R. Yantosca Treat GEOS-5.7.x in the same way as MERRA/GEOS-5
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object

9.1.6 is_water

Function IS_WATER returns TRUE if surface grid box (I,J) is an ocean or an ocean-ice box.

INTERFACE:

```
FUNCTION IS_WATER( I, J, State_Met ) RESULT ( WATER )
```

USES:

USE State_Met_Mod, ONLY : MetState USE TIME_MOD, ONLY : GET_YEAR

INPUT PARAMETERS:

RETURN VALUE:

LOGICAL :: WATER ! =T if this is a water box

- 30 Jan 1998 R. Yantosca Initial version
- (1) Now use ALBEDO field to determine water or water ice boxes for GEOS-3. (bmy, 4/4/01)
- (2) For 4x5 data, regridded albedo field can cause small inaccuracies near the poles (bmy, 4/4/01)
- (3) Add references to CMN_SIZE and CMN, so that we can use the JYEAR variable to get the current year. Also, for 1998, we need to compute if is an ocean box or not from the surface albedo, since for this year the LWI/SURFTYPE field is not given. For other years than 1998, we use LWI(I,J) >= 50 as our ocean box criterion. Deleted obsolete code and updated comments. (mje, bmy, 1/9/02)
- (4) Deleted GEOS-2 #ifdef statement. GEOS-2 met fields never really materialized, we use GEOS-3 instead. (bmy, 9/18/02)
- (5) Now uses function GET_YEAR from "time_mod.f". Removed reference to CMN header file. (bmy, 3/11/03)
- (6) Added code to determine water boxes for GEOS-4 (bmy, 6/18/03)
- (7) Now modified for GEOS-5 and GCAP met fields (swu, bmy, 5/25/05)
- (8) Now remove test for sea ice (bmy, 8/10/05)
- (9) Now use NINT to round LWI for GEOS-4/GEOS-5 (1tm, bmy, 5/9/06)
- (10) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06
- 16 Aug 2010 R. Yantosca Added ProTeX headers
- 25 Aug 2010 R. Yantosca Treat MERRA in the same way as GEOS-5
- 06 Feb 2012 R. Yantosca Treat GEOS-5.7.x in the same way as MERRA/GEOS-5
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object

9.1.7 is_ice

Function IS_ICE returns TRUE if surface grid box (I,J) contains either land-ice or sea-ice.

INTERFACE:

```
FUNCTION IS_ICE( I, J, State_Met ) RESULT ( ICE )
```

USES:

USE State_Met_Mod, ONLY : MetState USE TIME_MOD, ONLY : GET_YEAR

INPUT PARAMETERS:

RETURN VALUE:

LOGICAL :: ICE ! =T if this is an ice box

REVISION HISTORY:

```
09 Aug 2005 - R. Yantosca - Initial version
(1 ) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
16 Aug 2010 - R. Yantosca - Added ProTeX headers
25 Aug 2010 - R. Yantosca - Treat MERRA in the same way as GEOS-5
06 Feb 2012 - R. Yantosca - Treat GEOS-5.7.x in the same way as MERRA/GEOS-5
28 Feb 2012 - R. Yantosca - Removed support for GEOS-3
```

9.1.8 is_near

Function IS_NEAR returns TRUE if surface grid box (I,J) contains any land above a certain threshold (THRESH) or any of the adjacent boxes up to NEIGHBOR boxes away contain land.

INTERFACE:

```
FUNCTION IS_NEAR( I, J, THRESH, NEIGHBOR, State_Met ) & RESULT ( NEAR )
```

USES:

USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

```
! Arguments

INTEGER, INTENT(IN) :: I, J ! Lon & lat grid box indices

INTEGER, INTENT(IN) :: NEIGHBOR ! # of neighbor boxes to consider

REAL(fp), INTENT(IN) :: THRESH ! LWI threshold for near-land

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

RETURN VALUE:

LOGICAL :: NEAR ! # of near land boxes

REMARKS:

```
Typical values for:

GCAP : THRESH = 0.2, NEIGHBOR = 1
```

GEOS-3: THRESH = 80.0, NEIGHBOR = 1 GEOS-4: THRESH = 0.2, NEIGHBOR = 1 GEOS-5: THRESH = 0.2, NEIGHBOR = 1

NOTE: This routine is mostly obsolete now.

```
09 May 2006 - R. Yantosca - Initial version
(1 ) Modified for GCAP and GEOS-3 met fields (bmy, 5/16/06)
(2 ) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
16 Aug 2010 - R. Yantosca - Added ProTeX headers
19 Aug 2010 - R. Yantosca - Rewrote logic of #if block for clarity
25 Aug 2010 - R. Yantosca - Treat MERRA in same way as GEOS-5
06 Feb 2012 - R. Yantosca - Treat GEOS-5.7.x in the same way as MERRA/GEOS-5
28 Feb 2012 - R. Yantosca - Removed support for GEOS-3
09 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met derived type object
```

$9.1.9 \text{ get_obk}$

Function GET_OBK returns the Monin-Obhukov length at a grid box (I,J).

INTERFACE:

```
FUNCTION GET_OBK( I, J, State_Met ) RESULT( OBK )
```

USES:

USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I ! Longitude index INTEGER, INTENT(IN) :: J ! Latitude index
```

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

RETURN VALUE:

REAL(fp) :: OBK ! Monin-Obhukhov length

REMARKS:

REVISION HISTORY:

```
25 May 2005 - R. Yantosca - Initial version

16 Aug 2010 - R. Yantosca - Added ProTeX headers

09 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met

derived type object
```

9.1.10 get_cosine_sza

Routine GET_COSINE_SZA is a driver for calling the COSSZA routine from dao_mod.F. This routine calls COSSZA twice. The first call computes the sun angles at the current time and midpoint of the current chemistry time step. The second call computes the sun angles 5 hours prior to the current time (for the PARANOX ship emissions plume model).

INTERFACE:

```
SUBROUTINE GET_COSINE_SZA( am_I_Root, Input_Opt, State_Met, RC )
  USES:
      USE ErrCode_Mod
      USE Input_Opt_Mod,
                              ONLY : OptInput
      USE JULDAY_MOD,
                              ONLY : JULDAY
      USE State_Met_Mod,
                              ONLY : MetState
      USE TIME_MOD,
                              ONLY : GET_DAY_OF_YEAR
      USE TIME_MOD,
                              ONLY : GET_DAY
      USE TIME_MOD,
                              ONLY : GET_GMT
      USE TIME_MOD,
                              ONLY : GET_HOUR
      USE TIME_MOD,
                              ONLY : GET_MINUTE
      USE TIME_MOD,
                              ONLY : GET_MONTH
      USE TIME_MOD,
                              ONLY : GET_YEAR
INPUT PARAMETERS:
      LOGICAL,
                      INTENT(IN)
                                    :: am_I_Root ! Are we on the root CPU?
      TYPE(OptInput), INTENT(IN)
                                    :: Input_Opt    ! Input Options object
INPUT/OUTPUT PARAMETERS:
      TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
OUTPUT PARAMETERS:
                                                   ! Success or failure?
      INTEGER,
                      INTENT(OUT)
                                    :: RC
REVISION HISTORY:
   07 Feb 2012 - R. Yantosca - Initial version
   27 Nov 2012 - R. Yantosca - Add am_I_root, Input_Opt, State_Met, RC args
   27 Nov 2012 - R. Yantosca - Now pass State_Met to COSSZA so that the
                               SUNCOS fields may be updated
   28 Nov 2012 - R. Yantosca - Removed references to 1-D SUNCOS arrays
   04 Dec 2014 - M. Yannetti - REAL*8 needs to stay *8 due to JULDAY
```

9.1.11 cossza

COSSZA computes the cosine of the solar zenith angle, given the day of the year and GMT hour. The cosine of the solar zenith angle is returned at both the current time and at the midpoint of the chemistry timestep (i.e. for the centralized chemistry timestep option).

INTERFACE:

```
SUBROUTINE COSSZA( DOY, GMT_HOUR, DO_5hr_AGO, State_Met )
```

USES:

```
USE GC_GRID_MOD, ONLY: GET_YMID_R
USE State_Met_Mod, ONLY: MetState
USE TIME_MOD, ONLY: GET_MINUTE
USE TIME_MOD, ONLY: GET_LOCALTIME
USE TIME_MOD, ONLY: GET_TS_CHEM
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: DOY ! Day of the year
INTEGER, INTENT(IN) :: GMT_HOUR ! Hour of day
LOGICAL, INTENT(IN) :: DO_5hr_AGO ! Compute 5h ago?
```

INPUT/OUTPUT PARAMETERS:

TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State

REMARKS:

Hour angle (AHR) is a function of longitude. AHR is zero at solar noon, and increases by 15 deg for every hour before or after solar noon. Hour angle can be thought of as the time in hours since the sun last passed the meridian (i.e. the time since the last local noon).

The cosine of the solar zenith angle (SZA) is given by:

```
cos(SZA) = sin(LAT)*sin(DEC) + cos(LAT)*cos(DEC)*cos(AHR)
```

where LAT = the latitude angle,

DEC = the solar declination angle,

AHR = the hour angle, all in radians.

If SUNCOS < 0, then the sun is below the horizon, and therefore does not contribute to any solar heating.

- 21 Jan 1998 R. Yantosca Initial version
- (1) COSSZA is written in Fixed-Form Fortran 90.
- (2) Use IMPLICIT NONE
- (3) Use C-preprocessor #include statement to include CMN_SIZE, which has IIPAR, JJPAR, LLPAR, IIPAR, JJPAR, LGLOB.
- (4) Use IM and JM (in CMN_SIZE) as loop limits.
- (5) Include Harvard CTM common blocks and rename variables where needed.
- (6) Use SUNCOS(MAXIJ) instead of a 2D array, in order for compatibility with the Harvard CTM subroutines. SUNCOS loops over J, then I.
- (7) Added DO WHILE loops to reduce TIMLOC into the range Oh 24h.
- (8) Cosmetic changes. Also use F90 declaration statements (bmy, 6/5/00)
- (9) Added to "dao_mod.f". Also updated comments. (bmy, 9/27/01)
- (10) Replaced all instances of IM with IIPAR and JM with JJPAR, in order to prevent namespace confusion for the new TPCORE (bmy, 6/25/02)
- (11) Deleted obsolete code from 6/02 (bmy, 8/21/02)
- (12) Removed RLAT and XLON from the arg list. Now compute these using functions from "grid_mod.f" (bmy, 2/3/03)
- (13) Now uses GET_LOCALTIME from "time_mod.f" to get the local time.

 Added parallel DO loop. Removed NHMSb, NSEC arguments. (bmy, 2/13/07)
- (14) Now compute SUNCOS at the midpoint of the relevant time interval (i.e. the chemistry timestep). Also make the A and B coefficients

```
parameters instead of variables. (bmy, 4/27/10)
16 Aug 2010 - R. Yantosca - Added ProTeX headers
05 Oct 2011 - R. Yantosca - Now also return the cosine of the solar
                            zenith angle at 30m after the GMT hour.
07 Oct 2011 - R. Yantosca - Now return SUNCOS_MID, the cos(SZA) at the
                            midpt of the chem step (not always at 00:30).
07 Feb 2012 - R. Yantosca - Now add GMT_HOUR as a new argument, which !
                            will facilitate computing sun angles 5h ago
01 Mar 2012 - R. Yantosca - Now use GET_YMID_R(I,J,L) from grid_mod.F90
01 Mar 2012 - R. Yantosca - Now use GET_LOCALTIME(I,J,L) from time_mod.F90
27 Nov 2012 - R. Yantosca - Update SUNCOS fields of the State_Met object
```

9.1.12 copy_i3_i6_fields

Subroutine COPY_I3_I6_FIELDS copies the I-6 fields at the end of a 6-hr timestep. The I-6 fields at the end of a given 6-hr timestep become the fields at the beginning of the next 6-hr timestep.

INTERFACE:

```
SUBROUTINE COPY_I3_I6_FIELDS( State_Met )
```

USES:

```
USE State_Met_Mod,
                          ONLY : MetState
```

13 Apr 2004 - R. Yantosca - Initial version (1) Added parallel DO-loops (bmy, 4/13/04)

INPUT PARAMETERS:

TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object

REVISION HISTORY:

09 Nov 2012 - M. Payer

```
(2) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
(3 ) Added TROPP (phs 11/10/06)
(4) Don't copy TROPP2 to TROPP1 for GEOS-5 (bmy, 1/17/07)
16 Aug 2010 - R. Yantosca - Added ProTeX headers
20 Aug 2010 - R. Yantosca - Rewrite #if block for clarity
20 Aug 2010 - R. Yantosca - Added #if block for MERRA met fields
06 Feb 2012 - R. Yantosca - Added #if block for GEOS-5.7.x met fields
07 Feb 2012 - R. Yantosca - Renamed to COPY_I3_I6_FIELDS
28 Feb 2012 - R. Yantosca - Removed support for GEOS-3
```

```
derived type object
26 Sep 2013 - R. Yantosca - Renamed GEOS_57 Cpp switch to GEOS_FP
```

- Replaced all met field arrays with State_Met

11 Aug 2015 - R. Yantosca - MERRA2 behaves in the same way as GEOS-FP

03 May 2016 - E. Lundgren - Add PS1_DRY update

9.2 Fortran: Module Interface merra2_read_mod.F90

Module MERRA2_READ_MOD contains subroutines for reading the MERRA2 data from disk (in netCDF format).

INTERFACE:

```
MODULE Merra2_Read_Mod
```

USES:

```
! NcdfUtil modules for netCDF I/O
                                         ! netCDF open
 USE m_netcdf_io_open
                                         ! netCDF dimension queries
 USE m_netcdf_io_get_dimlen
                                         ! netCDF data reads
 USE m_netcdf_io_read
 USE m_netcdf_io_close
                                         ! netCDF close
  ! GEOS-Chem modules
 USE CMN_SIZE_MOD
                                         ! Size parameters
#if defined( BPCH_DIAG )
 USE CMN_DIAG_MOD
                                         ! Diagnostic arrays & counters
                                         ! Array for ND21 diagnostic
 USE DIAG_MOD, ONLY : AD21
                                         ! Array for ND66 diagnostic
 USE DIAG_MOD,
                    ONLY : AD66
 USE DIAG_MOD,
                                         ! Array for ND67 diagnostic
                    ONLY : AD67
#endif
                                         ! Stop w/ error message
 USE ERROR_MOD,
                    ONLY : ERROR_STOP
                                         ! Physical constants
 USE PhysConstants
                                          ! Flexible precision definitions
 USE Precision_Mod
 USE TIME_MOD
                                          ! Date & time routines
                                          ! Routines for casting
 USE TRANSFER_MOD
 IMPLICIT NONE
 PR.TVATE.
# include "netcdf.inc"
                                         ! Include file for netCDF library
```

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: Check_Dimensions
PRIVATE :: Merra2_Read_A3cld
PRIVATE :: Merra2_Read_A3dyn
PRIVATE :: Merra2_Read_A3mstC
PRIVATE :: Merra2_Read_A3mstE
PRIVATE :: Get_Resolution_String

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: Merra2_Read_CN
PUBLIC :: Merra2_Read_A1
PUBLIC :: Merra2_Read_A3
PUBLIC :: Merra2_Read_I3_1

PUBLIC :: Merra2_Read_I3_2
PUBLIC :: Cleanup_Merra2_Read

REMARKS:

Assumes that you have a netCDF library (either v3 or v4) installed on your system.

REVISION HISTORY:

9.2.1 Get_Resolution_String

Function Get_Resolution_String returns the proper filename extension for the GEOS-Chem horizontal grid resolution. This is used to construct the various file names.

INTERFACE:

```
FUNCTION Get_Resolution_String() RESULT( resString )
```

RETURN VALUE:

```
CHARACTER(LEN=255) :: resString
```

REVISION HISTORY:

```
12 Aug 2015 - R. Yantosca - Initial version, based on geosfp_read_mod.F90 13 Aug 2015 - R. Yantosca - MERRA2 data is now storead as netCDF4 (.nc4)
```

9.2.2 Check_Dimensions

Subroutine CHECK_DIMENSIONS checks to see if dimensions read from the netCDF file match the defined GEOS-Chem dimensions. If not, then it will stop the GEOS-Chem simulation with an error message.

INTERFACE:

```
SUBROUTINE Check_Dimensions(lon, lat, lev, time, time_expected, caller)
```

INPUT PARAMETERS:

```
INTEGER, OPTIONAL, INTENT(IN) :: lon ! Lon dimension INTEGER, OPTIONAL, INTENT(IN) :: lat ! Lat dimension INTEGER, OPTIONAL, INTENT(IN) :: lev ! Alt dimension
```

REMARKS:

```
Call this routine with keyword arguments, e.g
    CALL CHECK_DIMENSION( lon=X, lat=Y, lev=Z, time=T, time_expected=8, caller=caller )
```

REVISION HISTORY:

```
02 Feb 2012 - R. Yantosca - Initial version
03 Feb 2012 - R. Yantosca - Now pass the caller routine name as an argument
```

9.2.3 Merra2_Read_cn

Routine to read variables and attributes from a MERRA2 met fields file containing constant (CN) data.

INTERFACE:

```
SUBROUTINE Merra2_Read_CN( Input_Opt, State_Met )
```

USES:

```
USE Input_Opt_Mod, ONLY : OptInput
USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

```
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

REMARKS:

Even though the netCDF file is self-describing, the MERRA2 data, dimensions, and units are pre-specified according to the GMAO MERRA2 file specification. Therefore we can "cheat" a little bit and not have to read netCDF attributes to find what these values are.

```
12 Aug 2015 - R. Yantosca - Initial version, based on geosfp_read_mod.F90 13 Aug 2015 - R. Yantosca - Bug fix: change CN date to 2015/01/01
```

9.2.4 Merra2_Read_a1

Routine to read variables and attributes from a MERRA2 met fields file containing 1-hr time-averaged (A1) data.

INTERFACE:

```
SUBROUTINE Merra2_Read_A1( YYYYMMDD, HHMMSS, Input_Opt, State_Met )
```

USES:

```
USE Input_Opt_Mod, ONLY : OptInput USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

REMARKS:

Even though the netCDF file is self-describing, the MERRA2 data, dimensions, and units are pre-specified according to the GMAO MERRA2 file specification. Therefore we can "cheat" a little bit and not have to read netCDF attributes to find what these values are.

Special handling for surface precipitation fields:

In MERRA2 (and in MERRA), the PRECTOT etc. surface precipitation met fields fields have units of [kg/m2/s]. In all other GEOS versions, PREACC and PRECON have units of [mm/day].

Therefore, for backwards compatibility with existing code, apply the following unit conversion to the GEOS-5 PRECTOT and PRECCON fields:

```
kg | m3 | 86400 s | 1000 mm
------ = 86400
m2 s | 1000 kg | day | m

1 / density of water
```

REMARKS:

MERRA2 pressure quantities are stored on disk with units of Pa. For now we will convert to hPa for compatibility with GEOS-Chem. But in the near future we will probably recode GEOS-Chem to use the native units, which facilitate GEOS-Chem HP development.

REVISION HISTORY:

```
12 Aug 2015 - R. Yantosca - Initial version, based on geosfp_read_mod.F90 23 Sep 2015 - E. Lundgren - Now assign SWGDN to State_Met SWGDN not RADSWG 03 Dec 2015 - R. Yantosca - Now open file only once per day
```

9.2.5 Merra2_Read_a3

Convenience wrapper for the following routines which read 3-hour time averaged data from disk:

- Merra2_Read_A3cld
- Merra2_Read_A3dyn
- Merra2_Read_A3mstC
- Merra2_Read_A3mstE

INTERFACE:

```
SUBROUTINE Merra2_Read_A3( YYYYMMDD, HHMMSS, Input_Opt, State_Met )
```

USES:

```
USE Input_Opt_Mod, ONLY : OptInput USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

REVISION HISTORY:

```
12 Aug 2015 - R. Yantosca - Initial version, based on geosfp_read_mod.F90
```

9.2.6 Merra2_Read_a3cld

Routine to read variables and attributes from a MERRA2 met fields file containing 3-hr time-averaged (A3) data (cloud fields).

INTERFACE:

```
SUBROUTINE Merra2_Read_A3cld( YYYYMMDD, HHMMSS, Input_Opt, State_Met )
```

USES:

```
USE Input_Opt_Mod, ONLY : OptInput
USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

REMARKS:

Even though the netCDF file is self-describing, the MERRA2 data, dimensions, and units are pre-specified according to the GMAO MERRA2 file specification. Therefore we can "cheat" a little bit and not have to read netCDF attributes to find what these values are.

REVISION HISTORY:

```
12 Aug 2015 - R. Yantosca - Initial version, based on geosfp_read_mod.F90
03 Dec 2015 - R. Yantosca - Now open file only once per day
17 Mar 2016 - M. Sulprizio- Read optical depth into State_Met%OPTD instead of State_Met%OPTDEP (obsolete).
```

9.2.7 Merra2_Read_a3dyn

Routine to read variables and attributes from a MERRA2 met fields file containing 3-hr time-averaged (A3) data (dynamics fields).

INTERFACE:

```
SUBROUTINE Merra2_Read_A3dyn( YYYYMMDD, HHMMSS, Input_Opt, State_Met )
```

USES:

```
USE Input_Opt_Mod, ONLY : OptInput USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: YYYYMMDD ! GMT date in YYYY/MM/DD format
INTEGER, INTENT(IN) :: HHMMSS ! GMT time in hh:mm:ss format
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

REMARKS:

Even though the netCDF file is self-describing, the MERRA2 data, dimensions, and units are pre-specified according to the GMAO MERRA2 file specification. Therefore we can "cheat" a little bit and not have to read netCDF attributes to find what these values are.

REVISION HISTORY:

```
12 Aug 2015 - R. Yantosca - Initial version, based on geosfp_read_mod.F90 03 Dec 2015 - R. Yantosca - Now open file only once per day
```

9.2.8 Merra2_Read_a3mstc

Routine to read variables and attributes from a MERRA2 met fields file containing 3-hr time-averaged (A3) data (moist fields, saved on level centers).

INTERFACE:

```
SUBROUTINE Merra2_Read_A3mstC( YYYYMMDD, HHMMSS, Input_Opt, State_Met )
```

USES:

```
USE Input_Opt_Mod, ONLY : OptInput USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

REMARKS:

Even though the netCDF file is self-describing, the MERRA2 data, dimensions, and units are pre-specified according to the GMAO MERRA2 file specification. Therefore we can "cheat" a little bit and not have to read netCDF attributes to find what these values are.

```
12 Aug 2015 - R. Yantosca - Initial version, based on geosfp_read_mod.F90 03 Dec 2015 - R. Yantosca - Now open file only once per day
```

9.2.9 Merra2_Read_a3mste

Routine to read variables and attributes from a MERRA2 met fields file containing 3-hr time-averaged (A3) data (moist fields, saved on level edges).

INTERFACE:

```
SUBROUTINE Merra2_read_A3mstE( YYYYMMDD, HHMMSS, Input_Opt, State_Met )
```

USES:

```
USE Input_Opt_Mod, ONLY : OptInput
USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: YYYYMMDD ! GMT date in YYYY/MM/DD format INTEGER, INTENT(IN) :: HHMMSS ! GMT time in hh:mm:ss format
```

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

REMARKS:

This routine was automatically generated by the Perl script ncCodeRead, and was subsequently hand-edited for compatibility with GEOS-Chem.

Even though the netCDF file is self-describing, the MERRA2 data, dimensions, and units are pre-specified according to the GMAO MERRA2 file specification. Therefore we can "cheat" a little bit and not have to read netCDF attributes to find what these values are.

REVISION HISTORY:

```
12 Aug 2015 - R. Yantosca - Initial version, based on geosfp_read_mod.F90 03 Dec 2015 - R. Yantosca - Now open file only once per day
```

9.2.10 Merra2 Read I3 1

Routine to read variables and attributes from a MERRA2 met fields file containing 3-hr instantaneous (I3) data.

INTERFACE:

```
SUBROUTINE Merra2_Read_I3_1( YYYYMMDD, HHMMSS, Input_Opt, State_Met )
```

USES:

```
USE Input_Opt_Mod, ONLY : OptInput
USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

REMARKS:

Even though the netCDF file is self-describing, the MERRA2 data, dimensions, and units are pre-specified according to the GMAO MERRA2 file specification. Therefore we can "cheat" a little bit and not have to read netCDF attributes to find what these values are.

MERRA2 pressure quantities are stored on disk with units of Pa. For now we will convert to hPa for compatibility with GEOS-Chem. But in the near future we will probably recode GEOS-Chem to use the native units, which facilitate GEOS-Chem HP development.

REVISION HISTORY:

```
12 Aug 2015 - R. Yantosca - Initial version, based on geosfp_read_mod.F90 03 Dec 2015 - R. Yantosca - Now open file only once per day
```

9.2.11 Merra2_Read_I3_2

Routine to read variables and attributes from a MERRA2 met fields file containing 3-hr instantaneous (I3) data.

INTERFACE:

```
SUBROUTINE Merra2_Read_I3_2( YYYYMMDD, HHMMSS, Input_Opt, State_Met )
```

USES:

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: YYYYMMDD ! GMT date in YYYY/MM/DD format
INTEGER, INTENT(IN) :: HHMMSS ! GMT time in hh:mm:ss format
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

REMARKS:

Even though the netCDF file is self-describing, the MERRA2 data, dimensions, and units are pre-specified according to the GMAO MERRA2 file specification. Therefore we can "cheat" a little bit and not have to read netCDF attributes to find what these values are.

MERRA2 pressure quantities are stored on disk with units of Pa. For now we will convert to hPa for compatibility with GEOS-Chem. But in the near future we will probably recode GEOS-Chem to use the native units, which facilitate GEOS-Chem HP development.

REVISION HISTORY:

```
12 Aug 2015 - R. Yantosca - Initial version, based on geosfp_read_mod.F90 03 Dec 2015 - R. Yantosca - Now open file only once per day 20 Sep 2016 - R. Yantosca - Bug fix: FIRST must be declared as LOGICAL
```

9.2.12 Cleanup_Merra2_Read

Closes any open netCDF files at the end of a simulation. This can occur if the simulation ends at a time other than 00:00 GMT.

INTERFACE:

```
SUBROUTINE Cleanup_Merra2_Read()
```

REVISION HISTORY:

```
06 Jan 2015 - R. Yantosca - Initial version
```

9.3 Fortran: Module Interface geosfp_read_mod.F90

Module GEOSFP_READ_MOD contains subroutines for reading the GEOS-FP data from disk (in netCDF format).

INTERFACE:

```
MODULE GeosFp_Read_Mod
```

USES:

```
#if defined( BPCH_DIAG )
 USE CMN_DIAG_MOD
                                          ! Diagnostic arrays & counters
 USE DIAG_MOD,
                    ONLY : AD21
                                          ! Array for ND21 diagnostic
 USE DIAG_MOD,
USE DIAG_MOD,
                                        ! Array for ND66 diagnostic
                    ONLY : AD66
                    ONLY : AD67
                                        ! Array for ND67 diagnostic
#endif
 USE ERROR_MOD,
                    ONLY : ERROR_STOP
                                         ! Stop w/ error message
 USE PhysConstants
                                          ! Physical constants
                                          ! Date & time routines
 USE TIME_MOD
 USE TRANSFER_MOD
                                          ! Routines for casting
 IMPLICIT NONE
 PRIVATE
# include "netcdf.inc"
                                         ! Include file for netCDF library
```

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: Check_Dimensions
PRIVATE :: GeosFp_Read_A3cld
PRIVATE :: GeosFp_Read_A3dyn
PRIVATE :: GeosFp_Read_A3mstC
PRIVATE :: GeosFp_Read_A3mstE
PRIVATE :: Get_Resolution_String

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: GeosFp_Read_CN
PUBLIC :: GeosFp_Read_A1
PUBLIC :: GeosFp_Read_A3
PUBLIC :: GeosFp_Read_I3_1
PUBLIC :: GeosFp_Read_I3_2
PUBLIC :: Cleanup_GeosFp_Read

REMARKS:

Assumes that you have a netCDF library (either v3 or v4) installed on your system.

```
30 Jan 2012 - R. Yantosca - Initial version

03 Feb 2012 - R. Yantosca - Add Geos57_Read_A3 wrapper function

07 Feb 2012 - R. Yantosca - Now echo info after reading fields from disk

10 Feb 2012 - R. Yantosca - Add function Get_Resolution_String

05 Apr 2012 - R. Yantosca - Convert units for specific humidity properly

15 Nov 2012 - R. Yantosca - Now replace dao_mod.F arrays with State_Met

11 Apr 2013 - R. Yantosca - Now pass directory fields via Input_Opt

26 Sep 2013 - R. Yantosca - Renamed to geosfp_read_mod.F90

14 Jan 2014 - R. Yantosca - Remove "define GEOS572_FILES #ifdef blocks

14 Aug 2014 - R. Yantosca - Compute CLDTOPS field in GeosFp_Read_A3mstE
```

```
03 Dec 2015 - R. Yantosca - Add file ID's as module variables
03 Dec 2015 - R. Yantosca - Add CLEANUP_GEOSFP_READ to close any open
netCDF files left at the end of a simulation
02 Feb 2016 - E. Lundgren - Block of diagnostics with if defined BPCH
```

9.3.1 Get_Resolution_String

Function Get_Resolution_String returns the proper filename extension for the GEOS-Chem horizontal grid resolution. This is used to construct the various file names.

INTERFACE:

```
FUNCTION Get_Resolution_String() RESULT( resString )
```

RETURN VALUE:

```
CHARACTER(LEN=255) :: resString
```

REVISION HISTORY:

```
10 Feb 2012 - R. Yantosca - Initial version
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
26 Sep 2013 - R. Yantosca - Remove SEAC4RS C-preprocssor switch
```

9.3.2 Check Dimensions

Subroutine CHECK_DIMENSIONS checks to see if dimensions read from the netCDF file match the defined GEOS-Chem dimensions. If not, then it will stop the GEOS-Chem simulation with an error message.

INTERFACE:

```
SUBROUTINE Check_Dimensions(lon, lat, lev, time, time_expected, caller)
```

INPUT PARAMETERS:

```
OPTIONAL, INTENT(IN) :: lon
INTEGER,
                                                         ! Lon dimension
                 OPTIONAL, INTENT(IN)
                                                         ! Lat dimension
INTEGER,
                                      :: lat
                                                         ! Alt dimension
                 OPTIONAL, INTENT(IN) :: lev
INTEGER,
                 OPTIONAL, INTENT(IN) :: time
                                                         ! Time dimension
INTEGER,
                 OPTIONAL, INTENT(IN) :: time_expected ! Expected # of
INTEGER,
                                                         ! time slots
CHARACTER(LEN=*), OPTIONAL, INTENT(IN) :: caller
                                                         ! Name of caller
                                                         ! routine
```

REMARKS:

REVISION HISTORY:

```
02 Feb 2012 - R. Yantosca - Initial version
```

03 Feb 2012 - R. Yantosca - Now pass the caller routine name as an argument

9.3.3 GeosFp_Read_cn

Routine to read variables and attributes from a GEOS-FP met fields file containing constant (CN) data.

INTERFACE:

```
SUBROUTINE GeosFp_Read_CN( Input_Opt, State_Met )
```

USES:

```
USE Input_Opt_Mod, ONLY : OptInput USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

```
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met   ! Meteorology State object
```

REMARKS:

This routine was automatically generated by the Perl script ncCodeRead, and was subsequently hand-edited for compatibility with GEOS-Chem.

Even though the netCDF file is self-describing, the GEOS-FP data, dimensions, and units are pre-specified according to the GMAO GEOS-FP file specification. Therefore we can "cheat" a little bit and not have to read netCDF attributes to find what these values are.

```
30 Jan 2012 - R. Yantosca - Initial version

07 Feb 2012 - R. Yantosca - Now echo info after reading fields from disk

10 Feb 2012 - R. Yantosca - Now get a string for the model resolution

09 Nov 2012 - M. Payer - Copy all met fields to the State_Met derived type object

15 Nov 2012 - R. Yantosca - Now replace dao_mod.F arrays with State_Met

11 Apr 2013 - R. Yantosca - Now pass directory fields with Input_Opt

26 Sep 2013 - R. Yantosca - Renamed to GeosFp_Read_CN

06 Nov 2014 - R. Yantosca - Replace TRANSFER_2D with direct casts
```

9.3.4 GeosFp_Read_a1

Routine to read variables and attributes from a GEOS-FP met fields file containing 1-hr time-averaged (A1) data.

INTERFACE:

```
SUBROUTINE GeosFp_Read_A1( YYYYMMDD, HHMMSS, Input_Opt, State_Met )
```

USES:

```
USE Input_Opt_Mod, ONLY : OptInput USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

REMARKS:

This routine was automatically generated by the Perl script ncCodeRead, and was subsequently hand-edited for compatibility with GEOS-Chem.

Even though the netCDF file is self-describing, the GEOS-FP data, dimensions, and units are pre-specified according to the GMAO GEOS-FP file specification. Therefore we can "cheat" a little bit and not have to read netCDF attributes to find what these values are.

```
Special handling for surface precipitation fields:
```

In GEOS-FP (and in MERRA), the PRECTOT etc. surface precipitation met fields fields have units of [kg/m2/s]. In all other GEOS versions, PREACC and PRECON have units of [mm/day].

Therefore, for backwards compatibility with existing code, apply the following unit conversion to the GEOS-5 PRECTOT and PRECCON fields:

```
kg | m3 | 86400 s | 1000 mm
------ = 86400
m2 s | 1000 kg | day | m

1 / density of water
```

```
30 Jan 2012 - R. Yantosca - Initial version
07 Feb 2012 - R. Yantosca - Now echo info after reading fields from disk
10 Feb 2012 - R. Yantosca - Now get a string for the model resolution
                         - Copy all met fields to the State_Met derived type
09 Nov 2012 - M. Payer
                            object
15 Nov 2012 - R. Yantosca - Now replace dao_mod.F arrays with State_Met
04 Jan 2013 - M. Payer
                         - Bug fix: Use State_Met%TSKIN for ND67 surface
                            skin temperature diagnostic, not State_MET%TS
11 Apr 2013 - R. Yantosca - Now pass directory fields with Input_Opt
02 Dec 2013 - S. Philip - Correction for GEOS-FP boundary layer height
04 Dec 2013 - R. Yantosca - Now comment out GEOS-FP BL height correction
06 Nov 2014 - R. Yantosca - Replace TRANSFER_2D with direct casts
23 Sep 2015 - E. Lundgren - Now assign SWGDN to State_Met SWGDN not RADSWG
03 Dec 2015 - R. Yantosca - Now open file only once per day
```

9.3.5 GeosFp_Read_a3

Convenience wrapper for the following routines which read 3-hour time averaged data from disk:

- GeosFp_Read_A3cld
- GeosFp_Read_A3dyn
- GeosFp_Read_A3mstC
- GeosFp_Read_A3mstE

INTERFACE:

```
SUBROUTINE GeosFp_Read_A3( YYYYMMDD, HHMMSS, Input_Opt, State_Met )
```

USES:

```
USE Input_Opt_Mod, ONLY : OptInput USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

```
30 Jan 2012 - R. Yantosca - Initial version
11 Apr 2013 - R. Yantosca - Now pass directory fields with Input_Opt
26 Sep 2013 - R. Yantosca - Renamed to GeosFp_Read_A3
```

9.3.6 GeosFp_Read_a3cld

Routine to read variables and attributes from a GEOS-FP met fields file containing 3-hr time-averaged (A3) data (cloud fields).

INTERFACE:

```
SUBROUTINE GeosFp_Read_A3cld( YYYYMMDD, HHMMSS, Input_Opt, State_Met )
```

USES:

```
USE Input_Opt_Mod, ONLY : OptInput USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

REMARKS:

This routine was automatically generated by the Perl script ncCodeRead, and was subsequently hand-edited for compatibility with GEOS-Chem.

Even though the netCDF file is self-describing, the GEOS-FP data, dimensions, and units are pre-specified according to the GMAO GEOS-FP file specification. Therefore we can "cheat" a little bit and not have to read netCDF attributes to find what these values are.

```
30 Jan 2012 - R. Yantosca - Initial version

07 Feb 2012 - R. Yantosca - Now echo info after reading fields from disk

10 Feb 2012 - R. Yantosca - Now get a string for the model resolution

05 Apr 2012 - R. Yantosca - Fixed bug: TAUCLI was overwritten w/ TAUCLW

09 Nov 2012 - M. Payer - Copy all met fields to the State_Met derived type object

15 Nov 2012 - R. Yantosca - Now replace dao_mod.F arrays with State_Met

11 Apr 2013 - R. Yantosca - Now pass directory fields with Input_Opt

26 Sep 2013 - R. Yantosca - Renamed to GeosFp_Read_A3Cld

06 Nov 2014 - R. Yantosca - Replace TRANSFER_A6 with TRANSFER_3D

03 Dec 2015 - R. Yantosca - Now open file only once per day

17 Mar 2016 - M. Sulprizio- Read optical depth into State_Met%OPTD instead of State_Met%OPTDEP (obsolete).
```

9.3.7 GeosFp_Read_a3dyn

Routine to read variables and attributes from a GEOS-FP met fields file containing 3-hr time-averaged (A3) data (dynamics fields).

INTERFACE:

```
SUBROUTINE GeosFp_Read_A3dyn( YYYYMMDD, HHMMSS, Input_Opt, State_Met )
```

USES:

```
USE Input_Opt_Mod, ONLY : OptInput USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

REMARKS:

This routine was automatically generated by the Perl script ncCodeRead, and was subsequently hand-edited for compatibility with GEOS-Chem.

Even though the netCDF file is self-describing, the GEOS-FP data, dimensions, and units are pre-specified according to the GMAO GEOS-FP file specification. Therefore we can "cheat" a little bit and not have to read netCDF attributes to find what these values are.

```
30 Jan 2012 - R. Yantosca - Initial version

07 Feb 2012 - R. Yantosca - Now echo info after reading fields from disk

10 Feb 2012 - R. Yantosca - Now get a string for the model resolution

09 Nov 2012 - M. Payer - Copy all met fields to the State_Met derived type object

15 Nov 2012 - R. Yantosca - Now replace dao_mod.F arrays with State_Met

11 Apr 2013 - R. Yantosca - Now pass directories with Input_Opt

26 Sep 2013 - R. Yantosca - Renamed to GeosFp_Read_A3dyn

15 Nov 2013 - R. Yantosca - Now convert RH from [1] to [%], in order to be consistent with GEOS-Chem convention

14 Aug 2014 - R. Yantosca - Now compute CLDTOPS in GeosFP_Read_A3mstE

03 Dec 2015 - R. Yantosca - Now open file only once per day
```

9.3.8 GeosFp_Read_a3mstc

Routine to read variables and attributes from a GEOS-FP met fields file containing 3-hr time-averaged (A3) data (moist fields, saved on level centers).

INTERFACE:

```
SUBROUTINE GeosFp_Read_A3mstC( YYYYMMDD, HHMMSS, Input_Opt, State_Met )
```

USES:

```
USE Input_Opt_Mod, ONLY: OptInput USE State_Met_Mod, ONLY: MetState
```

INPUT PARAMETERS:

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

REMARKS:

This routine was automatically generated by the Perl script ncCodeRead, and was subsequently hand-edited for compatibility with GEOS-Chem.

Even though the netCDF file is self-describing, the GEOS-FP data, dimensions, and units are pre-specified according to the GMAO GEOS-FP file specification. Therefore we can "cheat" a little bit and not have to read netCDF attributes to find what these values are.

REVISION HISTORY:

```
30 Jan 2012 - R. Yantosca - Initial version

07 Feb 2012 - R. Yantosca - Now echo info after reading fields from disk

10 Feb 2012 - R. Yantosca - Now get a string for the model resolution

09 Nov 2012 - M. Payer - Copy all met fields to the State_Met derived type object

15 Nov 2012 - R. Yantosca - Now replace dao_mod.F arrays with State_Met

11 Apr 2013 - R. Yantosca - Now pass directory fields with Input_Opt

26 Sep 2013 - R. Yantosca - Renamed to GeosFp_Read_A3mstC

03 Dec 2015 - R. Yantosca - Now open file only once per day
```

9.3.9 GeosFp_Read_a3mste

Routine to read variables and attributes from a GEOS-FP met fields file containing 3-hr time-averaged (A3) data (moist fields, saved on level edges).

SUBROUTINE GeosFp_Read_A3mstE(YYYYMMDD, HHMMSS, Input_Opt, State_Met)

USES:

```
USE Input_Opt_Mod, ONLY : OptInput
USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: YYYYMMDD ! GMT date in YYYY/MM/DD format INTEGER, INTENT(IN) :: HHMMSS ! GMT time in hh:mm:ss format
```

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

REMARKS:

This routine was automatically generated by the Perl script ncCodeRead, and was subsequently hand-edited for compatibility with GEOS-Chem.

Even though the netCDF file is self-describing, the GEOS-FP data, dimensions, and units are pre-specified according to the GMAO GEOS-FP file specification. Therefore we can "cheat" a little bit and not have to read netCDF attributes to find what these values are.

REVISION HISTORY:

```
30 Jan 2012 - R. Yantosca - Initial version

07 Feb 2012 - R. Yantosca - Now echo info after reading fields from disk

10 Feb 2012 - R. Yantosca - Now get a string for the model resolution

09 Nov 2012 - M. Payer - Copy all met fields to the State_Met derived type object

15 Nov 2012 - R. Yantosca - Now replace dao_mod.F arrays with State_Met

11 Apr 2013 - R. Yantosca - Now pass directory fields with Input_Opt

26 Sep 2013 - R. Yantosca - Renamed to GeosFp_Read_A3mstE

26 Sep 2013 - R. Yantosca - Now read CMFMC from GEOSFP*.nc files

14 Aug 2014 - R. Yantosca - Now compute CLDTOPS here; it depends on CMFMC

03 Dec 2015 - R. Yantosca - Now open file only once per day
```

$9.3.10 \quad GeosFp_Read_I3_1$

Routine to read variables and attributes from a GEOS-FP met fields file containing 3-hr instantaneous (I3) data.

INTERFACE:

```
SUBROUTINE GeosFp_Read_I3_1( YYYYMMDD, HHMMSS, Input_Opt, State_Met )
```

```
USE Input_Opt_Mod, ONLY : OptInput
USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met  ! Meteorology State object
```

REMARKS:

This routine was automatically generated by the Perl script ncCodeRead, and was subsequently hand-edited for compatibility with GEOS-Chem.

Even though the netCDF file is self-describing, the GEOS-FP data, dimensions, and units are pre-specified according to the GMAO GEOS-FP file specification. Therefore we can "cheat" a little bit and not have to read netCDF attributes to find what these values are.

REVISION HISTORY:

```
30 Jan 2012 - R. Yantosca - Initial version
07 Feb 2012 - R. Yantosca - Now echo info after reading fields from disk
10 Feb 2012 - R. Yantosca - Now get a string for the model resolution
05 Apr 2012 - R. Yantosca - Now convert QV1 from [kg/kg] to [g/kg]
09 Nov 2012 - M. Payer
                          - Copy all met fields to the State_Met derived type
                            object
15 Nov 2012 - R. Yantosca - Now replace dao_mod.F arrays with State_Met
11 Apr 2013 - R. Yantosca - Now pass directory fields with Input_Opt
06 Sep 2013 - R. Yantosca - Bug fix: we need to initialize State_Met%T
                            with State_Met%TMPU1 to avoid errors. The
                            State_Met%T field will be set again in INTERP.
26 Sep 2013 - R. Yantosca - Renamed to GeosFp_Read_I3_1
29 Oct 2013 - R. Yantosca - Now read T_FULLGRID_1 for offline simulations
06 Nov 2014 - R. Yantosca - Replace TRANSFER_2D with direct casts
16 Apr 2015 - R. Yantosca - Remove reference to T_FULLGRID; it's obsolete
12 Jun 2015 - E. Lundgren - Initialize State_MET%SPHU with State_Met%SPHU1
03 Dec 2015 - R. Yantosca - Now open file only once per day
```

9.3.11 GeosFp_Read_I3_2

Routine to read variables and attributes from a GEOS-FP met fields file containing 3-hr instantaneous (I3) data.

SUBROUTINE GeosFp_Read_I3_2(YYYYMMDD, HHMMSS, Input_Opt, State_Met) USES:

```
USE Input_Opt_Mod, ONLY : OptInput
USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: YYYYMMDD ! GMT date in YYYY/MM/DD format INTEGER, INTENT(IN) :: HHMMSS ! GMT time in hh:mm:ss format
```

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

REMARKS:

This routine was automatically generated by the Perl script ncCodeRead, and was subsequently hand-edited for compatibility with GEOS-Chem.

Even though the netCDF file is self-describing, the GEOS-FP data, dimensions, and units are pre-specified according to the GMAO GEOS-FP file specification. Therefore we can "cheat" a little bit and not have to read netCDF attributes to find what these values are.

REVISION HISTORY:

```
30 Jan 2012 - R. Yantosca - Initial version

07 Feb 2012 - R. Yantosca - Now echo info after reading fields from disk

10 Feb 2012 - R. Yantosca - Now get a string for the model resolution

05 Apr 2012 - R. Yantosca - Now convert QV2 from [kg/kg] to [g/kg]

09 Nov 2012 - M. Payer - Copy all met fields to the State_Met derived type object

15 Nov 2012 - R. Yantosca - Now replace dao_mod.F arrays with State_Met

11 Apr 2013 - R. Yantosca - Now pass directory fields with Input_Opt

26 Sep 2013 - R. Yantosca - Rename to GeosFp_Read_I3_2

29 Oct 2013 - R. Yantosca - Now read T_FULLGRID_2 for offline simulations

06 Nov 2014 - R. Yantosca - Replace TRANSFER_2D with direct casts

03 Dec 2015 - R. Yantosca - Now open file only once per day

20 Sep 2016 - R. Yantosca - Bug fix: FIRST must be declared as LOGICAL
```

9.3.12 Cleanup_GeosFp_Read

Closes any open netCDF files at the end of a simulation. This can occur if the simulation ends at a time other than 00:00 GMT.

INTERFACE:

SUBROUTINE Cleanup_GeosFp_Read()

```
06 Jan 2015 - R. Yantosca - Initial version
```

9.4 Fortran: Module Interface merra_a1_mod.F90

Module MERRA_A1_MOD contains subroutines for reading the 1-hour time averaged (aka "A1") fields from the MERRA data archive.

INTERFACE:

```
MODULE MERRA_A1_MOD
```

USES:

```
USE inquireMod, ONLY: findFreeLUN
USE PRECISION_MOD! For GEOS-Chem Precision (fp)

IMPLICIT NONE
```

PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: GET_MERRA_A1_FIELDS
PUBLIC :: OPEN_MERRA_A1_FIELDS
```

PRIVATE MEMBER FUNCTIONS:

```
PRIVATE :: A1_CHECK
PRIVATE :: DO_OPEN_A1
PRIVATE :: READ_A1
```

REMARKS:

Don't bother with the file unzipping anymore.

REVISION HISTORY:

PRIVATE

```
19 Aug 2010 - R. Yantosca - Initial version, based on a3_read_mod.f
03 Aug 2012 - R. Yantosca - Now make IU_A1 a private module variable
15 Nov 2012 - R. Yantosca - Now replace dao_mod.F arrays with State_Met
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
17 Nov 2014 - M. Yannetti - Added PRECISION_MOD
```

9.4.1 do_open_a1

Function DO_OPEN_A1 returns TRUE if is time to open the A1 met field file or FALSE otherwise. This prevents us from opening a file which has already been opened.

INTERFACE:

```
FUNCTION DO_OPEN_A1( NYMD, NHMS, RESET ) RESULT( DO_OPEN )
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NYMD ! YYYYMMDD and hhmmss to test
INTEGER, INTENT(IN) :: NHMS ! if it's time to open file
LOGICAL, INTENT(IN), OPTIONAL :: RESET ! Reset the
```

RETURN VALUE:

LOGICAL :: DO_OPEN ! =T if it's time to open file

REVISION HISTORY:

```
19 Aug 2010 - R. Yantosca - Initial version, based on a3_read_mod.f
21 Sep 2010 - R. Yantosca - Add RESET via the argument list to reset
the FIRST flag if so desired.
```

9.4.2 open_merra_a1_fields

Subroutine OPEN_MERRA_A1_FIELDS opens the A1 met fields file for date NYMD and time NHMS.

INTERFACE:

```
SUBROUTINE OPEN_MERRA_A1_FIELDS( NYMD, NHMS, Input_Opt, & RESET, IUNIT )
```

USES:

```
USE BPCH2_MOD, ONLY : GET_RES_EXT
USE ERROR_MOD, ONLY : ERROR_STOP
USE FILE_MOD, ONLY : FILE_EXISTS
USE FILE_MOD, ONLY : IOERROR
USE Input_Opt_Mod, ONLY : OptInput
USE TIME_MOD, ONLY : EXPAND_DATE
```

INPUT PARAMETERS:

LOGICAL, INTENT(IN), OPTIONAL :: RESET ! Reset first A1 flag?

INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT), OPTIONAL :: IUNIT ! Returns IU_A1
```

```
19 Aug 2010 - R. Yantosca - Initial version, based on a3_read_mod.f
03 Aug 2012 - R. Yantosca - Now use findFreeLUN to define IU_A1 locally
06 Aug 2012 - R. Yantosca - Add optional IUNIT to pass LUN to calling routine
07 Aug 2012 - R. Yantosca - Now print LUN used to open file
11 Apr 2013 - R. Yantosca - Now pass directory fields with Input_Opt
```

9.4.3 get_merra_a1_fields

Subroutine GET_MERRA_A1_FIELDS is a wrapper for routine READ_A1.

INTERFACE:

```
SUBROUTINE GET_MERRA_A1_FIELDS( NYMD, NHMS, Input_Opt, State_Met )
```

USES:

```
USE CMN_SIZE_MOD
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NYMD ! YYYYMMDD and
```

INTEGER, INTENT(IN) :: NHMS ! hhmmss of data to read
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met   ! Meteorology State object
```

REVISION HISTORY:

```
19 Aug 2010 - R. Yantosca - Initial version, based on a3_read_mod.f
```

```
25 Aug 2010 - R. Yantosca - Now pass LWI down to READ_A1
```

09 Nov 2012 - M. Payer - Copy all met fields to the State_Met derived type object

15 Nov 2012 - R. Yantosca - Remove reference to dao_mod.F module arrays

22 Sep 2015 - E. Lundgren - Now also read SWGDN

$9.4.4 \quad read_a1$

Subroutine READ_A1 reads MERRA 1-hour time averaged ("A1") met fields from disk.

READ_A1(NYMD,	NHMS,	Input_Opt	,	
	ALBEDO,	CLDTOT,	EFLUX,	EVAP,	
	FRSEAICE,	FRSNO,	GRN,	GWETROOT,	
	GWETTOP,	HFLUX,	LAI,	LWGNT,	
	LWI,	PARDF,	PARDR,	PBLH,	
	PRECANV,	PRECTOT,	PRECCON,	PRECLSC,	
	PRECSNO,	SEAICE00,	SEAICE10,	SEAICE20,	
	SEAICE30,	SEAICE40,	SEAICE50,	SEAICE60,	
	SEAICE70,	SEAICE80,	SEAICE90,	SLP,	
	SNODP,	SNOMAS,	SWGDN,	SWGNT,	
	TROPPT,	T2M,	TS,	U1OM,	
	USTAR,	V1OM,	ZOM)
		ALBEDO, FRSEAICE, GWETTOP, LWI, PRECANV, PRECSNO, SEAICE30, SEAICE70, SNODP, TROPPT,	ALBEDO, CLDTOT, FRSEAICE, FRSNO, GWETTOP, HFLUX, LWI, PARDF, PRECANV, PRECTOT, PRECSNO, SEAICE00, SEAICE30, SEAICE40, SEAICE70, SEAICE80, SNODP, SNOMAS, TROPPT, T2M,	ALBEDO, CLDTOT, EFLUX, FRSEAICE, FRSNO, GRN, GWETTOP, HFLUX, LAI, LWI, PARDF, PARDR, PRECANV, PRECTOT, PRECCON, PRECSNO, SEAICE00, SEAICE10, SEAICE30, SEAICE40, SEAICE50, SEAICE70, SEAICE80, SEAICE90, SNODP, SNOMAS, SWGDN, TROPPT, T2M, TS,	• • •

USES:

USE CMN_SIZE_MOD

#if defined(BPCH_DIAG)

USE CMN_DIAG_MOD

USE DIAG_MOD, ONLY : AD67

#endif

USE FILE_MOD, ONLY : IOERROR

USE Input_Opt_Mod, ONLY : OptInput

USE TIME_MOD, ONLY : SET_CT_A1

INPUT PARAMETERS:

USE TIME_MOD,

ONLY : TIMESTAMP_STRING

OUTPUT PARAMETERS:

```
REAL(fp),
           INTENT(OUT) :: ALBEDO
                                   (IIPAR, JJPAR)
                                                  ! Sfc albedo [unitless]
REAL(fp),
           INTENT(OUT) :: CLDTOT
                                   (IIPAR, JJPAR)
                                                  ! Column cld fraction
REAL(fp),
           INTENT(OUT) :: EFLUX
                                                  ! Latent heat flux [W/m2]
                                   (IIPAR, JJPAR)
           INTENT(OUT) :: EVAP
REAL(fp),
                                   (IIPAR, JJPAR)
                                                  ! Surface evap [kg/m2/s]
REAL(fp), INTENT(OUT) :: FRSEAICE(IIPAR,JJPAR)
                                                  ! Sfc sea ice fraction
                                                  ! Sfc snow fraction
REAL(fp),
          INTENT(OUT) :: FRSNO
                                   (IIPAR, JJPAR)
REAL(fp), INTENT(OUT) :: GRN
                                                  ! Greenness fraction
                                   (IIPAR, JJPAR)
REAL(fp), INTENT(OUT) :: GWETROOT(IIPAR,JJPAR)
                                                  ! Root soil wetness [frac]
REAL(fp), INTENT(OUT) :: GWETTOP (IIPAR, JJPAR)
                                                  ! Topsoil wetness [frac]
REAL(fp), INTENT(OUT) :: HFLUX
                                   (IIPAR, JJPAR)
                                                  ! Sensible H-flux [W/m2]
REAL(fp), INTENT(OUT) :: LAI
                                   (IIPAR, JJPAR)
                                                  ! Leaf area index [m2/m2]
REAL(fp), INTENT(OUT) :: LWI
                                   (IIPAR, JJPAR)
                                                  ! Leaf area index [m2/m2]
                                                  ! Net LW rad @ sfc [W/m2]
REAL(fp), INTENT(OUT) :: LWGNT
                                   (IIPAR, JJPAR)
REAL(fp), INTENT(OUT) :: PARDF
                                   (IIPAR, JJPAR)
                                                  ! Diffuse PAR [W/m2]
REAL(fp), INTENT(OUT) :: PARDR
                                   (IIPAR, JJPAR)
                                                  ! Direct PAR [W/m2]
REAL(fp), INTENT(OUT) :: PBLH
                                   (IIPAR, JJPAR)
                                                  ! PBL height [m]
REAL(fp),
                                                  ! Anv prec @ sfc [kg/m2/s]
           INTENT(OUT) :: PRECANV (IIPAR, JJPAR)
REAL(fp),
           INTENT(OUT) :: PRECTOT (IIPAR, JJPAR)
                                                  ! Tot prec @ sfc [kg/m2/s]
REAL(fp),
                                                  ! CV prec @ sfc [kg/m2/s]
           INTENT(OUT) :: PRECCON (IIPAR, JJPAR)
REAL(fp),
           INTENT(OUT) :: PRECLSC (IIPAR, JJPAR)
                                                  ! LS prec @ sfc [kg/m2/s]
REAL(fp),
           INTENT(OUT) :: PRECSNO (IIPAR, JJPAR)
                                                  ! Snow precip [kg/m2/s]
REAL(fp),
           INTENT(OUT) :: SEAICEOO(IIPAR, JJPAR)
                                                  ! Sea ice coverage 00-10%
REAL(fp), INTENT(OUT) :: SEAICE10(IIPAR, JJPAR)
                                                  ! Sea ice coverage 10-20%
REAL(fp),
          INTENT(OUT) :: SEAICE20(IIPAR, JJPAR)
                                                  ! Sea ice coverage 20-30%
REAL(fp), INTENT(OUT) :: SEAICE30(IIPAR,JJPAR)
                                                  ! Sea ice coverage 30-40%
REAL(fp), INTENT(OUT) :: SEAICE40(IIPAR, JJPAR)
                                                  ! Sea ice coverage 40-50%
REAL(fp), INTENT(OUT) :: SEAICE50(IIPAR, JJPAR)
                                                  ! Sea ice coverage 50-60%
REAL(fp), INTENT(OUT) :: SEAICE60(IIPAR,JJPAR)
                                                  ! Sea ice coverage 60-70%
REAL(fp), INTENT(OUT) :: SEAICE70(IIPAR, JJPAR)
                                                  ! Sea ice coverage 70-80%
           INTENT(OUT) :: SEAICE80(IIPAR, JJPAR)
                                                  ! Sea ice coverage 80-90%
REAL(fp),
```

```
REAL(fp), INTENT(OUT) :: SEAICE90(IIPAR, JJPAR)
                                                 ! Sea ice coverage 90-100%
REAL(fp), INTENT(OUT) :: SLP
                                  (IIPAR, JJPAR)
                                                 ! Sea level pressure [hPa]
REAL(fp), INTENT(OUT) :: SNODP
                                  (IIPAR, JJPAR)
                                                 ! Snow depth [m]
REAL(fp), INTENT(OUT) :: SNOMAS
                                  (IIPAR, JJPAR)
                                                 ! Snow mass [kg/m2]
REAL(fp), INTENT(OUT) :: SWGDN
                                  (IIPAR, JJPAR)
                                                 ! Incident SW rad @ sfc
                                                 [W/m2]
REAL(fp), INTENT(OUT) :: SWGNT
                                                 ! Net SW rad @ sfc [W/m2]
                                  (IIPAR, JJPAR)
REAL(fp), INTENT(OUT) :: TROPPT
                                  (IIPAR, JJPAR)
                                                 ! T'pause pressure [hPa]
REAL(fp), INTENT(OUT) :: T2M
                                  (IIPAR, JJPAR)
                                                 ! T @ 2m height [K]
                                                 ! Sfc skin T [K]
REAL(fp), INTENT(OUT) :: TS
                                  (IIPAR, JJPAR)
REAL(fp), INTENT(OUT) :: U10M
                                  (IIPAR, JJPAR)
                                                 ! U-wind @ 10m [m/s]
REAL(fp), INTENT(OUT) :: USTAR
                                  (IIPAR, JJPAR)
                                                 ! Friction velocity [m/s]
REAL(fp), INTENT(OUT) :: V10M
                                  (IIPAR, JJPAR)
                                                ! V-wind @ 10m [m/s]
REAL(fp), INTENT(OUT) :: ZOM
                                  (IIPAR, JJPAR)
                                                ! Roughness height [m]
```

REVISION HISTORY:

```
19 Aug 2010 - R. Yantosca - Initial version, based on a3_read_mod.f
25 Aug 2010 - R. Yantosca - Now read LWI (land/water/ice) from disk
15 Aug 2011 - R. Yantosca - Now save SWGDN in 2nd slot of ND67 diagnostic
25 Mar 2011 - R. Yantosca - Bug fix: make local SWGDN array for ND67 diag
08 Jun 2012 - S. Philip - Correction for MERRA boundary layer height
03 Aug 2012 - R. Yantosca - Now use locally-defined IU_A1 file LUN
07 Aug 2012 - R. Yantosca - Now print LUN used to open file
24 Jun 2014 - R. Yantosca - Now accept Input_Opt via the arg list
06 Nov 2014 - R. Yantosca - Replace TRANSFER_2D with direct casts
22 Sep 2015 - E. Lundgren - Now save SWGDN globally
02 Feb 2016 - E. Lundgren - Block off bpch diagnostics with if defined bpch
```

9.4.5 al_check

Subroutine A1_CHECK prints an error message if not all of the A-3 met fields are found. The run is also terminated.

INTERFACE:

```
SUBROUTINE A1_CHECK( NFOUND, N_A1 )
```

USES:

```
USE ERROR_MOD, ONLY : GEOS_CHEM_STOP
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NFOUND   ! Number of met fields read in from disk
INTEGER, INTENT(IN) :: N_A1    ! Number of expected met fields
```

```
19 Aug 2010 - R. Yantosca - Initial version, based on a3_read_mod.f
```

9.5 Fortran: Module Interface merra_a3_mod.F90

Module MERRA_A3_MOD contains subroutines for reading the 3-hour time averaged (aka "A3") fields from the MERRA data archive.

INTERFACE:

```
MODULE MERRA_A3_MOD
```

USES:

```
USE inquireMod, ONLY : findFreeLUN
USE PRECISION_MOD ! For GEOS-Chem Precision (fp)
```

IMPLICIT NONE

PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: GET_MERRA_A3_FIELDS
PUBLIC :: OPEN_MERRA_A3_FIELDS

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: A3_CHECK
PRIVATE :: DO_OPEN_A3
PRIVATE :: READ_A3

REMARKS:

Don't bother with the file unzipping anymore.

REVISION HISTORY:

```
19 Aug 2010 - R. Yantosca - Initial version, based on i6_read_mod.f
03 Aug 2012 - R. Yantosca - Now make IU_A3 a private module variable
15 Nov 2012 - R. Yantosca - Now replace dao_mod.F arrays with State_Met
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
17 Nov 2014 - M. Yannetti - Added PRECISION_MOD
```

9.5.1 do_open_a3

unction DO_OPEN_A3 returns TRUE if is time to open the A3 met field file or FALSE otherwise. This prevents us from opening a file which has already been opened.

INTERFACE:

```
FUNCTION DO_OPEN_A3( NYMD, NHMS ) RESULT( DO_OPEN )
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NYMD     ! YYYYMMDD and hhmmss to be tested
INTEGER, INTENT(IN) :: NHMS     ! to see if it's time to open A3 file
```

RETURN VALUE:

LOGICAL :: DO_OPEN ! = T if it is time to open the file

REVISION HISTORY:

20 Aug 2010 - R. Yantosca - Initial version, based on a3_read_mod.f

9.5.2 open_merra_a3_fields

USE BPCH2_MOD,

Subroutine OPEN_MERRA_A3_FIELDS opens the A3 met fields file for date NYMD and time NHMS.

INTERFACE:

```
SUBROUTINE OPEN_MERRA_A3_FIELDS( NYMD, NHMS, Input_Opt )
```

USES:

ONLY : GET_RES_EXT USE CMN_SIZE_MOD USE ERROR_MOD, ONLY : ERROR_STOP USE FILE_MOD, ONLY : FILE_EXISTS
USE FILE_MOD, ONLY : IOERROR
USE Input_Opt_Mod, ONLY : OptInput USE TIME_MOD, ONLY : EXPAND_DATE

INPUT PARAMETERS:

INTENT(IN) :: NYMD INTEGER, ! YYYYMMDD and hhmmss INTENT(IN) :: NHMS ! to test for A3 file open INTEGER, TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

REVISION HISTORY:

```
20 Aug 2010 - R. Yantosca - Initial version, based on a6_read_mod.f
03 Aug 2012 - R. Yantosca - Now use findFreeLUN to define IU_A3 locally
07 Aug 2012 - R. Yantosca - Now print LUN used to open file
11 Apr 2013 - R. Yantosca - Now pass fields with Input_Opt
```

9.5.3 get_merra_a3_fields

Subroutine GET_MERRA_A3_FIELDS is a wrapper for routine READ_A3.

```
SUBROUTINE GET_MERRA_A3_FIELDS( NYMD, NHMS, Input_Opt, State_Met )
```

USES:

```
USE CMN_SIZE_MOD

USE Input_Opt_Mod, ONLY : OptInput

USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NYMD ! YYYYMMDD and
```

INTEGER, INTENT(IN) :: NHMS ! hhmmss of desired data
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met   ! Meteorology State object
```

REVISION HISTORY:

```
20 Aug 2010 - R. Yantosca - Initial version, based on a3_read_mod.f

09 Nov 2012 - M. Payer - Copy all met fields to the State_Met derived type object

15 Nov 2012 - R. Yantosca - Now replace dao_mod.F arrays with State_met

23 Oct 2013 - R. Yantosca - Now accept Input_Opt as an argument

23 Oct 2013 - R. Yantosca - Now read T_FULLGRID for specialty (offline) sims

16 Apr 2015 - R. Yantosca - Remove reference to T_FULLGRID; it's obsolete

17 Mar 2016 - M. Sulprizio- Read optical depth into State_Met%OPTD instead of State_Met%OPTDEP (obsolete).
```

$9.5.4 \quad read_a3$

Subroutine READ_A3 reads the MERRA 3-hour time-averaged (aka "A3") met fields from disk.

INTERFACE:

SUBROUTINE H	READ_A3(NYMD,	NHMS,	Input_Opt	,	
&		CLOUD,	CLDTOPS,	CMFMC,	DQRCU,	
&		DQRLSAN,	DQIDTMST,	DQLDTMST,	DQVDTMST,	
&		DTRAIN,	MOISTQ,	OPTDEPTH,	PFICU,	
&		PFILSAN,	PFLCU,	PFLLSAN,	QI,	
&		QL,	QV,	REEVAPCN,	REEVAPLS,	
&		Τ,	TAUCLI,	TAUCLW,	U,	
&		V)

```
USE CMN_SIZE_MOD
#if defined( BPCH_DIAG )
USE CMN_DIAG_MOD
```

```
USE DIAG_MOD,
                               ONLY: AD21
       USE DIAG_MOD,
                               ONLY: AD66
      USE DIAG_MOD,
                               ONLY: AD67
 #endif
       USE FILE_MOD,
                               ONLY : IOERROR
      USE Input_Opt_Mod,
                               ONLY : OptInput
      USE TIME_MOD,
                               ONLY : SET_CT_A3
      USE TIME_MOD,
                               ONLY: TIMESTAMP_STRING
       USE TRANSFER_MOD,
                               ONLY: TRANSFER_3D_Lp1
       USE TRANSFER_MOD,
                               ONLY: TRANSFER_3D
      USE TRANSFER_MOD,
                               ONLY: TRANSFER_G5_PLE
INPUT PARAMETERS:
                       INTENT(IN) :: NYMD
                                                  ! YYYYMMDD & hhmmss
       INTEGER,
                       INTENT(IN) :: NHMS
                                                     of desired data
       INTEGER,
                                                  ! Input Options object
       TYPE(OptInput), INTENT(IN) :: Input_Opt
OUTPUT PARAMETERS:
       ! Fields dimensioed as (I,J)
       INTEGER, INTENT(OUT) :: CLDTOPS
                                          (IIPAR, JJPAR
                                                              )
       ! Fields dimensioned as (I,J,L)
       REAL(fp), INTENT(OUT) :: CMFMC
                                            (IIPAR, JJPAR, LLPAR+1)
       REAL(fp), INTENT(OUT) :: DQRCU
                                            (IIPAR, JJPAR, LLPAR
       REAL(fp), INTENT(OUT) :: DQRLSAN
                                            (IIPAR, JJPAR, LLPAR
      REAL(fp), INTENT(OUT) :: DQIDTMST
                                            (IIPAR, JJPAR, LLPAR
       REAL(fp), INTENT(OUT) :: DQLDTMST
                                            (IIPAR, JJPAR, LLPAR
                                                                )
       REAL(fp), INTENT(OUT) :: DQVDTMST
                                            (IIPAR, JJPAR, LLPAR
       REAL(fp), INTENT(OUT) :: DTRAIN
                                            (IIPAR, JJPAR, LLPAR
       REAL(fp), INTENT(OUT) :: PFICU
                                            (IIPAR, JJPAR, LLPAR
                                                                )
       REAL(fp), INTENT(OUT) :: PFILSAN
                                            (IIPAR, JJPAR, LLPAR
       REAL(fp), INTENT(OUT) :: PFLCU
                                            (IIPAR, JJPAR, LLPAR
                                                                )
       REAL(fp), INTENT(OUT) :: PFLLSAN
                                            (IIPAR, JJPAR, LLPAR
                                                                )
       REAL(fp), INTENT(OUT) :: QI
                                            (IIPAR, JJPAR, LLPAR
                                                                )
       REAL(fp), INTENT(OUT) :: QL
                                            (IIPAR, JJPAR, LLPAR
       REAL(fp), INTENT(OUT) :: QV
                                            (IIPAR, JJPAR, LLPAR
       REAL(fp), INTENT(OUT) :: REEVAPCN
                                            (IIPAR, JJPAR, LLPAR
                                            (IIPAR, JJPAR, LLPAR
       REAL(fp), INTENT(OUT) :: REEVAPLS
       REAL(fp), INTENT(OUT) :: T
                                            (IIPAR, JJPAR, LLPAR
                                                                )
      REAL(fp), INTENT(OUT) :: TAUCLI
                                            (IIPAR, JJPAR, LLPAR
       REAL(fp), INTENT(OUT) :: TAUCLW
                                            (IIPAR, JJPAR, LLPAR
                                                                )
       REAL(fp), INTENT(OUT) :: U
                                            (IIPAR, JJPAR, LLPAR
       REAL(fp), INTENT(OUT) :: V
                                            (IIPAR, JJPAR, LLPAR
       REAL(fp), INTENT(OUT) :: CLOUD
                                            (IIPAR, JJPAR, LLPAR
       REAL(fp), INTENT(OUT) :: MOISTQ
                                            (IIPAR, JJPAR, LLPAR
       REAL(fp), INTENT(OUT) :: OPTDEPTH
                                            (IIPAR, JJPAR, LLPAR )
```

REVISION HISTORY:

9.5.5 a3_check

Subroutine A3_CHECK prints an error message if not all of the A-6 met fields are found. The run is also terminated.

INTERFACE:

```
SUBROUTINE A3_CHECK( NFOUND, N_A3 )
```

USES:

```
USE ERROR_MOD, ONLY : GEOS_CHEM_STOP
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NFOUND   ! # of fields found in file
INTEGER, INTENT(IN) :: N_A3    ! # of expected fields
```

REVISION HISTORY:

```
20 Aug 2010 - R. Yantosca - Initial version, based on a6_read_mod.f
```

9.6 Fortran: Module Interface merra_cn_mod.F90

Module MERRA_CN_MOD contains subroutines for reading the constant (aka "CN") fields from the MERRA data archive.

INTERFACE:

```
MODULE MERRA_CN_MOD
```

USE CMN_SIZE_MOD ! Size parameters
USE CMN_DIAG_MOD ! NDxx flags

USE inquireMod, ONLY : findFreeLUN ! Routine to find free LUNs

USE PhysConstants ! g0

USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

IMPLICIT NONE PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: GET_MERRA_CN_FIELDS
PUBLIC :: OPEN_MERRA_CN_FIELDS

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: CN_CHECK PRIVATE :: READ_CN

REMARKS:

Don't bother with the file unzipping anymore.

REVISION HISTORY:

```
19 Aug 2010 - R. Yantosca - Initial version, based on i6_read_mod.f
20 Aug 2010 - R. Yantosca - Moved include files to top of module
03 Aug 2012 - R. Yantosca - Now make IU_A3 a private module variable
09 Nov 2012 - R. Yantosca - Now get met fields from State_Met object
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
17 Nov 2014 - M. Yannetti - Added PRECISION_MOD
```

9.6.1 open_merra_cn_fields

Subroutine OPEN_MERRA_CN_FIELDS opens the MERRA "CN" met fields file for date NYMD and time NHMS.

INTERFACE:

```
SUBROUTINE OPEN_MERRA_CN_FIELDS( NYMD, NHMS, Input_Opt )
```

USES:

```
USE BPCH2_MOD, ONLY : GET_RES_EXT
USE ERROR_MOD, ONLY : ERROR_STOP
USE FILE_MOD, ONLY : FILE_EXISTS
USE FILE_MOD, ONLY : IOERROR
USE Input_Opt_Mod, ONLY : OptInput
USE TIME_MOD, ONLY : EXPAND_DATE
```

INPUT PARAMETERS:

REVISION HISTORY:

```
19 Aug 2010 - R. Yantosca - Initial version, based on i6_read_mod.f
03 Aug 2012 - R. Yantosca - Now use findFreeLUN to define IU_CN locally
07 Aug 2012 - R. Yantosca - Now print LUN used to open file
11 Apr 2013 - R. Yantosca - Now pass directory fields via Input_Opt
```

9.6.2 get_merra_cn_fields

Subroutine GET_MERRA_CN_FIELDS is a wrapper for routine READ_CN.

INTERFACE:

```
SUBROUTINE GET_MERRA_CN_FIELDS( NYMD, NHMS, Input_Opt, State_Met )
```

USES:

```
USE Input_Opt_Mod, ONLY : OptInput
USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met   ! Meteorology State object
```

REVISION HISTORY:

9.6.3 read_cn

Subroutine READ_CN reads the MERRA CN (constant) fields from disk.

```
SUBROUTINE READ_CN( NYMD, NHMS, Input_Opt, & FRLAKE, FRLAND, FRLANDIC, FROCEAN, PHIS )
```

USES:

```
#if defined( BPCH_DIAG )
```

USE DIAG_MOD, ONLY : AD67

#endif

USE FILE_MOD, ONLY : IOERROR
USE Input_Opt_Mod, ONLY : OptInput

USE TIME_MOD, ONLY : TIMESTAMP_STRING

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: NYMD ! YYYYMMDD and

INTEGER, INTENT(IN) :: NHMS ! hhmmss time of desired data

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

OUTPUT PARAMETERS:

```
! Fraction of grid box covered by lakes [unitless]
REAL(fp), INTENT(OUT) :: FRLAKE (IIPAR, JJPAR)
```

```
! Fraction of grid box covered by land ice [unitless] REAL(fp), INTENT(OUT) :: FRLAND (IIPAR,JJPAR)
```

```
! Fraction of grid box covered by land ice [unitless] REAL(fp), INTENT(OUT) :: FRLANDIC(IIPAR, JJPAR)
```

```
! Fraction of grid box covered by ocean [unitless] REAL(fp), INTENT(OUT) :: FROCEAN (IIPAR, JJPAR)
```

```
! Surface geopotential height [m2/s2]
```

REAL(fp), INTENT(OUT) :: PHIS (IIPAR, JJPAR)

REVISION HISTORY:

```
19 Aug 2010 - R. Yantosca - Initial version, based on i6\_read\_mod.f
```

03 Aug 2012 - R. Yantosca - Now use locally-defined IU_CN file LUN

07 Aug 2012 - R. Yantosca - Now print LUN used to open file

06 Nov 2014 - R. Yantosca - Replace TRANSFER_2D with direct casts

02 Feb 2015 - E. Lundgren - Block off bpch diagnostics with if defined bpch

9.6.4 cn_check

Subroutine CN_CHECK prints an error message if not all of the CN met fields are found. The run is also terminated.

INTERFACE:

```
SUBROUTINE CN_CHECK( NFOUND, N_CN )
```

```
USE ERROR_MOD, ONLY : GEOS_CHEM_STOP
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NFOUND   ! Number of met fields read in from disk
INTEGER, INTENT(IN) :: N_CN    ! Number of expected met fields
```

REVISION HISTORY:

```
19 Aug 2010 - R. Yantosca - Initial version, based on i6\_read\_mod.f
```

9.7 Fortran: Module Interface merra_i6_mod.F90

Module MERRA_I6_MOD contains subroutines for reading the 6-hour instantaneous (aka "I6") fields from the MERRA data archive.

INTERFACE:

```
MODULE MERRA_I6_MOD
```

USES:

```
USE inquireMod, ONLY: findFreeLUN

USE PRECISION_MOD! For GEOS-Chem Precision (fp)

IMPLICIT NONE

PRIVATE
```

PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: GET_MERRA_16_FIELDS_1
PUBLIC :: GET_MERRA_16_FIELDS_2
PUBLIC :: OPEN_MERRA_16_FIELDS
```

PRIVATE MEMBER FUNCTIONS:

```
PRIVATE :: 16_CHECK
PRIVATE :: READ_16
```

REMARKS:

Don't bother with the file unzipping anymore.

```
19 Aug 2010 - R. Yantosca - Initial version, based on i6_read_mod.f
03 Aug 2012 - R. Yantosca - Now make IU_I6 a private module variable
15 Nov 2012 - R. Yantosca - Now replace dao_mod.F arrays with State_Met
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
17 Nov 2014 - M. Yannetti - Added PRECISION_MOD
```

9.7.1 open_merra_i6_fields

Subroutine OPEN_MERRA_I6_FIELDS opens the MERRA "I6" met fields file for date NYMD and time NHMS.

INTERFACE:

```
SUBROUTINE OPEN_MERRA_I6_FIELDS( NYMD, NHMS, Input_Opt )
```

USES:

```
USE BPCH2_MOD, ONLY : GET_RES_EXT
USE ERROR_MOD, ONLY : ERROR_STOP
USE FILE_MOD, ONLY : FILE_EXISTS
USE FILE_MOD, ONLY : IOERROR
USE Input_Opt_Mod, ONLY : OptInput
USE TIME_MOD, ONLY : EXPAND_DATE
```

INPUT PARAMETERS:

REVISION HISTORY:

```
19 Aug 2010 - R. Yantosca - Initial version, based on i6_read_mod.f
03 Aug 2012 - R. Yantosca - Now use findFreeLUN to define IU_I6 locally
07 Aug 2012 - R. Yantosca - Now print LUN used to open file
11 Apr 2013 - R. Yantosca - Now pass directory fields with Input_Opt
```

9.7.2 get_merra_i6_fields_1

Subroutine GET_MERRA_I6_FIELDS_1 is a wrapper for routine READ_I6. It reads the initial data at the start of a GEOS-Chem simulation.

INTERFACE:

USES:

```
USE Input_Opt_Mod, ONLY : OptInput
USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NYMD ! YYYYMMDD date
```

INTEGER, INTENT(IN) :: NHMS ! hhmmss time of desired data

INPUT/OUTPUT PARAMETERS:

```
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

REVISION HISTORY:

9.7.3 get_merra_i6_fields_2

Subroutine GET_MERRA_I6_FIELDS_2 is a wrapper for routine READ_I6. It reads the data every 6 hours during a GEOS-Chem simulation.

INTERFACE:

```
SUBROUTINE GET_MERRA_I6_FIELDS_2( NYMD, NHMS, & Input_Opt, State_Met )
```

USES:

INPUT PARAMETERS:

INPUT/OUTPUT PARAMETERS:

```
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

REVISION HISTORY:

$9.7.4 \quad read_i6$

Subroutine READ_I6 reads GEOS-Chem I-6 (instantaneous 6-hour) met fields from disk.

```
SUBROUTINE READ_I6( NYMD, NHMS, Input_Opt, PS, RH)
```

USES:

```
USE CMN_SIZE_MOD
USE CMN_DIAG_MOD
```

USE FILE_MOD, ONLY : IOERROR
USE Input_Opt_Mod, ONLY : OptInput
USE TIME_MOD, ONLY : SET_CT_I6
USE TIME_MOD, ONLY : TIMESTAMP_STRING
USE TRANSFER_MOD, ONLY : TRANSFER_3D

INPUT PARAMETERS:

INTEGER. INTENT(IN) :: NYMD ! YYYYMMDD and hhmmss INTENT(IN) :: NHMS INTEGER, ! time of desired data TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT) :: PS(IIPAR, JJPAR ) ! Surface pressure [hPa]
REAL(fp), INTENT(OUT) :: RH(IIPAR, JJPAR, LLPAR) ! Rel. humidity
```

REVISION HISTORY:

```
19 Aug 2010 - R. Yantosca - Initial version, based on i6_read_mod.f
03 Aug 2012 - R. Yantosca - Now use locally-defined IU_I6 file LUN
07 Aug 2012 - R. Yantosca - Now print LUN used to open file
15 Nov 2013 - R. Yantosca - Now convert RH from [1] to [%], in order
                            to be consistent with GEOS-Chem convention
24 Jun 2014 - R. Yantosca - Now accept Input_Opt via the arg list
```

9.7.5 i6_check

Subroutine I6_CHECK prints an error message if not all of the I6 met fields are found. The run is also terminated.

INTERFACE:

```
SUBROUTINE I6_CHECK( NFOUND, N_I6 )
```

USES:

```
USE ERROR_MOD, ONLY : GEOS_CHEM_STOP
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NFOUND   ! Number of met fields read in from disk
INTEGER, INTENT(IN) :: N_I6    ! Number of expected met fields
```

```
19 Aug 2010 - R. Yantosca - Initial version, based on i6_read_mod.f
```

9.8 Fortran: Module Interface a3_read_mod.F

Module A3_READ_MOD contains routines that unzip, open, and read the GEOS-Chem A3 (avg 3-hour) met fields from disk.

INTERFACE:

MODULE A3_READ_MOD

USES:

USE inquireMod, ONLY : findFreeLUN USE PRECISION_MOD

IMPLICIT NONE PRIVATE

PUBLIC DATA MEMBERS:

PUBLIC :: GET_A3_FIELDS
PUBLIC :: OPEN_A3_FIELDS
PUBLIC :: UNZIP_A3_FIELDS

!PRIVATE DATA MEMBERS:

PRIVATE :: A3_CHECK
PRIVATE :: CHECK_TIME
PRIVATE :: DO_OPEN_A3
PRIVATE :: GET_N_A3
PRIVATE :: READ_A3

REMARKS:

This module reads GEOS-4, GEOS-5, and GCAP met fields MERRA met fields are read in routines merra_*_mod.F GEOS-FP met fields are read in geosfp_read_mod.F

- 23 Jun 2003 R. Yantosca Initial version
- (1) Adapted from "dao_read_mod.f" (bmy, 6/23/03)
- (2) Now can read from either zipped or unzipped files. (bmy, 12/11/03)
- (3) Now skips past the GEOS-4 met field ident string (bmy, 12/12/03)
- (5) Now references FILE_EXISTS from "file_mod.f" (bmy, 3/23/05)
- (6) Now modified for GEOS-5 and GCAP met fields (bmy, 5/25/05)
- (7) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (8) Fixed typos for GCAP fields and ND67 diagnostics (bmy, 2/9/06)
- (9) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (10) Now read PARDF, PARDR for GCAP met fields (swu, bmy, 10/4/06)
- (11) Extra modifications for GEOS-5 met fields (bmy, 1/17/07)
- (12) Now get the # of A-3 fields from the file ident string (bmy, 10/7/08)
- (13) Remove references to IN_CLOUD_OD (bmy, 10/15/09)

```
21 Sep 2010 - R. Yantosca - Added ProTeX headers
28 Feb 2012 - R. Yantosca - Removed support for GEOS-3
03 Aug 2012 - R. Yantosca - Move calls to findFreeLUN out of DEVEL block
03 Aug 2012 - R. Yantosca - Now make IU_A3 a private module variable
15 Nov 2012 - R. Yantosca - Now replace dao_mod.F arrays with State_Met
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
05 Nov 2014 - M. Yannetti - Added PRECISION_MOD
12 May 2016 - M. Sulprizio- Remove routine ARCHIVE_ND67_1D. It is obsolete and it not called from any other routine.
```

9.8.1 unzip_a3_fields

Subroutine UNZIP_A3_FIELDS invokes a FORTRAN system call to uncompress GEOS-Chem A3 met field files and store the uncompressed data in a temporary directory, where GEOS-CHEM can read them. The original data files are not disturbed.

INTERFACE:

SUBROUTINE UNZIP_A3_FIELDS(Input_Opt, OPTION, NYMD)

USES:

```
USE BPCH2_MOD, ONLY : GET_RES_EXT
USE CMN_SIZE_MOD
USE ERROR_MOD, ONLY : ERROR_STOP
```

USE Input_Opt_Mod, ONLY: OptInput
USE TIME_MOD, ONLY: EXPAND_DATE

INPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(IN) :: OPTION ! Unzip option
INTEGER, OPTIONAL, INTENT(IN) :: NYMD ! YYYY/MM/DD of file to unzip
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

- 15 Jun 1998 R. Yantosca Initial version
- (1) Adapted from UNZIP_MET_FIELDS of "dao_read_mod.f" (bmy, 6/23/03)
- (2) Directory information YYYY/MM or YYYYMM is now contained w/in GEOS_1_DIR, GEOS_S_DIR, GEOS_3_DIR, GEOS_4_DIR (bmy, 12/11/03)
- (3) Now reference "directory_mod.f" and "unix_cmds_mod.f". Now prevent EXPAND_DATE from overwriting directory paths with Y/M/D tokens in them (bmy, 7/20/04)
- (4) Now modified for GEOS-5 and GCAP met fields (swu, bmy, 5/25/05)
- (5) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (6) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- 21 Sep 2010 R. Yantosca Added ProTeX headers
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3

9.8.2 do_open_a3

Function DO_OPEN_A3 returns TRUE if is time to open the A3 met field file or FALSE otherwise. This prevents us from opening a file which has already been opened.

INTERFACE:

```
FUNCTION DO_OPEN_A3( NYMD, NHMS, RESET ) RESULT( DO_OPEN )
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NYMD ! YYYY/MM/DD date
INTEGER, INTENT(IN) :: NHMS ! hh:mm:ss time
```

LOGICAL, INTENT(IN), OPTIONAL :: RESET ! Reset first-time flag?

REVISION HISTORY:

```
23 Jun 2003 - R. Yantosca - Initial version
```

- (1) Now modified for GEOS-5 and GCAP met fields (swu, bmy, 5/25/05)
- 21 Sep 2010 R. Yantosca Added ProTeX headers
- 21 Sep 2010 R. Yantosca Bug fix: If we are using MEGAN (which reads many days of A3 data @ start of run), then reset the first-time flag. This will prevent an error if if the start time is not 00 GMT.
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3

9.8.3 open_a3_fields

Subroutine OPEN_A3_FIELDS opens the A3 met fields file for date NYMD and time NHMS.

INTERFACE:

SUBROUTINE OPEN_A3_FIELDS(NYMD, NHMS, Input_Opt, RESET, IUNIT)

USES:

```
USE BPCH2_MOD, ONLY : GET_RES_EXT
```

USE CMN_SIZE_MOD ! Size parameters

USE ERROR_MOD, ONLY : ERROR_STOP

USE FILE_MOD, ONLY : IOERROR, FILE_EXISTS

USE Input_Opt_Mod, ONLY : OptInput
USE TIME_MOD, ONLY : EXPAND_DATE

INPUT PARAMETERS:

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT), OPTIONAL :: IUNIT ! Returns IU_A1

REVISION HISTORY:

- 15 Jun 1998 R. Yantosca Initial version
- (1) Adapted from OPEN_MET_FIELDS of "dao_read_mod.f" (bmy, 6/13/03)
- (2) Now opens either zipped or unzipped files (bmy, 12/11/03)
- (3) Now skips past the GEOS-4 ident string (bmy, 12/12/03)
- (4) Now references "directory_mod.f" instead of CMN_SETUP. Also now references LUNZIP from "logical_mod.f". Also now prevents EXPAND_DATE from overwriting Y/M/D tokens in directory paths. (bmy, 7/20/04)
- (5) Now use FILE_EXISTS from "file_mod.f" to determine if file unit IU_A3 refers to a valid file on disk (bmy, 3/23/05)
- (6) Now modified for GEOS-5 and GCAP met fields (swu, bmy, 5/25/05)
- (7) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (8) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (9) Now get the # of A-3 fields from the file ident string (bmy, 10/7/08)
- 21 Sep 2010 R. Yantosca Added ProTeX headers
- 21 Sep 2010 R. Yantosca Now pass RESET flag to DO_OPEN_A3
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 03 Aug 2012 R. Yantosca Move calls to findFreeLUN out of DEVEL block
- 03 Aug 2012 R. Yantosca Now use findFreeLUN to define IU_A3 locally
- 06 Aug 2012 R. Yantosca Add IUNIT to pass IU_A3 to calling routine
- 07 Aug 2012 R. Yantosca Now print LUN used to open file
- 11 Apr 2013 R. Yantosca Now pass Input_Opt object

9.8.4 get_a3_fields

Subroutine GET_A3_FIELDS is a wrapper for routine READ_A3. GET_A3_FIELDS calls READ_A3 properly for reading GEOS-3, GEOS-4, GEOS-5, or GCAP met data sets.

INTERFACE:

SUBROUTINE GET_A3_FIELDS(NYMD, NHMS, Input_Opt, State_Met)

USES:

USE CMN_SIZE_MOD

USE Input_Opt_Mod, ONLY : OptInput
USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: NYMD ! YYYY/MM/DD

INTEGER, INTENT(IN) :: NHMS ! and hh:mm:ss of desired data

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INPUT/OUTPUT PARAMETERS:

TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object

REVISION HISTORY:

- 23 Jun 2003 R. Yantosca Initial version
- (1) Now save RADSWG to the RADSWG array (instead of RADIAT). Now save CLDFRC to the CLDFRC array (instead of CFRAC). Now get RADLWG, SNOW arrays. Also updated comments. (bmy, 12/9/03)
- (2) Now modified for GEOS-5 and GCAP met fields (swu, bmy, 5/25/05)
- (3) Bug fix: replace RADSWG in call to READ_A3 for GCAP met fields. (bmy, 2/9/06)
- (4) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (5) Now read PARDF, PARDR for GCAP met fields (swu, bmy, 10/4/06)
- (6) Now read SNOW and GETWETTOP for GCAP met fields (swu, phs, 11/15/06)
- (7) Now read extra fields for GEOS-5 (bmy, 1/17/07)
- (8) Now read EFLUX field for non-local PBL scheme (only GEOS5). (ccc, 5/14/09)
- (9) Now read FRLAND, FROCEAN, FRLANDIC and FRLAKE for methane (kjw, 8/18/09)
- 21 Sep 2010 R. Yantosca Added ProTeX headers
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 09 Nov 2012 M. Payer Copy all met fields to the State_Met derived type object
- 15 Nov 2012 R. Yantosca Now replace dao_mod.F arrays with State_Met
- 02 Jul 2013 R. Yantosca For GCAP, PBL is now State_Met%PBLH (similarly for State_Met%PRECCON and State_Met%PRECTOT)
- 13 Aug 2013 R. Yantosca For GEOS-4, PBL is now State_Met%PBLH (similarly for State_Met%PRECCON and State_Met%PRECTOT)
- 24 Jun 2014 R. Yantosca Now accept Input_Opt via the arg list

$9.8.5 \text{ get}_n_3$

Function GET_N_A3 returns the number of A3 fields per met data set.

INTERFACE:

FUNCTION GET_N_A3(NYMD) RESULT(N_A3)

USES:

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: NYMD ! YYYY/MM/DD date

RETURN VALUE:

INTEGER :: N_A3 ! Number of A3 fields in file

REMARKS:

REVISION HISTORY:

- 23 Jun 2003 R. Yantosca Initial version
- (1) GEOS-4/fvDAS now has 19 A-3 fields; we added LAI, RADLWG, SNOW. (bmy, 12/9/03)
- (2) Now modified for GEOS-5 and GCAP met fields (bmy, 5/25/05)
- (3) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (4) Increase # of fields for GCAP from 12 to 16 (swu, bmy, 10/4/06)
- (5) Increase # of fields for GEOS-5 to 25 (bmy, 1/17/07)
- (6) Increase # of fields for GEOS-5 to 26 (EFLUX) (ccc, 5/21/09)
- 21 Sep 2010 R. Yantosca Added ProTeX headers
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3

9.8.6 check_time

Function CHECK_TIME checks to see if the timestamp of the A3 field just read from disk matches the current time. If so, then it's time to return the A3 field to the calling program.

INTERFACE:

```
FUNCTION CHECK_TIME( XYMD, XHMS, NYMD, NHMS ) RESULT( ITS_TIME )
```

USES:

USE CMN_SIZE_MOD

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: XYMD    ! YYYY/MM/DD and hh:mm:ss
INTEGER, INTENT(IN) :: XHMS    ! timestamp of A3 data in file
INTEGER, INTENT(IN) :: NYMD    ! YYYY/MM/DD and hh:mm:ss
INTEGER, INTENT(IN) :: NHMS    ! timestamp for desired data
```

RETURN VALUE:

```
LOGICAL :: ITS_TIME ! =T if XYMD & XHMS match NYMD & NHMS
```

```
23 Jun 2003 - R. Yantosca - Initial version
```

- (1) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- 21 Sep 2010 R. Yantosca Added ProTeX headers

$9.8.7 \quad read_a3$

Subroutine READ_A3 reads GEOS A-3 (3-hr avg) fields from disk.

INTERFACE:

```
SUBROUTINE READ_A3( NYMD,
                               NHMS,
                                        Input_Opt,
                               CLDFRC, EVAP,
&
                      ALBEDO,
                                                 GRN,
                                                           GWETROOT,
                      GWETTOP, HFLUX,
&
                                        LAI,
                                                MOLENGTH, OICE,
&
                      PARDF,
                               PARDR,
                                        PBL,
                                                           PRECON,
                                                PREACC,
&
                      PRECSNO, RADLWG, RADSWG, RADSWT,
                                                           SNICE,
                                SNOMAS, SNOW,
                                                 TROPP,
                                                           TS,
&
                      SNODP,
&
                      TSKIN,
                                U10M,
                                        USTAR,
                                                V1OM,
                                                           Ζ0,
                      EFLUX,
                                FRLAND, FRLAKE, FROCEAN,
                                                           FRLANDIC )
&
```

USES:

```
USE CMN_SIZE_MOD

#if defined( BPCH_DIAG )

USE CMN_DIAG_MOD

USE DIAG_MOD, ONLY : AD67
```

#endif

USE FILE_MOD, ONLY : IOERROR
USE Input_Opt_Mod, ONLY : OptInput!
USE TIME_MOD, ONLY : SET_CT_A3

USE TIME_MOD, ONLY : TIMESTAMP_STRING

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NYMD ! YYYYMMDD
```

INTEGER, INTENT(IN) :: NHMS ! and hhmmss of desired data

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

OUTPUT PARAMETERS:

```
INTENT(OUT), OPTIONAL :: ALBEDO
                                             (IIPAR, JJPAR)
REAL(fp),
REAL(fp),
           INTENT(OUT), OPTIONAL :: CLDFRC
                                             (IIPAR, JJPAR)
REAL(fp),
           INTENT(OUT), OPTIONAL :: EVAP
                                             (IIPAR, JJPAR)
REAL(fp),
           INTENT(OUT), OPTIONAL :: GRN
                                             (IIPAR, JJPAR)
           INTENT(OUT), OPTIONAL :: GWETROOT(IIPAR, JJPAR)
REAL(fp),
REAL(fp), INTENT(OUT), OPTIONAL :: GWETTOP (IIPAR, JJPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: HFLUX
                                             (IIPAR, JJPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: LAI
                                             (IIPAR, JJPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: MOLENGTH(IIPAR, JJPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: OICE
                                             (IIPAR, JJPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: PARDF
                                             (IIPAR, JJPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: PARDR
                                             (IIPAR, JJPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: PBL
                                             (IIPAR, JJPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: PREACC
                                             (IIPAR, JJPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: PRECON
                                             (IIPAR, JJPAR)
```

```
REAL(fp),
           INTENT(OUT), OPTIONAL :: PRECSNO (IIPAR, JJPAR)
REAL(fp),
           INTENT(OUT), OPTIONAL :: RADLWG
                                              (IIPAR, JJPAR)
REAL(fp),
           INTENT(OUT), OPTIONAL :: RADSWG
                                              (IIPAR, JJPAR)
REAL(fp),
           INTENT(OUT), OPTIONAL :: RADSWT
                                               (IIPAR, JJPAR)
REAL(fp),
           INTENT(OUT), OPTIONAL :: SNICE
                                               (IIPAR, JJPAR)
REAL(fp),
           INTENT(OUT), OPTIONAL :: SNODP
                                               (IIPAR, JJPAR)
REAL(fp),
           INTENT(OUT), OPTIONAL :: SNOMAS
                                               (IIPAR, JJPAR)
           INTENT(OUT), OPTIONAL :: SNOW
REAL(fp),
                                               (IIPAR, JJPAR)
REAL(fp),
           INTENT(OUT), OPTIONAL :: TROPP
                                               (IIPAR, JJPAR)
REAL(fp),
           INTENT(OUT), OPTIONAL :: TS
                                               (IIPAR, JJPAR)
           INTENT(OUT), OPTIONAL :: TSKIN
REAL(fp),
                                               (IIPAR, JJPAR)
REAL(fp),
           INTENT(OUT), OPTIONAL :: U10M
                                               (IIPAR, JJPAR)
           INTENT(OUT), OPTIONAL :: USTAR
REAL(fp),
                                               (IIPAR, JJPAR)
REAL(fp),
           INTENT(OUT), OPTIONAL :: V10M
                                               (IIPAR, JJPAR)
REAL(fp),
           INTENT(OUT), OPTIONAL :: ZO
                                               (IIPAR, JJPAR)
REAL(fp),
           INTENT(OUT), OPTIONAL :: EFLUX
                                               (IIPAR, JJPAR)
           INTENT(OUT), OPTIONAL :: FRLAND
REAL(fp),
                                              (IIPAR, JJPAR)
REAL(fp),
           INTENT(OUT), OPTIONAL :: FRLAKE
                                              (IIPAR, JJPAR)
REAL(fp),
           INTENT(OUT), OPTIONAL :: FROCEAN (IIPAR, JJPAR)
           INTENT(OUT), OPTIONAL :: FRLANDIC(IIPAR, JJPAR)
REAL(fp),
```

REMARKS:

(1)	ALBEDO	:	(2-D)	GMAO	surface albedo at 10 m	[unitless]
(2)	CLDFRC	:	(2-D)	GMAO	column cloud fraction @ ground	[unitless]
(3)	EVAP	:	(2-D)	GMAO	evapotranspiration flux	
(4)	GRN	:	(2-D)	GMAO	greenness index	
(5)	GWETROOT	:	(2-D)	GMAO	root soil wetness	[unitless]
(6)	GWETTOP	:	(2-D)	GMAO	topsoil wetness	[unitless]
(7)	HFLUX	:	(2-D)	GMAO	sensible heat flux	[W/m2]
(8)	LAI	:	(2-D)	GMAO	leaf area index	[m2/m2]
(9)	${\tt MOLENGTH}$:	(2-D)	GCAP	Monin-Obhukov length	[m]
(10)	OICE	:	(2-D)	GCAP	fraction of ocean ice	[unitless]
(11)	PARDF	:	(2-D)	GMAO	${\tt photosyn} \ {\tt active} \ {\tt diffuse} \ {\tt radiation}$	[W/m2]
(12)	PARDR	:	(2-D)	GMAO	photosyn active direct radiation	[W/m2]
(13)	PBL	:	(2-D)	GMAO	planetary boundary layer depth	[mb]
(14)	PREACC	:	(2-D)	GMAO	accumulated precip @ ground	[mm H2O/day]
(15)	PRECON	:	(2-D)	GMAO	convective precip @ ground	[mm H2O/day]
(16)	PRECSNO	:	(2-D)	GMAO	"snow" precip @ ground	
(17)	RADLWG	:	(2-D)	GMAO	upward LW flux @ ground	[W/m2]
(18)	RADSWG	:	(2-D)	GMAO	downward SW flux @ ground	[W/m2]
(19)	RADSWT	:	(2-D)	GMAO	downward SW flux @ atm top	[W/m2]
(20)	SNICE	:	(2-D)	GCAP	fraction of snow/ice	[unitless]
(21)	SNODP	:	(2-D)	GMAO	GEOS-5 geometric snow depth	[m]
(22)	SNOMAS	:	(2-D)	GMAO	GEOS-5 H2O equiv snow depth	[m]
(23)	SNOW	:	(2-D)	GMAO	snow depth (H2O equivalent)	[mm H20]
(24)	TROPP	:	(2-D)	GMAO	tropopause pressure	[hPa]
(25)	TS	:	(2-D)	GMAO	surface air temperature	[K]
(26)	TSKIN	:	(2-D)	GMAO	radiance temperature	[K]

(27)	USTAR	:	(2-D)	GMAO	friction velocity	[m/s]
(28)	U10M	:	(2-D)	GMAO	U-wind at 10 m	[m/s]
(29)	V10M	:	(2-D)	GMAO	V-wind at 10 m	[m/s]
(30)	Z0	:	(2-D)	GMAO	roughness height	[m]
(31)	EFLUX	:	(2-D)	GMAO	latent heat flux	[W/m2]
(32)	FRLAND	:	(2-D)	GMAO	fraction of land	[unitless]
(33)	FROCEAN	:	(2-D)	GMAO	fraction of ocean	[unitless]
(34)	FRLANDIC	:	(2-D)	GMAO	fraction of land ice	[unitless]
(35)	FRLAKE	:	(2-D)	GMAO	fraction of lake water	[unitless]

REVISION HISTORY:

- 08 May 1998 R. Yantosca Initial version
- (1) Now use function TIMESTAMP_STRING from "time_mod.f" for formatted date/time output. (bmy, 10/28/03)
- (2) RADSWG, CLDFRC, USTAR, and ZO. are now 2-D arrays. Also added RADLWG and SNOW arrays via the arg list. Now skip over LAI. (bmy, 12/9/03)
- (3) Now modified for GEOS-5 and GCAP met fields. Added GCAP MOLENGTH, SNICE, OICE optional arguments. (swu, bmy, 5/25/05)
- (4) Fixed typo in the ND67 diagnostic for RADSWG (swu, bmy, 2/9/06)
- (5) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (6) Add "PARDIF", "PARDIR" to case statement for GCAP (swu, bmy, 10/4/06)
- (7) Add EVAP, GRN, GWETROOT, LAI, PRECSNO, SNODP, SNOMAS, and TROPP as optional arguments. Also update the CASE statement accordingly for GEOS-5 fields. Convert GEOS-5 PRECTOT and PRECCON fields from [kg/m2/s] to [mm/day] for backwards compatibility. (bmy, 1/17/07)
- (8) Now get the # of A-3 fields from the file ident string (bmy, 10/7/08)
- (9) Now read EFLUX for non-local PBL scheme for GEOS5 (ccc, 5/14/09)
- (10) Now read FRLAND, FROCEAN, FRLANDIC, FRLAKE for methane (kjw, 8/18/09)
- (11) Remove reference to IN_CLOUD_OD (bmy, 10/15/09)
- 21 Sep 2010 R. Yantosca Added ProTeX headers
- 08 Jun 2012 S. Philip Correction for GEOS_5 boundary layer height
- 03 Aug 2012 R. Yantosca Now use locally-defined IU_A3 file LUN
- 07 Aug 2012 R. Yantosca Now print LUN used to open file
- 05 Nov 2014 M. Yannetti Changed REAL*8 to REAL(fp)
- 06 Nov 2014 R. Yantosca Replace TRANSFER_2D with direct casts
- 02 Feb 2016 E. Lundgren Block off bpch diagnostics with if defined bpch

9.8.8 a3_check

Subroutine A3_CHECK prints an error message if not all of the A-3 met fields are found. The run is also terminated.

INTERFACE:

SUBROUTINE A3_CHECK(NFOUND, N_A3)

USE ERROR_MOD, ONLY : GEOS_CHEM_STOP

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NFOUND   ! Number of A3 fields found in file
INTEGER, INTENT(IN) :: N_A3    ! Expected number of A3 fields
```

REVISION HISTORY:

```
27 Oct 2000 - R. Yantosca - Initial version
(1 ) Adapted from DAO_CHECK from "dao_read_mod.f" (bmy, 6/23/03)
21 Sep 2010 - R. Yantosca - Added ProTeX headers
```

9.9 Fortran: Module Interface a6_read_mod.F

Module A6_READ_MOD contains subroutines that unzip, open, and read GEOS-CHEM A-6 (avg 6-hour) met fields from disk.

INTERFACE:

MODULE A6_READ_MOD

USES:

```
USE inquireMod, ONLY : findFreeLUN
USE PRECISION_MOD

IMPLICIT NONE
PRIVATE
```

PUBLIC DATA MEMBERS:

PUBLIC :: GET_A6_FIELDS
PUBLIC :: OPEN_A6_FIELDS
PUBLIC :: UNZIP_A6_FIELDS

REMARKS:

This module reads GEOS-4, GEOS-5, and GCAP met fields MERRA met fields are read in routines merra_*_mod.F GEOS-FP met fields are read in geosfp_read_mod.F

- 19 Jun 2003 R. Yantosca Initial version
- (1) Adapted from "dao_read_mod.f" (bmy, 6/19/03)
- (2) Now use TIMESTAMP_STRING for formatted output (bmy, 10/28/03)
- (3) CLDFRC is now a 2-D array in MAKE_CLDFRC< GET_A6_FIELDS. Also now read from either zipped or unzipped files. (bmy, 12/9/03)
- (4) Now skips past the GEOS-4 ident string (bmy, 12/12/03)

- (5) Bug fix: need to determine CLDTOPS for GEOS-4. (bmy, 3/4/04)
- (6) Now modified for GEOS-4 "a_llk_03" and "a_llk_04" data (bmy, 3/4/04)
- (8) Now references FILE_EXISTS from "file_mod.f" (bmy, 3/23/05)
- (9) Now modified for GEOS-5 and GCAP met fields. Added MAKE_GCAP_CLDFRC routine. (swu, bmy, 5/25/05)
- (10) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (11) Bug fix in ND66 diagnostic for ZMMU (bmy, 2/1/06)
- (12) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (13) Now set negative Q (i.e. SPHU) to a small positive # (bmy, 9/8/06)
- (14) Now read extra fields for GEOS-5. Bug fix: we must convert RH from unitless to % to be compatible w/ present drydep etc. algorithms. (phs, bmy, 3/28/08)
- (15) Now get the # of A-6 fields from the file ident string (bmy, 10/7/08)
- (16) Remove references to IN_CLOUD_OD (bmy, 10/15/09)
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 03 Aug 2012 R. Yantosca Now make IU_A6 a private module variable
- 15 Nov 2012 R. Yantosca Now replace dao_mod.F arrays with State_Met
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 25 Feb 2014 M. Sulprizio- Added ProTeX headers
- 05 Nov 2014 M. Yannetti Added PRECISION_MOD

9.9.1 unzip_a6_fields

Subroutine UNZIP_A6_FIELDS invokes a FORTRAN system call to uncompress GEOS-Chem A6 met field files and store the uncompressed data in a temporary directory, where GEOS-CHEM can read them. The original data files are not disturbed.

INTERFACE:

SUBROUTINE UNZIP_A6_FIELDS(Input_Opt, OPTION, NYMD)

USES:

USE BPCH2_MOD, ONLY : GET_RES_EXT

USE CMN_SIZE_MOD

USE ERROR_MOD, ONLY : ERROR_STOP
USE Input_Opt_Mod, ONLY : OptInput
USE TIME_MOD, ONLY : EXPAND_DATE

INPUT PARAMETERS:

CHARACTER(LEN=*), INTENT(IN) :: OPTION ! Unzip option

INTEGER, OPTIONAL, INTENT(IN) :: NYMD ! YYYY/MM/DD of file to unzip

- 15 Jun 1998 R. Yantosca Initial version
- (1) Adapted from UNZIP_MET_FIELDS of "dao_read_mod.f" (bmy, 6/19/03)
- (2) Directory information YYYY/MM or YYYYMM is now contained w/in GEOS_1_DIR, GEOS_S_DIR, GEOS_3_DIR, GEOS_4_DIR (bmy, 12/11/03)
- (3) Now reference "directory_mod.f" and "unix_cmds_mod.f". Now prevent EXPAND_DATE from overwriting directory paths with Y/M/D tokens in them (bmy, 7/20/04)
- (4) Removed code for GEOS-4 a_llk_03 data. Also modified for GEOS-5 and GCAP met fields. (bmy, 5/25/05)
- (5) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (6) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 11 Apr 2013 R. Yantosca Now replace directory_mod.F and unix_cmds_mod.F with the Input_Opt derived type object
- 25 Feb 2014 M. Sulprizio- Added ProTeX headers

9.9.2 do_open_a6

Function DO_OPEN_A6 returns TRUE if is time to open the A6 met field file or FALSE otherwise. This prevents us from opening a file which has already been opened.

INTERFACE:

```
FUNCTION DO_OPEN_A6( NYMD, NHMS ) RESULT( DO_OPEN )
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NYMD   ! YYYY/MM/DD date
INTEGER, INTENT(IN) :: NHMS    ! hh:mm:ss time
```

REVISION HISTORY:

- 19 Jun 2003 R. Yantosca Initial version
- (1) Now modified for GEOS-4 "a_llk_03" or "a_llk_04" data (bmy, 3/22/04)
- (2) Remove code for obsolete GEOS-4 a_llk_03 data. Also modified for GEOS-5 and GCAP met fields. (swu, bmy, 5/25/05)
- 25 Feb 2014 M. Sulprizio- Added ProTeX headers

9.9.3 open_a6_fields

Subroutine OPEN_A6_FIELDS opens the A6 met fields file for date NYMD and time NHMS.

INTERFACE:

```
SUBROUTINE OPEN_A6_FIELDS( NYMD, NHMS, Input_Opt )
```

USE BPCH2_MOD, ONLY : GET_RES_EXT

USE CMN_SIZE_MOD

USE ERROR_MOD, ONLY : ERROR_STOP

USE FILE_MOD, ONLY : IOERROR, FILE_EXISTS

USE Input_Opt_Mod, ONLY : OptInput
USE TIME_MOD, ONLY : EXPAND_DATE

INPUT PARAMETERS:

REVISION HISTORY:

15 Jun 1998 - R. Yantosca - Initial version

- (1) Adapted from OPEN_MET_FIELDS of "dao_read_mod.f" (bmy, 6/19/03)
- (2) Now opens either zipped or unzipped files (bmy, 12/11/03)
- (3) Now skips past the GEOS-4 ident string (bmy, 12/12/03)
- (4) Now references "directory_mod.f" instead of CMN_SETUP. Also now references LUNZIP from "logical_mod.f". Also now prevents EXPAND_DATE from overwriting Y/M/D tokens in directory paths. (bmy, 7/20/04)
- (5) Now use FILE_EXISTS from "file_mod.f" to determine if file unit IU_A6 refers to a valid file on disk (bmy, 3/23/05)
- (6) Now modified for GEOS-5 and GCAP met fields (swu, bmy, 5/25/05)
- (7) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (8) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (9) Now get the # of A-3 fields from the file ident string (bmy, 10/7/08)
- (10) Set N_A6_FIELDS=21 for GEOS-5 and IN_CLOUD_OD (jmao, bmy, 2/12/09)
- (11) Remove references to IN_CLOUD_OD (bmy, 10/15/09)
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 03 Aug 2012 R. Yantosca Now use findFreeLUN to define IU_A6 locally
- 07 Aug 2012 R. Yantosca Now print LUN used to open file
- 11 Apr 2013 R. Yantosca Now pass directory fields with Input_Opt
- 25 Feb 2014 M. Sulprizio- Added ProTeX headers

9.9.4 get_a6_fields

Subroutine GET_A6_FIELDS is a wrapper for routine READ_A6. GET_A6_FIELDS calls READ_A6 properly for reading A-6 fields from GEOS-1, GEOS-STRAT, GEOS-3, GEO b S-4, GEOS-5, or GCAP met data sets.

INTERFACE:

SUBROUTINE GET_A6_FIELDS(NYMD, NHMS, Input_Opt, State_Met)

```
USE CMN_SIZE_MOD

USE Input_Opt_Mod, ONLY : OptInput

USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

```
! Arguments
```

INTEGER, INTENT(IN) :: NYMD ! YYYY/MM/DD

INTEGER, INTENT(IN) :: NHMS ! and hh:mm:ss of desired data

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input_Options

INPUT/OUTPUT PARAMETERS:

TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object

REVISION HISTORY:

- 19 Jun 2003 R. Yantosca Initial version
- (1) CFRAC has been removed from CMN_DEP. Now use CLDFRC(I,J) from "dao_mod.f" (bmy, 12/9/03)
- (2) Now pass CLDTOPS to READ_A6 for GEOS-4 (bmy, 3/4/04)
- (3) Now modified for GEOS-5 and GCAP met fields (swu, bmy, 5/25/05)
- (4) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (5) Now read CMFMC, DQIDTMST, DQLDTMST, DQRCON, DQRLSC, DQVDTMST, MFXC, MFYC, MFZ, PV, QI, QL, RH, TAUCLI, TAUCLW for GEOS-5 (bmy, 10/30/07)
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 19 Oct 2012 R. Yantosca Now reference gigc_state_met_mod.F90
- 23 Oct 2012 R. Yantosca Add QI, QL to the State_Met object
- 09 Nov 2012 M. Payer Copy all met fields to the State_Met derived type object
- 15 Nov 2012 R. Yantosca Now replace dao_mod.F arrays with State_Met
- 14 Mar 2013 M. Payer Now read T_FULLGRID for vertical regridding of OH for offline simulations (C. Holmes)
- 02 Jul 2013 R. Yantosca Now use State_Met%U and State_Met%V to hold
- the GCAP U and V wind fields
- 02 Jul 2013 R. Yantosca Now use State_Met%U and State_Met%V to hold the GEOS-4 U and V wind fields
- 25 Feb 2014 M. Sulprizio- Added ProTeX headers
- 16 Apr 2015 R. Yantosca Remove reference to T_FULLGRID; it's obsolete
- 17 Mar 2016 M. Sulprizio- Read optical depth into State_Met%OPTD instead of State_Met%OPTDEP (obsolete).

9.9.5 make_gcap_cldfrc

Subroutine MAKE_CLDFRC constructs the GCAP CLDFRC field from the 3-D cloud fraction field.

SUBROUTINE MAKE_GCAP_CLDFRC(CLDF, CLDFRC)

USES:

```
USE CMN_SIZE_MOD ! Size parameters
#if defined( BPCH_DIAG )
            USE CMN_DIAG_MOD ! ND67
            USE DIAG_MOD, ONLY : AD67
#endif
```

INPUT PARAMETERS:

```
! GCAP 3-D cloud fraction field [unitless]
REAL(fp), INTENT(IN) :: CLDF(IIPAR, JJPAR, LLPAR)
```

OUTPUT PARAMETERS:

```
! GCAP column cloud fraction field [unitless]
REAL(fp), INTENT(OUT) :: CLDFRC(IIPAR, JJPAR)
```

REVISION HISTORY:

```
25 May 2005 - R. Yantosca - Initial version
25 Feb 2014 - M. Sulprizio- Added ProTeX headers
06 Nov 2014 - R. Yantosca - Now use CLDF(I,J,L)
```

9.9.6 get_n_a6

Function GET_N_A6 returns the number of A6 fields per met data set.

INTERFACE:

```
FUNCTION GET_N_A6() RESULT( N_A6 )
```

USES:

USE CMN_SIZE_MOD

RETURN VALUE:

INTEGER :: N_A6

- 19 Jun 2003 R. Yantosca Initial version
- (1) Now modified for GCAP and GEOS-5 met fields (swu, bmy, 5/25/05)
- (2) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (3) Increase number of A-6 fields for GEOS-5 to 21 (bmy, 5/15/07)
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 25 Feb 2014 M. Sulprizio- Added ProTeX headers

9.9.7 check_time

Function CHECK_TIME checks to see if the timestamp of the A6 field just read from disk matches the current time. If so, then it's time to return the A6 field to the calling program.

INTERFACE:

```
FUNCTION CHECK_TIME( XYMD, XHMS, NYMD, NHMS ) RESULT( ITS_TIME )
```

USES:

USE CMN_SIZE_MOD

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: XYMD    ! YYYY/MM/DD and hh:mm:ss
INTEGER, INTENT(IN) :: XHMS    ! timestamp of A6 data in file
INTEGER, INTENT(IN) :: NYMD    ! YYYY/MM/DD and hh:mm:ss
INTEGER, INTENT(IN) :: NHMS    ! timestamp for desired data
```

RETURN VALUE:

```
LOGICAL :: ITS_TIME ! =T if XYMD & XHMS match NYMD & NHMS
```

REVISION HISTORY:

```
19 Jun 2003 - R. Yantosca - Initial version
```

- (1) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- 25 Feb 2014 M. Sulprizio- Added ProTeX headers

$9.9.8 \quad read_a6$

Subroutine READ_A6 reads GEOS A-6 (6-hr avg) fields from disk.

INTERFACE:

SUBROUTINE READ_A6(NYMD,	NHMS,	<pre>Input_Opt,</pre>	
&	CLDF,	CLDMAS,	CLDTOPS,	CMFMC,
&	DETRAINE,	DETRAINN,	DNDE,	DNDN,
&	DQIDTMST,	DQLDTMST,	DQRCON,	DQRLSC,
&	DQVDTMST,	DTRAIN,	ENTRAIN,	HKBETA,
&	HKETA,	MFXC,	MFYC,	MFZ,
&	MOISTQ,	OPTDEPTH,	PLE,	PV,
&	Q,	QI,	QL,	RH,
&	Τ,	TAUCLI,	TAUCLW,	U,
&	UPDE,	UPDN,	V,	ZMEU,
&	ZMMD,	ZMMU)		

USES:

```
USE CMN_SIZE_MOD
     USE PhysConstants
#if defined( BPCH_DIAG )
     USE CMN_DIAG_MOD
     USE DIAG_MOD,
                              ONLY: AD21
     USE DIAG_MOD,
                              ONLY: AD66
     USE DIAG_MOD,
                              ONLY: AD67
#endif
      USE FILE_MOD,
                              ONLY : IOERROR
     USE Input_Opt_Mod,
                              ONLY: OptInput
                              ONLY : SET_CT_A6
     USE TIME_MOD,
     USE TIME_MOD,
                              ONLY : TIMESTAMP_STRING
     USE TRANSFER_MOD,
                              ONLY : TRANSFER_3D_Lp1
     USE TRANSFER_MOD,
                              ONLY: TRANSFER_3D
     USE TRANSFER_MOD,
                              ONLY: TRANSFER_G5_PLE
```

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: NYMD ! YYYYMMDD

INTEGER, INTENT(IN) :: NHMS ! and hhmmss of desired data

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT), OPTIONAL :: CLDTOPS(IIPAR,JJPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: CLDF(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: CLDMAS(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: CMFMC(IIPAR,JJPAR,LLPAR+1)
REAL(fp), INTENT(OUT), OPTIONAL :: DETRAINE(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: DETRAINN(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: DNDE(IIPAR,JJPAR,LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: DNDN(IIPAR,JJPAR,LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: DQIDTMST(IIPAR,JJPAR,LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: DQLDTMST(IIPAR,JJPAR,LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: DQRCON(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: DQRLSC(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: DQVDTMST(IIPAR,JJPAR,LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: DTRAIN(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: ENTRAIN(IIPAR,JJPAR,LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: HKBETA(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: HKETA(IIPAR,JJPAR,LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: MFXC(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: MFYC(IIPAR,JJPAR,LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: MFZ(IIPAR,JJPAR,LLPAR+1)
REAL(fp), INTENT(OUT), OPTIONAL :: MOISTQ(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: OPTDEPTH(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: PLE(IIPAR, JJPAR, LLPAR+1)
REAL(fp), INTENT(OUT), OPTIONAL :: PV(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: Q(IIPAR, JJPAR, LLPAR)
```

```
REAL(fp), INTENT(OUT), OPTIONAL :: QI(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: QL(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: RH(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: T(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: TAUCLI(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: TAUCLW(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: U(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: UPDE(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: UPDN(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: ZMEU(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: ZMEU(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: ZMMD(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: ZMMU(IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: ZMMU(IIPAR, JJPAR, LLPAR)
```

REMARKS:

(3)	CLDF	:	(3-D)	Total cloud fractions	[unitless]
(4)	CLDMAS	:	(3-D)	Cloud mass flux field	[kg/m2/600s]
(5)	CLDTOPS	:	(2-D)	CTM Level in which cloud top occurs	[unitless]
(6)	CMFMC	:	(3-D)	GEOS-5 cloud mass flux	[kg/m2/s]
(7)	DETRAINE	:	(3-D)	GCAP detrainment (entraining plume)	[kg/m2/s]
(8)	DETRAINN	:	(3-D)	GCAP detrainment (non-entr'n plume)	
(9)	DNDE	:	(3-D)	GCAP downdraft (entraining plume)	
(10)	DNDN	:	(3-D)	GCAP downdraft (non-entr'n plume)	
(11)	DQIDTMST	:	(3-D)	GEOS-5 ice tendency in moist proc	[kg/kg/s]
(12)	DQLDTMST	:	(3-D)	GEOS-5 liquid tendency in moist proc	[kg/kg/s]
(13)	DQRCON	:	(3-D)	GEOS-5 precip formation rate / conv	
(14)	DQRLSC	:	(3-D)	GEOS-5 precip formation rate / lg scl	
(15)	DQVDTMST	:	(3-D)	GEOS-5 vapor tendency in moist proc	[kg/kg/s]
(16)	DTRAIN	:	(3-D)	Detrainment field	[kg/m2/s]
(17)	ENTRAIN	:	(3-D)	GCAP entrainment	
(18)	HKBETA	:	(3-D)	Hack overshoot parameter	[unitless]
(19)	HKETA	:	(3-D)	Hack convective mass flux	[kg/m2/s]
(20)	MFXC	:	(3-D)	GEOS-5 E-W mass flux	[Pa*m2/s]
(21)	MFYC	:	(3-D)	GEOS-5 N-S mass flux	[Pa*m2/s]
(22)	MFZ	:	(3-D)	GEOS-5 up/down mass flux	[kg/m2/s]
(23)	MOISTQ	:	(3-D)	DAO water vapor tendency d	[g/kg/day]
(24)	OPTDEPTH	:	(3-D)	GEOS grid box optical depth	[unitless]
(25)	PLE	:	(3-D)	GEOS-5 pressure edges	[hPa]
(26)	PV	:	(3-D)	GEOS-5 potential vorticity	[kg*m2/kg/s]
(27)	Q	:	(3-D)	Specific humidity	[g H2O/kg air]
(28)	T	:	(3-D)	Temperature	[K]
(29)	TAUCLI			GEOS ice path optical depth	[unitless]
(30)	TAUCLW	:	(3-D)	GEOS water path optical depth	[unitless]
(31)	U	:	(3-D)	Zonal winds	[m/s]
(32)	UPDE	:	(3-D)	GCAP updraft (entraining plume)	
(33)	UPDN	:	(3-D)	GCAP updraft (non-entr'n plume)	
(34)	V	:	(3-D)	Meridional winds	[m/s]
(35)	ZMEU	:	(3-D)	Zhang/McFarlane updraft entrainment	[Pa/s]

```
(36) ZMMD : (3-D) Zhang/McFarlane downdraft mass flux [Pa/s] (37) ZMMU : (3-D) Zhang/McFarlane updraft mass flux [Pa/s]
```

REVISION HISTORY:

- 05 Jun 1998 R. Yantosca Initial version
- (1) Adapted from READ_A6 of "dao_read_mod.f" (bmy, 6/19/03)
- (2) Now use function TIMESTAMP_STRING from "time_mod.f" for formatted date/time output. (bmy, 10/28/03)
- (3) Now compute CLDTOPS using ZMMU for GEOS-4 (bmy, 3/4/04)
- (4) Now modified for GEOS-5 and GCAP fields. Added DETRAINE, DETRAINN, DNDE, DNDN, ENTRAIN, UPDE, UPDN as optional arguments. Now references "CMN_DIAG". (swu, bmy, 5/25/05)
- (5) Bug fix in ND66 diagnostic for GEOS-4 (bmy, 2/1/06)
- (6) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (7) Now set negative SPHU to a small positive # (1d-32) instead of zero, so as not to blow up logarithms (bmy, 9/8/06)
- (8) Add CMFMC, DQIDTMST, DQLDTMST, DQRCON, DQRLSC, DQVDTMST, MFXC, MFYC, MFZ, PLE, PV, RH, TAUCLI, and TAUCLW as optional arguments. Also update the CASE statement accordingly for GEOS-5 met fields. Now reference TRANSFER_3D_Lp1 from "transfer_mod.f". Now convert GEOS-5 specific humidity from [kg/kg] to [g/kg] for compatibility with existing routines. Also recognize EPV, which is an alternate name for PV. Bug fix: convert GEOS-5 RH from unitless to %. (phs, bmy, 3/28/08)
- (8) Now get the # of A-6 fields from the file ident string (bmy, 10/7/08)
- (9) Remove references to IN_CLOUD_OD (bmy, 10/15/09)
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 03 Aug 2012 R. Yantosca Now use locally-defined IU_A3 file LUN
- 07 Aug 2012 R. Yantosca Now print LUN used to open file
- 14 Mar 2013 M. Payer Added T_FULLGRID as optional argument
- 29 Oct 2013 R. Yantosca Remove reference to TRANSFER_3D_NOLUMP
- 07 Nov 2013 R. Yantosca Now replace any NaN's in the MOISTQ field with zeroes. NaN's have occured near t-pause.
- 25 Feb 2014 M. Sulprizio- Added ProTeX headers
- 24 Jun 2014 R. Yantosca Now accept Input_Opt via the arg list
- 05 Nov 2014 M. Yannetti Changed REAL*8 to REAL(fp)
- 06 Nov 2014 R. Yantosca All input arguments are now declared as (I,J,L)
- 06 Nov 2014 R. Yantosca Replace TRANSFER_A6 with TRANSFER_3D
- 16 Apr 2015 R. Yantosca Remove reference to T_FULLGRID; it's obsolete
- 02 Feb 2016 E. Lundgren Block of diagnostics with if defined BPCH

9.9.9 a6_check

Subroutine A6_CHECK prints an error message if not all of the A-6 met fields are found. The run is also terminated.

INTERFACE:

```
SUBROUTINE A6_CHECK( NFOUND, N_A6 )
```

USES:

```
USE ERROR_MOD, ONLY : GEOS_CHEM_STOP
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NFOUND   ! Number of A6 fields found in file
INTEGER, INTENT(IN) :: N_A6    ! Expected number of A6 fields
```

REVISION HISTORY:

```
27 Oct 2000 - R. Yantosca - Initial version
(1 ) Adapted from DAO_CHECK from "dao_read_mod.f" (bmy, 6/19/03)
25 Feb 2014 - M. Sulprizio- Added ProTeX headers
```

9.10 Fortran: Module Interface i6_read_mod.F

Module I6_READ_MOD contains routines that unzip, open, and read the GEOS-Chem I6 (instantaneous 6-hour) met fields from disk.

INTERFACE:

```
MODULE I6_READ_MOD
```

USES:

```
USE inquireMod, ONLY: findFreeLUN
USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

IMPLICIT NONE
PRIVATE
```

PUBLIC DATA MEMBERS:

```
PUBLIC :: GET_I6_FIELDS_1
PUBLIC :: GET_I6_FIELDS_2
PUBLIC :: OPEN_I6_FIELDS
PUBLIC :: UNZIP_I6_FIELDS
```

REMARKS:

```
This module reads GEOS-4, GEOS-5, and GCAP met fields MERRA met fields are read in routines merra_*_mod.F GEOS-FP met fields are read in geosfp_read_mod.F
```

```
23 Jun 2003 - R. Yantosca - Initial version
(1) Adapted from "dao_read_mod.f" (bmy, 6/23/03)
(2) Now use TIMESTAMP_STRING for formatted date/time output (bmy, 10/28/03)
(3 ) Now reads either zipped or unzipped files (bmy, 12/11/03)
(4) Now skips past the GEOS-4 ident string (bmy, 12/12/03)
(5 ) Now references "directory_mod.f", "unix_cmds_mod.f", and
      "logical_mod.f" (bmy, 7/20/04)
(6 ) Now references FILE_EXISTS from "file_mod.f" (bmy, 3/23/05)
(7) Now modified for GEOS-5 and GCAP met fields (swu, bmy, 5/25/05)
(8) Now account for GEOS-4 coastal boxes in LWI properly (bmy, 8/10/05)
(9) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
(10) Now make LWI REAL(fp) for near-land formulation (ltm, bmy, 5/9/06)
(11) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
(12) Now set negative SPHU to a very small positive # (bmy, 9/8/06)
(13) Now read TROPP files for GEOS-4, and check tropopause level
     in case of a variable tropopause (phs, bmy, bdf, 9/14/06)
(14) Now get the # of A-3 fields from the file ident string (bmy, 10/7/08)
(15) Remove references to IN_CLOUD_OD (bmy, 10/15/09)
28 Feb 2012 - R. Yantosca - Removed support for GEOS-3
03 Aug 2012 - R. Yantosca - Now make IU_I6 a private module variable
15 Nov 2012 - R. Yantosca - Now replace dao_mod.F arrays with State_Met
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
25 Feb 2014 - M. Sulprizio- Added ProTeX headers
14 Nov 2014 - M. Yannetti - Added PRECISION_MOD
```

9.10.1 unzip_i6_fields

Subroutine UNZIP_I6_FIELDS invokes a FORTRAN system call to uncompress GEOS-Chem I-6 met field files and store the uncompressed data in a temporary directory, where GEOS-CHEM can read them. The original data files are not disturbed.

INTERFACE:

SUBROUTINE UNZIP_I6_FIELDS(Input_Opt, OPTION, NYMD)

USES:

```
USE BPCH2_MOD, ONLY : GET_RES_EXT

USE CMN_SIZE_MOD

USE ERROR_MOD, ONLY : ERROR_STOP

USE Input_Opt_Mod, ONLY : OptInput

USE TIME_MOD, ONLY : EXPAND_DATE
```

INPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(IN) :: OPTION ! Unzip option
INTEGER, OPTIONAL, INTENT(IN) :: NYMD ! YYYY/MM/DD of file to unzip
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

REVISION HISTORY:

- 15 Jun 1998 R. Yantosca Initial version
- (1) Adapted from UNZIP_MET_FIELDS of "dao_read_mod.f" (bmy, 6/23/03)
- (2) Directory information YYYY/MM or YYYYMM is now contained w/in GEOS_1_DIR, GEOS_S_DIR, GEOS_3_DIR, GEOS_4_DIR (bmy, 12/11/03)
- (3) Now reference "directory_mod.f" and "unix_cmds_mod.f". Now prevent EXPAND_DATE from overwriting directory paths with Y/M/D tokens in them (bmy, 7/20/04)
- (4) Now modified for GEOS-5 and GCAP met fields
- (5) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (6) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 11 Apr 2013 R. Yantosca Now pass fields via Input_Opt
- 25 Feb 2014 M. Sulprizio- Added ProTeX headers

9.10.2 open_i6_fields

Subroutine OPEN_I6_FIELDS opens the I-6 met fields file for date NYMD and time NHMS.

INTERFACE:

SUBROUTINE OPEN_I6_FIELDS(NYMD, NHMS, Input_Opt)

USES:

USE BPCH2_MOD, ONLY : GET_RES_EXT

USE CMN_SIZE_MOD

USE CMN_SIZE_MOD,

USE ERROR_MOD,

USE FILE_MOD,

USE Input_Opt_Mod,

USE TIME_MOD,

ONLY: EXPAND_DATE

INPUT PARAMETERS:

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

! YYYY/MM/dd and INTEGER, INTENT(IN) :: NYMD

- 15 Jun 1998 R. Yantosca Initial version
- (1) Adapted from OPEN_MET_FIELDS of "dao_read_mod.f" (bmy, 6/13/03)
- (2) Now opens either zipped or unzipped files (bmy, 12/11/03)
- (3) Now skips past the GEOS-4 ident string (bmy, 12/12/03)
- (4) Now references "directory_mod.f" instead of CMN_SETUP. Also now references LUNZIP from "logical_mod.f". Also now prevents EXPAND_DATE from overwriting Y/M/D tokens in directory paths. (bmy, 7/20/04)
- (5) Now use FILE_EXISTS from "file_mod.f" to determine if file unit IU_I6

refers to a valid file on disk (bmy, 3/23/05

- (6) Now modified for GEOS-5 and GCAP met fields (swu, bmy, 5/25/05)
- (7) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (8) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (9) Updated for variable tropopause (phs, bmy, 9/14/06)
- (10) Now get the # of A-3 fields from the file ident string (bmy, 10/7/08)
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 03 Aug 2012 R. Yantosca Now use findFreeLUN to define IU_I6 locally
- 07 Aug 2012 R. Yantosca Now print LUN used to open file
- 11 Apr 2013 R. Yantosca Now pass fields via Input_Opt
- 25 Feb 2014 M. Sulprizio- Added ProTeX headers

$9.10.3 \quad get_i6_fields_1$

Subroutine GET_I6_FIELDS_1 is a wrapper for routine READ_I6. This routine calls READ_I6 properly for reading I-6 fields from GEOS-3, GEOS-4, GEOS-5, or GCAP met data sets at the START of a GEOS-CHEM run.

INTERFACE:

SUBROUTINE GET_I6_FIELDS_1(NYMD, NHMS, Input_Opt, State_Met)

USES:

USE Input_Opt_Mod, ONLY : OptInput
USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: NYMD ! YYYY/MM/DD

INPUT/OUTPUT PARAMETERS:

TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object

- 23 Jun 2003 R. Yantosca Initial version
- (1) Now modified for GEOS-5 and GCAP met fields (swu, bmy, 5/25/05)
- (2) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (3) Now also read TO3 and TTO3 for GEOS-5 (bmy, 1/16/07)
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 09 Nov 2012 M. Payer Copy all met fields to the State_Met derived type object
- 15 Nov 2012 R. Yantosca Now replace dao_mod.F arrays with State_Met
- 25 Feb 2014 M. Sulprizio- Added ProTeX headers
- 24 Jun 2014 R. Yantosca Now pass Input_Opt to READ_I6

9.10.4 get_i6_fields_2

Subroutine GET_I6_FIELDS_2 is a wrapper for routine READ_I6. This routine calls READ_I6 properly for reading I-6 fields from GEOS-3, GEOS-4, GEOS-5, or GCAP met data sets every 6 hours during a GEOS-CHEM run.

INTERFACE:

```
SUBROUTINE GET_16_FIELDS_2( NYMD, NHMS, Input_Opt, State_Met )
```

USES:

```
USE Input_Opt_Mod, ONLY : OptInput
USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NYMD ! YYYY/MM/DD
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object
```

REVISION HISTORY:

```
23 Jun 2003 - R. Yantosca - Initial version
```

- (1) Now modified for GEOS-5 and GCAP met fields
- (2) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (3) Now read TO3 and TTO3 for GEOS-5 (bmy, 1/16/07)
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 09 Nov 2012 M. Payer Copy all met fields to the State_Met derived type object
- 15 Nov 2012 R. Yantosca Now replace dao_mod.F arrays with State_Met
- 25 Feb 2014 M. Sulprizio- Added ProTeX headers

9.10.5 get_n_i6

Function GET_N_I6 returns the number of I-6 fields per met data set.

INTERFACE:

```
FUNCTION GET_N_I6( NYMD ) RESULT( N_I6 )
```

USES:

USE CMN_SIZE_MOD

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: NYMD ! YYYY/MM/DD date

RETURN VALUE:

INTEGER :: N_I6 ! Number of I-6 fields in file

REVISION HISTORY:

- (1) Now modified for GCAP and GEOS-5 met fields (swu, bmy, 5/25/05)
- (2) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (3) Increase # of I-6 fields to 5 for GEOS-5 (bmy, 1/17/06)
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 25 Feb 2014 M. Sulprizio- Added ProTeX headers

9.10.6 check time

Function CHECK_TIME checks to see if the timestamp of the I6 field just read from disk matches the current time. If so, then it's time to return the I6 field to the calling program.

INTERFACE:

```
FUNCTION CHECK_TIME( XYMD, XHMS, NYMD, NHMS ) RESULT( ITS_TIME )
```

USES:

USE CMN_SIZE_MOD

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: XYMD    ! YYYY/MM/DD and hh:mm:ss
INTEGER, INTENT(IN) :: XHMS    ! timestamp of I6 data in file
INTEGER, INTENT(IN) :: NYMD    ! YYYY/MM/DD and hh:mm:ss
INTEGER, INTENT(IN) :: NHMS    ! timestamp for desired data
```

RETURN VALUE:

LOGICAL :: ITS_TIME ! =T if XYMD & XHMS match NYMD & NHMS

- 23 Jun 2003 R. Yantosca Initial version
- (1) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- 25 Feb 2014 M. Sulprizio- Added ProTeX headers

9.10.7 read_i6

Subroutine READ_I6 reads GEOS I-6 (inst. 6-hr) met fields from disk.

INTERFACE:

```
SUBROUTINE READ_16( NYMD, NHMS, Input_Opt,
& ALBD, LWI, PS, SLP, SPHU, TMPU,
& TO3, TROPP, TTO3, UWND, VWND )
```

USES:

```
USE CMN_SIZE_MOD

#if defined( BPCH_DIAG )

USE CMN_DIAG_MOD

USE DIAG_MOD, ONLY : AD66

USE DIAG_MOD, ONLY : AD67

#endif
```

USE FILE_MOD, ONLY : IOERROR
USE Input_Opt_Mod, ONLY : OptInput
USE TIME_MOD, ONLY : SET_CT_I6
USE TIME_MOD, ONLY : TIMESTAMP_STRING

USE TRANSFER_MOD, ONLY: TRANSFER_3D

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NYMD ! YYYYMMDD
```

INTEGER, INTENT(IN) :: NHMS ! and hhmmss of desired data

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT), OPTIONAL :: ALBD (IIPAR, JJPAR )
REAL(fp), INTENT(OUT), OPTIONAL :: LWI (IIPAR, JJPAR )
REAL(fp), INTENT(OUT), OPTIONAL :: PS (IIPAR, JJPAR )
REAL(fp), INTENT(OUT), OPTIONAL :: SLP (IIPAR, JJPAR )
REAL(fp), INTENT(OUT), OPTIONAL :: SPHU (IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: TMPU (IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: TO3 (IIPAR, JJPAR )
REAL(fp), INTENT(OUT), OPTIONAL :: TROPP(IIPAR, JJPAR )
REAL(fp), INTENT(OUT), OPTIONAL :: TTO3 (IIPAR, JJPAR )
REAL(fp), INTENT(OUT), OPTIONAL :: UWND (IIPAR, JJPAR, LLPAR)
REAL(fp), INTENT(OUT), OPTIONAL :: VWND (IIPAR, JJPAR, LLPAR)
```

REMARKS:

```
(3 ) ALBD : (2-D) GMAO Surface albedo [unitless]
(4 ) LWI : (2-D) GMAO Land-water indices [unitless]
(5 ) PS : (2-D) GMAO Surface pressure [hPa]
(6 ) SLP : (2-D) GMAO Sea-level pressures [hPa]
(7 ) SPHU : (3-D) GMAO Specific humidity field [g H2O/kg air]
```

ΓK]

(8) TMPU: (3-D) GMAO Temperature field

```
(9) TO3 : (2-D) GMAO GEOS-5 column ozone [DU]
(10) TROPP : (2-D) GMAO tropopause pressure pressures [hPa]
(11) TTO3 : (2-D) GMAO GEOS-5 trop column ozone [DU]
(12) UWND : (3-D) GMAO U-wind (zonal wind) [m/s]
(13) VWND : (3-D) GMAO V-wind (meridional wind) [m/s]
```

REVISION HISTORY:

- 08 May 1998 R. Yantosca Initial version
- (1) Adapted from "READ_I6" of "dao_read_mod.f" (bmy, 6/23/03)
- (2) Now use function TIMESTAMP_STRING from "time_mod.f" for formatted date/time output. (bmy, 10/28/03)
- (3) Round up to account for GEOS-4 coastal boxes properly (bmy, 8/10/05)
- (4) For near-land formulation: (a) make LWI a REAL(fp) and (b) do not round up LWI for GEOS-4 meteorology (ltm, bmy, 5/9/06)
- (5) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (6) Now set negative SPHU to a small positive number (1d-32) instead of zero, so as not to blow up logarithms (bmy, 9/8/06)
- (7) Now read TROPP files for GEOS-4 (phs, bmy, bdf, 9/12/06)
- (8) Now read TO3 and TTO3 for GEOS-5 (bmy, 1/16/07)
- (9) Now get the # of A-3 fields from the file ident string (bmy, 10/7/08)
- (10) Remove references to IN_CLOUD_OD (bmy, 10/15/09)
- 03 Aug 2012 R. Yantosca Now use locally-defined IU_I6, IU_TP file LUNs
- 07 Aug 2012 R. Yantosca Now print LUN used to open file
- 25 Feb 2014 M. Sulprizio- Added ProTeX headers
- 24 Jun 2014 R. Yantosca Now accept Input_Opt via the arg list
- 06 Nov 2014 R. Yantosca Replace TRANSFER_2D with direct casts
- 03 Dec 2014 R. Yantosca Bug fix: remove TRANSFER_2D from GEOS-4 block
- 02 Feb 2016 E. Lundgren Block of diagnostics with if defined BPCH

9.10.8 i6_check

Subroutine I6_CHECK prints an error message if not all of the I-6 met fields are found. The run is also terminated.

INTERFACE:

```
SUBROUTINE I6_CHECK( NFOUND, N_I6 )
```

USES:

USE ERROR_MOD, ONLY : GEOS_CHEM_STOP

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NFOUND   ! Number of I-6 fields found in file
INTEGER, INTENT(IN) :: N_I6    ! Expected number of I-6 fields
```

```
27 Oct 2000 - R. Yantosca - Initial version
(1 ) Adapted from DAO_CHECK from "dao_read_mod.f" (bmy, 6/23/03)
25 Feb 2014 - M. Sulprizio- Added ProTeX headers
```

9.11 Fortran: Module Interface gcap_read_mod.f

Module GCAP_READ_MOD contains file unit numbers, as well as file I/O routines for GEOS-Chem. FILE_MOD keeps all of the I/O unit numbers in a single location for convenient access.

INTERFACE:

```
MODULE GCAP_READ_MOD
```

USES:

```
USE inquireMod, ONLY : findFreeLUN
USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

IMPLICIT NONE
PRIVATE
```

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: CHECK_TIME
PRIVATE :: READ_GCAP
PRIVATE :: GCAP_CHECK

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: GET_GCAP_FIELDS
PUBLIC :: OPEN_GCAP_FIELDS
PUBLIC :: UNZIP_GCAP_FIELDS

REVISION HISTORY:

```
(1 ) Adapted from the obsolete "phis_read_mod.f" (bmy, 2/1/06)
03 Aug 2012 - R. Yantosca - Move calls to findFreeLUN out of DEVEL block
06 Aug 2012 - R. Yantosca - Now make IU_PH a local variable
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
13 Nov 2014 - M. Yannetti - Added PRECISION_MOD
```

9.11.1 unzip_gcap_fields

Subroutine UNZIP_GCAP_FIELDS invokes a FORTRAN system call to uncompress GCAP PHIS met field files and store the uncompressed data in a temporary directory, where GEOS-CHEM can read them. The original data files are not disturbed.

INTERFACE:

SUBROUTINE UNZIP_GCAP_FIELDS(Input_Opt, OPTION)

USES:

USE BPCH2_MOD, ONLY : GET_RES_EXT

USE CMN_SIZE_MOD

USE Input_Opt_Mod, ONLY : ERROR_STOP
USE TIME_MOD. ONLY : OptInput
ONLY : OptInput ONLY : EXPAND_DATE

INPUT PARAMETERS:

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object CHARACTER(LEN=*), INTENT(IN) :: OPTION ! Unzipping option

REVISION HISTORY:

- 15 Jun 1998 R. Yantosca Initial version
- (1) Adapted from UNZIP_MET_FIELDS of "dao_read_mod.f" (bmy, 6/16/03)
- (2) Directory information YYYY/MM or YYYYMM is now contained w/in GEOS_1_DIR, GEOS_S_DIR, GEOS_3_DIR, GEOS_4_DIR (bmy, 12/11/03)
- (3) Now reference "directory_mod.f" and "unix_cmds_mod.f". Now prevent EXPAND_DATE from overwriting directory paths with Y/M/D tokens in them (bmy, 7/20/04)
- (4) Now modified for GEOS-5 and GCAP met fields (swu, bmy, 5/25/05)
- 06 Aug 2012 R. Yantosca Added ProTeX headers
- 11 Apr 2013 R. Yantosca Now pass fields via Input_Opt

9.11.2 open_gcap_fields

Subroutine OPEN_GCAP_FIELDS opens the PHIS and LWI met fields file.

INTERFACE:

SUBROUTINE OPEN_GCAP_FIELDS(Input_Opt)

USES:

USE ERROR_MOD, ONLY : GET_RES_EXT

USE ERROR_MOD, ONLY : ERROR_STOP

USE FILE_MOD, ONLY : IOERROR, FILE_EXISTS

USE Input_Opt_Mod, ONLY : OptInput

USE TIME_MOD, ONLY : FYDAND

INPUT PARAMETERS:

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

- 01 Feb 2006 S. Wu Initial version
- (1) Adapted from OPEN_MET_FIELDS of "dao_read_mod.f" (bmy, 6/13/03)
- (2) Now opens either zipped or unzipped files (bmy, 12/11/03)
- (3) Now skips past the GEOS-4 ident string (bmy, 12/12/04)
- (4) Now references "directory_mod.f" instead of CMN_SETUP. Also now references LUNZIP from "logical_mod.f". Also now prevents EXPAND_DATE from overwriting Y/M/D tokens in directory paths. (bmy, 7/20/04)
- (5) Now use FILE_EXISTS from "file_mod.f" to determine if file unit IU_PH refers to a valid file on disk (bmy, 3/23/05)
- (6) Now modified for GEOS-5 and GCAP met fields (swu, bmy, 5/25/05)
- 06 Aug 2012 R. Yantosca Move calls to findFreeLUN out of DEVEL block
- 06 Aug 2012 R. Yantosca Added ProTeX headers

9.11.3 get_gcap_fields

Subroutine GET_GCAP_FIELDS calls READ_GCAP to read GCAP fields from disk at the start of a GEOS-Chem run.

INTERFACE:

SUBROUTINE GET_GCAP_FIELDS(Input_Opt, State_Met)

USES:

USE Input_Opt_Mod, ONLY : OptInput
USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INPUT/OUTPUT PARAMETERS:

TYPE(MetState), INTENT(INOUT) :: State_Met ! Meteorology State object

REVISION HISTORY:

- 01 Feb 2006 S. Wu Initial version
- (1) Now also read LWI_GISS for GCAP met fields (swu, bmy, 5/25/05)
- 06 Aug 2012 R. Yantosca Added ProTeX headers
- 09 Nov 2012 M. Payer Copy all met fields to the State_Met derived type object

9.11.4 check_time

Function CHECK_TIME checks to see if the timestamp of the GCAP field just read from disk matches the current time. If so, then it's time to return the GCAP field to the calling program. (bmy, 6/16/03)

INTERFACE:

FUNCTION CHECK_TIME(XYMD, XHMS, NYMD, NHMS) RESULT(ITS_TIME)

USES:

USE CMN_SIZE_MOD

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: XYMD     ! Date stamp in file (YYYYMMDD)

INTEGER, INTENT(IN) :: XHMS     ! Time stamp in file (hhmmss)

INTEGER, INTENT(IN) :: NYMD     ! Current model date (YYYYMMDD)

INTEGER, INTENT(IN) :: NHMS     ! Current model time (hhmmss)
```

RETURN VALUE:

! Function value

LOGICAL :: ITS_TIME ! = T is time to return fields

REVISION HISTORY:

```
16 Jun 2003 - R. Yantosca - Initial version
06 Aug 2012 - R. Yantosca - Added ProTeX headers
```

9.11.5 read_gcap

Subroutine READ_GCAP reads the PHIS (surface geopotential heights) field from disk. PHIS is an I-6 field, but is time-independent. Thus READ_GCAP only needs to be called once at the beginning of the model run.

INTERFACE:

```
SUBROUTINE READ_GCAP( NYMD, NHMS, PHIS, LWI )
```

USES:

```
#if defined( BPCH_DIAG )
    USE CMN_DIAG_MOD ! ND67
    USE DIAG_MOD, ONLY : AD67
#endif
    USE CMN_SIZE_MOD
    USE FILE_MOD, ONLY : IOERROR
    USE PhysConstants ! g0
    USE TIME_MOD, ONLY : TIMESTAMP_STRING
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NYMD ! YYYYMMDD date
INTEGER, INTENT(IN) :: NHMS ! hhmmss time
```

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT) :: PHIS(IIPAR,JJPAR) ! PHIS [m2/s2] REAL(fp), INTENT(OUT), OPTIONAL :: LWI(IIPAR,JJPAR) ! LWI flags
```

REVISION HISTORY:

```
01 Feb 2006 - S. Wu - Initial version
```

- (1) Adapted from READ_PHIS from "dao_read_mod.f" (bmy, 6/16/03)
- (2) Now use function TIMESTAMP_STRING from "time_mod.f" for formatted date/time output. (bmy, 10/28/03)
- (3) Now also read LWI_GISS for GCAP met fields. Added optional variable LWI to the arg list. (swu, bmy, 5/25/05)
- 06 Aug 2012 R. Yantosca Added ProTeX headers
- 07 Aug 2012 R. Yantosca Now print LUN used to open file
- 06 Nov 2014 R. Yantosca Replace TRANSFER_2D with direct casts
- 02 Feb 2015 E. Lundgren Block out bpch diagnostics with if defined bpch

9.11.6 gcap_check

Subroutine GCAP_CHECK prints an error message if not all of the GCAP met fields are found. The run is also terminated.

INTERFACE:

```
SUBROUTINE GCAP_CHECK( NFOUND, N_PHIS )
```

USES:

```
USE ERROR_MOD, ONLY : GEOS_CHEM_STOP
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NFOUND   ! # of fields read from disk
INTEGER, INTENT(IN) :: N_PHIS   ! # of of fields expected to be found
```

REMARKS:

REVISION HISTORY:

```
15 Jun 1998 - R. Yantosca - Initial version
(1 ) Adapted from DAO_CHECK from "dao_read_mod.f" (bmy, 6/16/03)
06 Aug 2012 - R. Yantosca - Added ProTeX headers
```

10 Specialty simulation modules

These modules contain routines used by the GEOS-Chem "specialty" simulations.

10.1 Fortran: Module Interface c2h6_mod.F

Module C2H6_MOD contains variables and routines used for the tagged C2H6 (ethane) simulation. (xyp, qli, bmy, 7/28/01, 4/5/06)

INTERFACE:

MODULE C2H6_MOD

USES:

USE PRECISION_MOD
USE PhysConstants, ONLY : AVO

IMPLICIT NONE PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: GET_C2H6_ANTHRO

PUBLIC :: CHEMC2H6
PUBLIC :: CLEANUP_C2H6
PUBLIC :: INIT_C2H6

PRIVATE DATA MEMBERS:

PRIVATE :: NGASC2H6
PRIVATE :: FMOL_C2H6
PRIVATE :: XNUMOL_C2H6

REMARKS:

Setting LSPLIT = T in "input.geos" will run with the following tracers:

- (1) Total C2H6
- (2) C2H6 from biomass burning
- (3) C2H6 from biofuel burning
- (4) C2H6 from natural gas leaking/venting (e.g. "anthro" C2H6)

Setting LSPLIT = F in "input.geos" will run w/ the following tracers:

(1) Total C2H6

- (1) Eliminated obsolete code from 1/02 (bmy, 2/27/02)
- (2) Now divide module header into MODULE PRIVATE, MODULE VARIABLES, and MODULE ROUTINES sections. Updated comments (bmy, 5/28/02)
- (3) Now reference BXHEIGHT and T from "dao_mod.f". Also references "error_mod.f". Removed obsolete code. Now references F90 module tracerid_mod.f". (bmy, 11/15/02)
- (4) Now references "grid_mod.f" and the new "time_mod.f" (bmy, 2/11/03)
- (5) Now references "directory_mod.f", "logical_mod.f", and "tracer_mod.f". (bmy, 7/20/04)
- (6) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (7) Now modified

10.1.1 chemc2h6

Subroutine CHEMC2H6 performs C2H6 chemistry. Loss of C2H6 is via reaction with OH. (xyp, qli, bmy, 10/19/99, 7/20/04)

INTERFACE:

```
SUBROUTINE CHEMC2H6( am_I_Root, Input_Opt,
& State_Met, State_Chm, RC )
```

USES:

```
USE CMN_SIZE_MOD

USE ErrCode_Mod

USE Error_Mod, ONLY : Error_Stop

USE HCO_Interface_Mod, ONLY : HcoState

USE HCO_EmisList_Mod, ONLY : HCO_GetPtr

USE Input_Opt_Mod, ONLY : OptInput

USE State_Chm_Mod, ONLY : ChmState

USE State_Met_Mod, ONLY : MetState

USE TIME_MOD, ONLY : GET_MONTH, GET_TS_CHEM
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

- (1) Now do chemistry all the way to the model top.
- (2) Use monthly mean OH fields for oxidation -- reference the monthly mean OH array and the routine which reads it from disk in "global_oh_mod.f" (bmy, 1/25/02)
- (3) Now reference T from "dao_mod.f". Also make FIRSTCHEM a local SAVEd variable. (bmy, 11/15/02)
- (4) Now use functions GET_MONTH and GET_TS_CHEM from "time_mod.f".
- (5) Now reference STT & N_TRACERS from "tracer_mod.f". Now reference LSPLIT from "logical_mod.f" (bmy, 7/20/04)
- 22 Mar 2012 M. Payer Added ProTeX headers
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 25 Mar 2013 R. Yantosca Now accept am_I_Root, Input_Opt, State_Chm, RC
- 23 Oct 2013 R. Yantosca Now pass objects to GET_GLOBAL_OH routine
- 06 Nov 2014 M. Yannetti Converted REAL*8 to REAL(fp)
- 29 Apr 2016 R. Yantosca Don't initialize pointers in declaration stmts
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.
- 10 Aug 2016 R. Yantosca Removed temporary tracer-removal code

10.1.2 get_c2h6_anthro

Function GET_C2H6_ANTHRO returns the monthly average anthropogenic C2H6 emissions at GEOS-Chem grid box (I,J). Data will be returned in units of [atoms C/cm2/s].

INTERFACE:

```
FUNCTION GET_C2H6_ANTHRO( I, J, N ) RESULT( C2H6_ANTHRO )
```

USES:

```
USE CMN_SIZE_MOD
```

USE State_Chm_Mod, ONLY : Ind_

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: I ! GEOS-Chem longitude index
INTEGER, INTENT(IN) :: J ! GEOS-Chem latitude index
INTEGER, INTENT(IN) :: N ! GEOS-Chem tracer index

RETURN VALUE:

REAL(fp) :: C2H6_ANTHRO

REVISION HISTORY:

22 Mar 2012 - M. Payer - Initial version adapted from GET_RETRO_ANTHRO

10.1.3 init_c2h6

Subroutine INIT_C2H6 allocates and zeroes the NGASC2H6 array, which holds global monthly mean natural gas C2H6 emissions.

INTERFACE:

```
SUBROUTINE INIT_C2H6( am_I_Root, Input_Opt, RC )
```

USES:

```
USE CMN_SIZE_MOD
USE ErrCode_Mod
```

USE ERROR_MOD, ONLY : ALLOC_ERR
USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?!
```

REMARKS:

This routine is now called from GC_INIT_EXTRA (in GeosCore/input_mod.F).

REVISION HISTORY:

```
(1 ) Now references ALLOC_ERR from "error_mod.f" (bmy, 10/15/02)
22 Mar 2012 - M. Payer - Added ProTeX headers
11 Apr 2014 - R. Yantosca - Now accept am_I_Root, Input_Opt, RC arguments
```

10.1.4 cleanup_c2h6

Subroutine CLEANUP_C2H6 deallocates the natural gas C2H6 emission array.

INTERFACE:

```
SUBROUTINE CLEANUP_C2H6
```

```
22 Mar 2012 - M. Payer - Added ProTeX headers
```

10.2 Fortran: Module Interface co2_mod.F

Module CO2_MOD contains variables and routines used for the CO2 simulation. A tagged CO2 simulation capability has now been added.

References:

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- Sausen, R. and Schumann, U. "Estimates of the Climate Response to Aircraft CO2 and NOx Emissions Scenarios", Climate Change, 44: 27-58, 2000
- Wilkersen, J.T. et al. Analysis of emission data from global commercial Aviation: 2004 and 2006, Atmos. chem. Phys. Disc., 10, 2945-2983, 2010.

INTERFACE:

MODULE CO2_MOD

USES:

USE PhysConstants ! Physical constants

USE inquireMod, ONLY : findFreeLUN

USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

IMPLICIT NONE PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: CLEANUP_CO2
PUBLIC :: INIT_CO2
PUBLIC :: EMISSCO2

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: DEF_BIOSPH_CO2_REGIONS_F
PRIVATE :: DEF_OCEAN_CO2_REGIONS_F
PRIVATE :: DEF_FOSSIL_CO2_REGIONS_F

REMARKS:

- 16 Aug 2005 P. Suntharalingam Initial version
- (1) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (2) Now references biomass_mod.f (bmy, 9/27/06)
- (3) Tagged CO2 capability developed (dbj)
- (4) Implemented monthly and annual fossil fuel inventories

```
(R.Nassar 2009-03-10)
(5) Implemented CO2 emissions from shipping and aviation (R.Nassar 2010)
(6) Implemented monthly CO2 chemical production and surface correction (R.Nassar 2010)
25 Feb 2011 - R. Nassar - Now read updated CDIAC CO2 emissions data
O7 Sep 2011 - P. Kasibhatla - Modified to include GFED3
O1 Aug 2012 - R. Yantosca - Add reference to findFreeLUN from inqure_mod.F90
O3 Aug 2012 - R. Yantosca - Move calls to findFreeLUN out of DEVEL block
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
20 Jun 2014 - R. Yantosca - Remove obsolete emissions code; we now use HEMCO
O7 Nov 2014 - M. Yannetti - Added PRECISION_MOD
```

10.2.1 emissco2

Subroutine EMISSCO2 is the driver routine for CO2 emissions.

INTERFACE:

```
SUBROUTINE EMISSCO2( am_I_Root, Input_Opt,
& State_Met, State_Chm, RC )
```

USES:

```
USE CMN_SIZE_MOD
USE ErrCode_Mod
USE ERROR_MOD,
                       ONLY : ERROR_STOP
USE DIAGO4_MOD,
                       ONLY: ADO4, NDO4
USE DIAGO4_MOD,
                       ONLY : ADO4_plane,
                                             AD04_chem
USE HCO_INTERFACE_MOD, ONLY : HcoState
USE HCO_EmisList_Mod, ONLY : HCO_GetPtr
                    ONLY : HCO_GetHcoID
USE HCO_STATE_MOD,
USE Input_Opt_Mod,
                       ONLY : OptInput
USE State_Chm_Mod,
                       ONLY : ChmState
USE State_Met_Mod,
                       ONLY : MetState
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REMARKS:

The initial condition for CO2 has to be at least 50 ppm or higher or else the balanced biosphere fluxes will make STT negative. (pns, bmy, 8/16/05)

REVISION HISTORY:

- 16 Aug 2005 P. Suntharalingam Initial version
- (1) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (2) We now get CO2 biomass emissions from biomass_mod.f. This allows us to use either GFED2 or default Duncan et al biomass emissions. (bmy, 9/27/06)
- (3) Tagged tracer capability added. This requires the editable region files Regions_land.dat and Regions_ocean.dat in the run directory (rnassar,dbj, 2009)
- (4) New tracers for emissions from international and domestic shipping, international and domestic aviation, and the chemical CO2 source from the oxidation of CO, CH4, and other organics (rnassar,dbj, 2009)
- 01 Mar 2012 R. Yantosca Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 25 Mar 2013 R. Yantosca Now accept am_I_Root, Input_Opt, State_Chm, RC
- 27 Aug 2014 C. Keller Now interface with HEMCO.
- 13 Apr 2015 R. Nassar Some bug fixes for HEMCO implementation, e.g. unit fixes for aviation and chem source
- 11 Sep 2015 E. Lundgren Tracer units are now kg/kg dry air (prev kg)
- 29 Apr 2016 R. Yantosca Don't initialize pointers in declaration stmts
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

10.2.2 def_biosph_co2_regions_f

Subroutine DEF_BIOSPH_CO2_REGIONS defines the land biospheric and ocean CO2 exchange regions.

INTERFACE:

SUBROUTINE DEF_BIOSPH_CO2_REGIONS_F(REGION)

USES:

USE CMN_SIZE_MOD ! Size parameters

USE FILE_MOD, ONLY : IOERROR

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: REGION(IIPAR, JJPAR)

REMARKS:

REVISION HISTORY:

```
18 May 2010 - R. Nassar, D. Jones - Initial version
```

03 Aug 2012 - R. Yantosca - Move calls to findFreeLUN out of DEVEL block

13 Apr 2013 - R. Nassar - minor fixes to region boundary indices

10.2.3 def_ocean_co2_regions_f

Subroutine DEF_OCEAN_CO2_REGIONS defines CO2 regions for ocean exchange.

INTERFACE:

```
SUBROUTINE DEF_OCEAN_CO2_REGIONS_F( REGION )
```

USES:

USE CMN_SIZE_MOD ! Size parameters

USE FILE_MOD, ONLY : IOERROR

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: REGION(IIPAR, JJPAR)

REMARKS:

REVISION HISTORY:

```
18 May 2010 - R. Nassar, D. Jones - Initial version
```

03 Aug 2012 - R. Yantosca - Move calls to findFreeLUN out of DEVEL block

10.2.4 def_fossil_co2_regions_f

Subroutine DEF_FOSSIL_CO2_REGIONS defines CO2 regions for anthropogenic emissions

INTERFACE:

```
SUBROUTINE DEF_FOSSIL_CO2_REGIONS_F( REGION )
```

USES:

USE CMN_SIZE_MOD ! Size parameters

USE FILE_MOD, ONLY : IOERROR

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: REGION(IIPAR, JJPAR)

REMARKS:

REVISION HISTORY:

```
18 May 2010 - R. Nassar, D. Jones - Initial version
03 Aug 2012 - R. Yantosca - Move calls to findFreeLUN out of DEVEL block
```

10.2.5 init_co2

Subroutine INIT_CO2 allocates memory to module arrays and reads in annual mean emissions.

INTERFACE:

```
SUBROUTINE INIT_CO2( am_I_Root, Input_Opt, RC )
```

USES:

```
! References to F90 modules \,
```

USE CMN_SIZE_MOD

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ALLOC_ERR USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

```
16 Aug 2005 - P. Suntharalingam - Initial version
```

18 May 2010 - R. Nassar, D. Jones - Updated

25 Mar 2013 - R. Yantosca - Now use logical fields from Input_Opt

10.2.6 cleanup_co2

Subroutine CLEANUP_CO2 deallocates all module arrays.

INTERFACE:

SUBROUTINE CLEANUP_CO2

REVISION HISTORY:

```
16 Aug 2005 - P. Suntharalingam - Initial version
18 May 2010 - R. Nassar, D. Jones - Updated
```

10.3 Fortran: Module Interface exchange_mod.F90

Module EXCHANGE_MOD contains variables and routines which are used to exchange data between two or more runs (Global Domain and Nested Domains), thus to combine them into TWO-WAY nested run. (yanyy, 6/18/14)

INTERFACE:

MODULE EXCHANGE_MOD

USES:

```
IMPLICIT NONE
PRIVATE
!PUBLIC MEMBER FUNCTIONS
```

PUBLIC :: EXCHANGE_GLOBAL_INIT
PUBLIC :: EXCHANGE_NESTED_INIT
PUBLIC :: EXCHANGE_GLOBAL_POST
PUBLIC :: EXCHANGE_NESTED_PRE
PUBLIC :: EXCHANGE_NESTED_POST
PUBLIC :: ITS_TIME_FOR_EXCHANGE

PUBLIC :: INIT_EXCHANGE
PUBLIC :: CLEANUP_EXCHANGE

PRIVATE MEMBER FUNCTIONS:

REMARKS:

```
Loop-----
     /----
  | phony_ex_global_pre
  | \----
        GEOSCHEM STUFF
     /----
     dump for nested
        done lock
                    wait for unlock
                     read LBCs ex_nested_pre
                      (regridded down) | apply LBCs |
  | ex_global_post
                          ----/
                      GEOSCHEM STUFF
                           ----\
                       dump for global(regridded up)
                                ex_nested_post
                      done lock
    | wait for unlock
                       ----/
     read & apply feedback
```

REVISION HISTORY:

- 30 Mar 2014 Y.Y. Yan Initial Version
- (1) Establish the frame of the data exchange between models (kuangye, yanyy, 6/10/12)
- (2) Now update for version 9-02 (yanyy, 6/21/14)
- 06 Jan 2015 R. Yantosca Added ProTeX headers

10.3.1 exchange_global_init

Global initialization for exchange

INTERFACE:

SUBROUTINE EXCHANGE_GLOBAL_INIT()

REVISION HISTORY:

10.3.2 exchange_nested_init

Nested initialization for exchange

INTERFACE:

```
SUBROUTINE EXCHANGE_NESTED_INIT()
```

REVISION HISTORY:

```
06 Jan 2015 - R. Yantosca - Added ProTeX headers
```

10.3.3 exchange_global_post

Carry out the process to communicate the nested simulated results back to global model.

INTERFACE:

```
SUBROUTINE EXCHANGE_GLOBAL_POST( am_I_Root, Input_Opt,
&
                                  State_Met, State_Chm, RC )
```

```
USES:
        USE CMN_SIZE_MOD
                                             ! Size parameters
        USE DAO_MOD
        USE ErrCode_Mod
        USE ERROR_MOD, ONLY : GC_Error
USE Input_Opt_Mod, ONLY : OptInput
USE State Chm Mod. ONLY : ChmState
        USE State_Chm_Mod,
                                      ONLY : ChmState
                                      ONLY : MetState
        USE State_Met_Mod,
        USE TPCORE_BC_MOD
        USE UnitConv_Mod
```

INPUT PARAMETERS:

```
LOGICAL,
               INTENT(IN)
                          :: am_I_Root
TYPE(OptInput), INTENT(IN) :: Input_Opt
                            :: State_Met
TYPE(MetState), INTENT(IN)
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm
```

OUTPUT PARAMETERS:

```
INTEGER,
               INTENT(OUT) :: RC
```

REMARKS:

```
06 Jan 2015 - R. Yantosca - Added ProTeX headers
13 Aut 2015 - E. Lundgren - Now input tracer conc in kg/kg not v/v.
```

10.3.4 exchange_nested_pre

Before nested grid exchange

INTERFACE:

SUBROUTINE EXCHANGE_NESTED_PRE()

REVISION HISTORY:

06 Jan 2015 - R. Yantosca - Added ProTeX headers

10.3.5 exchange_nested_post

After nested-grid exchange

INTERFACE:

```
SUBROUTINE EXCHANGE_NESTED_POST( am_I_Root, Input_Opt, State_Met, State_Chm, RC )
```

USES:

```
USE CMN_SIZE_MOD ! Size parameters
```

USE DAO_MOD

USE ErrCode_Mod

USE ERROR_MOD, ONLY : GC_Error
USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState

USE UnitConv_Mod

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root
TYPE(OptInput), INTENT(IN) :: Input_Opt
TYPE(MetState), INTENT(IN) :: State_Met
```

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC

RETURN VALUE:

REMARKS:

```
06 Jan 2015 - R. Yantosca - Added ProTeX headers
13 Aug 2015 - E. Lundgren - Input tracer conc in kg/kg not v/v
```

10.3.6 its_time_for_exchange

Returns TRUE if it's time to do the 2-way exchange of data.

INTERFACE:

FUNCTION ITS_TIME_FOR_EXCHANGE()

USES:

USE TIME_MOD, ONLY : ITS_TIME_FOR_EXCH

RETURN VALUE:

LOGICAL :: ITS_TIME_FOR_EXCHANGE

REVISION HISTORY:

06 Jan 2015 - R. Yantosca - Added ProTeX headers

10.3.7 init_exchange

Initialization routine.

INTERFACE:

SUBROUTINE INIT_EXCHANGE(am_I_Root)

USES:

USE CMN_SIZE_MOD ! Size parameters USE ERROR_MOD

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root

REVISION HISTORY:

06 Jan 2015 - R. Yantosca - Now only print output on the root CPU

06 Jan 2015 - R. Yantosca - Added ProTeX headers

24 Mar 2015 - E. Lundgren - Remove tracer_mod dependency since unused

10.3.8 cleanup_exchange

Cleanup routine.

INTERFACE:

SUBROUTINE CLEANUP_EXCHANGE(am_I_Root)

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root
```

REVISION HISTORY:

```
06 Jan 2015 - R. Yantosca - Now only write output on the root CPU 06 Jan 2015 - R. Yantosca - Added ProTeX headers
```

10.3.9 ex_dump_for_global

?

INTERFACE:

```
SUBROUTINE EX_DUMP_FOR_GLOBAL( am_I_Root, Input_Opt, & State_Met, State_Chm, RC )
```

USES:

USE CMN_SIZE_MOD ! Size parameters

USE ERROR_MOD

USE Input_Opt_Mod, ONLY: OptInput
USE State_Chm_Mod, ONLY: ChmState
USE State_Met_Mod, ONLY: MetState

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root
TYPE(OptInput), INTENT(IN) :: Input_Opt
TYPE(MetState), INTENT(IN) :: State_Met

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC

REVISION HISTORY:

```
06 Jan 2015 - R. Yantosca - Added ProTeX headers
06 Jun 2016 - M. Sulprizio- Replace NTSPEC with State_Chm%nSpecies
15 Aug 2016 - E. Lundgren - Replace tracers with species
```

10.3.10 ex_read_and_apply_feedback

?

INTERFACE:

USES:

USE CMN_SIZE_MOD ! Size parameters

USE ERROR_MOD

USE Input_Opt_Mod, ONLY : OptInput USE State_Chm_Mod, ONLY : ChmState USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root
TYPE(OptInput), INTENT(IN) :: Input_Opt
TYPE(MetState), INTENT(IN) :: State_Met
INTEGER, INTENT(IN) :: DOMAIN

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC

REVISION HISTORY:

```
06 Jan 2015 - R. Yantosca - Now get LPRT from Input_Opt
06 Jan 2015 - R. Yantosca - Added ProTeX headers
24 Mar 2015 - E. Lundgren - Remove tracer_mod dependency since not used
06 Jun 2016 - M. Sulprizio- Replace NTSPEC with State_Chm%nSpecies
15 Aug 2016 - E. Lundgren - Replace tracers with species
```

$10.3.11 \text{ ex_regrid_up}$

This subroutine will be called within EX_DUMP_FOR_GLOBAL, Using module's global vars: REGRID_MAT_L, REGRID_MAT_R

INTERFACE:

```
SUBROUTINE EX_REGRID_UP( NX_ORIG, NY_ORIG, NX_NEW, NY_NEW, NZ, ORIG_ARRAY, NEW_ARRAY)
```

REVISION HISTORY:

10.3.12 ex_convert_units_cspec

Converts molec/cm3/box to fakemass (e.g. convert especfull to a masslike unit)

INTERFACE:

```
SUBROUTINE EX_CONVERT_UNITS_CSPEC( am_I_Root, Input_Opt, & State_Met, State_Chm, RC, FLAG, NX, NY, NZ)
```

USES:

```
USE CMN_SIZE_MOD ! Size parameters
```

USE DAO_MOD

USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root
TYPE(OptInput), INTENT(IN) :: Input_Opt
TYPE(MetState), INTENT(IN) :: State_Met

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC

RETURN VALUE:

REMARKS:

REVISION HISTORY:

```
06 Jan 2015 - R. Yantosca - Added ProTeX headers
06 Jun 2016 - M. Sulprizio- Replace NTSPEC with State_Chm%nSpecies
```

10.3.13 wait_for_unlock

Waits for MPI unlock.

INTERFACE:

SUBROUTINE WAIT_FOR_UNLOCK()

REVISION HISTORY:

10.3.14 done_lock_me_up

?

INTERFACE:

SUBROUTINE DONE_LOCK_ME_UP()

REVISION HISTORY:

06 Jan 2015 - R. Yantosca - Added ProTeX headers

10.3.15 no_more_lock

?

INTERFACE:

SUBROUTINE NO_MORE_LOCK()

REVISION HISTORY:

06 Jan 2015 - R. Yantosca - Added ProTeX headers

10.3.16 alert_for_kill_command

Stops if there is a kill command issued.

INTERFACE:

SUBROUTINE ALERT_FOR_KILL_COMMAND()

USES:

USE ERROR_MOD

REVISION HISTORY:

06 Jan 2015 - R. Yantosca - Added ProTeX headers

10.3.17 touch_file

Touches a file (i.e. updates the timestamp on disk).

INTERFACE:

SUBROUTINE TOUCH_FILE(FNAME)

INPUT PARAMETERS:

CHARACTER(LEN=*), INTENT(IN) :: FNAME

REVISION HISTORY:

10.3.18 open_bin_file_for_read

Opens a binary file for reading.

INTERFACE:

SUBROUTINE OPEN_BIN_FILE_FOR_READ(FNAME)

USES:

USE FILE_MOD

REVISION HISTORY:

06 Jan 2015 - R. Yantosca - Added ProTeX headers

10.3.19 open_bin_file_for_write

Opens a binary file for writing.

INTERFACE:

SUBROUTINE OPEN_BIN_FILE_FOR_WRITE(FNAME)

USES:

USE FILE_MOD

INPUT PARAMETERS:

CHARACTER(LEN=*), INTENT(IN) :: FNAME

REVISION HISTORY:

06 Jan 2015 - R. Yantosca - Added ProTeX headers

10.3.20 open_bin_file_for_append

Opens a binary file for appending.

INTERFACE:

SUBROUTINE OPEN_BIN_FILE_FOR_APPEND(FNAME)

USES:

USE FILE_MOD

INPUT PARAMETERS:

CHARACTER(LEN=*), INTENT(IN) :: FNAME

REVISION HISTORY:

06 Jan 2015 - R. Yantosca - Added ProTeX headers

10.3.21 close_bin_file

Closes a binary file.

INTERFACE:

SUBROUTINE CLOSE_BIN_FILE()

REVISION HISTORY:

06 Jan 2015 - R. Yantosca - Added ProTeX headers

10.3.22 write_3d_real8_array

Writes data to a 3-D REAL*8 array.

INTERFACE:

SUBROUTINE WRITE_3D_REAL8_ARRAY(NI, NJ, NK, ARRAY)

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: NI, NJ, NK

REAL*8, INTENT(IN) :: ARRAY(NI,NJ,NK)

REVISION HISTORY:

06 Jan 2015 - R. Yantosca - Added ProTeX headers

10.3.23 read_3d_real8_array

Reads data from 3-D REAL*8 array.

INTERFACE:

SUBROUTINE READ_3D_REAL8_ARRAY(NI, NJ, NK, ARRAY)

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: NI, NJ, NK

OUTPUT PARAMETERS:

REAL*8, INTENT(OUT) :: ARRAY(NI,NJ,NK)

REVISION HISTORY:

06 Jan 2015 - R. Yantosca - Added ProTeX headers

10.3.24 gen_regrid_mat

Regridding utility.

INTERFACE:

SUBROUTINE GEN_REGRID_MAT(N1, N2, RATIO, OFFSET, RES)

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: N1, N2

REAL*8, INTENT(IN) :: RATIO, OFFSET

OUTPUT PARAMETERS:

REAL*8, INTENT(OUT) :: RES(N1, N2)

REMARKS:

REVISION HISTORY:

06 Jan 2015 - R. Yantosca - Added ProTeX headers

10.4 Fortran: Module Interface global_ch4_mod.F

Module GLOBAL_CH4_MOD contains variables and routines for simulating CH4 chemistry in the troposphere.

INTERFACE:

MODULE GLOBAL_CH4_MOD

USES:

USE HCO_ERROR_MOD ! For HEMCO error reporting

USE PhysConstants, ONLY : AVO, AIRMW

USE PRECISION_MOD ! For GEOS-Chem Precision (fp, f4, f8)

IMPLICIT NONE

PRIVATE

%%% Normally we will not save out the CH4_BUDGET diagnostics (esp. when

%% using the nested grid simulations) in order to save memory. If you

%%% want to use CH4_BUDGET, then uncomment the following line of code:

%%% (kjw, bmy, 2/12/14)

#define USE_CH4_BUDGET_DIAG 1

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: CH4_AVGTP
PUBLIC :: EMISSCH4
PUBLIC :: CHEMCH4

PUBLIC :: INIT_GLOBAL_CH4
PUBLIC :: CLEANUP_GLOBAL_CH4

PUBLIC DATA MEMBERS:

- 17 Jan 2001- J. Wang, B. Duncan, R. Yantosca -- Initial version
- (2) XNUMOL_CH4 and TCH4 have to be public all other variables can be made private, so as not to conflict with other common-block definitions (bmy, 1/17/01)
- (3) Minor fixes from jsw added (jsw, bmy, 2/17/01)
- (4) Removed some F90 module references from EMISSCH4 (bmy, 3/20/01)
- (5) Eliminate obsolete commented-out code (bmy, 4/20/01)
- (6) Updated comments (bmy, 9/4/01)
- (7) Fixes for binary punch file in READ_COPROD (bmy, 9/26/01)
- (8) Removed obsolete code from READ_COPROD (bmy, 10/24/01)
- (9) Minor bug fixes for compilation on ALPHA (bmy, 11/15/01)
- (10) Eliminate obsolete code from 11/01 (bmy, 2/27/02)
- (11) Now eliminate PS from the arg list to CH4_AVGTP (4/11/02)
- (12) Now divide module header into MODULE PRIVATE, MODULE VARIABLES, and MODULE ROUTINES sections. Updated comments (bmy, 5/28/02)
- (13) Replaced all instances of IM with IIPAR and JM with JJPAR, in order to prevent namespace confusion for the new TPCORE (bmy, 6/25/02)
- (14) Now reference "file_mod.f". Also removed obsolete code. (bmy, 6/27/02)
- (15) Now references "pressure_mod.f" (bmy, 8/21/02)
- (16) Now reference AD and T from "dao_mod.f". Now reference "error_mod.f". Remove obsolete code from various routines. Remove reference to header file "comtrid.h" -- it's not used. (bmy, 11/6/02)
- (17) Minor bug fix in FORMAT statements (bmy, 3/23/03)
- (18) Now references "grid_mod.f" and "time_mod.f" (bmy, 3/27/03)
- (19) Updates to GET_GLOBAL_CH4 (bmy, 7/1/03)
- (20) Now references "directory_mod.f", "tracer_mod.f", and "diag_oh_mod.f"

```
(bmy, 7/20/04)
```

(21) Now can read data for both GEOS and GCAP grids (bmy, 8/16/05) (22) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05) (23) Updated CH4 simulation (kjw, cph, ccarouge, 10/1/09) (24) Added modifications for MERRA (bmy, 8/13/10) 08 Feb 2012 - R. Yantosca - Added modifications for GEOS-5.7.x 01 Mar 2012 - R. Yantosca - Now reference new grid_mod.F90 07 Mar 2012 - M. Payer - Added ProTeX headers 01 Aug 2012 - R. Yantosca - Add reference to findFreeLUN from inqure_mod.F90 03 Aug 2012 - R. Yantosca - Move calls to findFreeLUN out of DEVEL block 20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete 12 Feb 2014 - K. Wecht - Add modifications for 0.25 x 0.3125 NA grid 12 Feb 2014 - K. Wecht - Disable CH4 budget diagnostic (bracket the code out with #ifdef blocks so it can be used) 20 Jun 2014 - R. Yantosca - Remove obsolete emissions code; we now use HEMCO 09 Sep 2014 - C. Keller - Implemented HEMCO for emissions. 16 Sep 2014 - C. Keller - Now also get chemical fields (OH and CH4 prod) through HEMCO. Removed READ_COPROD and READ_CH4LOSS (now obsolete) 16 Sep 2014 - C. Keller - Removed all references to Clarisa's OH climatology (not used anywhere) 14 Nov 2014 - M. Yannetti - Added PRECISION_MOD 04 Mar 2015 - R. Yantosca - Now use REAL(f4) for HCO_GetPtr pointer args 06 Jan 2016 - E. Lundgren - Use global physical parameters 16 Jun 2016 - M. Sulprizio- Now define IDTCH4 locally 20 Jun 2016 - R. Yantosca - Rename IDTCH4 to id_CH4 for consistency 29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90

DEFINED PARAMETERS:

BOC

! Module Variables: ! N_CH4 : Number of budget items in TCH4 ! BAIRDENS : Array for air density [molec/cm3] ! BOH : Array for OH values [kg/m3] : Array for zonal mean P(CO) ! COPROD [v/v/s]! CH4LOSS : Array for monthly average CH4 loss freq [1/s]: Array for 24-h avg surface pressure [mb] ! PAVG ! TAVG : Array for 24-h avg temperature [K] ! TCH4 : Array for CH4 budget (N_CH4 items) [molec/box] ! FMOL_CH4 : Molecular weight of CH4 [kg/mole] ! XNUMOL_CH4 : Molecules CH4 / kg CH4 [molec/kg] : Array for CH4 Emissions ! CH4_EMIS [kg/m2/s]**|-----**

[!] Number of CH4 budget types

```
INTEGER, PARAMETER :: N_CH4
                                      = 12
      REAL(fp), PARAMETER :: XNUMOL_OH = AVO / 17e-3_fp ! molec OH / kg OH
                                                       ! hard-coded MW
      REAL(fp), PARAMETER :: CM3PERM3 = 1.e+6_fp
LOCAL VARIABLES:
      ! Species ID flag
      INTEGER
                         :: id_CH4
      ! Various arrays
      REAL(fp), ALLOCATABLE :: BAIRDENS(:,:,:)
      REAL(fp), ALLOCATABLE :: PAVG(:,:,:)
      REAL(fp), ALLOCATABLE :: TAVG(:,:,:)
      ! Pointers to fields in the HEMCO data structure.
      ! These need to be declared as REAL(f4), aka REAL*4.
      ! NOTE: These are globally SAVEd variables so we can
      ! nullify these in the declaration statement (bmy, 4/29/16)
                                    (:,:,:) => NULL()
      REAL(f4), POINTER :: BOH
                        :: CH4LOSS(:,:,:) => NULL()
      REAL(f4), POINTER
      ! Online CH4 only
      REAL(fp), ALLOCATABLE :: SUMANTHRO(:,:)
      REAL(fp), ALLOCATABLE :: SUMBIOG(:,:)
      REAL(fp)
                   :: TROPOCH4
      CONTAINS
 EOC
                  GEOS-Chem Global Chemical Transport Model
\mbox{}\hrulefill\
 \subsubsection [ch4\_avgtp] {ch4\_avgtp}
 Subroutine CH4\_AVGTP gets the 24-h average surface pressure
   and temperature needed for the CH4 simulation. (jsw, bnd, bmy, 1/16/01,
   7/20/04)
 \\{\bf INTERFACE:}
\begin{verbatim} SUBROUTINE CH4_AVGTP( State_Met )
USES:
```

```
USE CMN_SIZE_MOD
                                      ! Size parameters
USE ERROR_MOD, ONLY : GEOS_CHEM_STOP
USE State_Met_Mod, ONLY : MetState
```

USE TIME_MOD, ONLY : GET_TS_DYN, GET_TS_CHEM

USE TIME_MOD, ONLY : GET_ELAPSED_MIN

INPUT PARAMETERS:

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

REVISION HISTORY:

- (1) Created by Bryan Duncan (1/99). Adapted for CH4 chemistry and placed into module "global_ch4_mod.f" by Bob Yantosca. (bmy, 1/16/01)
- (2) CH4_AVGTP is independent of "CMN_OH", "CMN_CO", and "CMN_CO_BUDGET". (bmy, 1/16/01)
- (3) Removed duplicate definition for NTDT, NMIN (bmy, 11/15/01)
- (4) Removed PS from argument list. Now use P(I,J)+PTOP instead of PS, this ensures that we have consistency between P and AD. (bmy, 4/11/02)
- (5) Removed obsolete code (bmy, 6/27/02)
- (6) Now uses GET_PCENTER from "pressure_mod.f" to return the pressure at the midpoint of the box (I,J,L). Also added parallel DO-loops. Updated comments. (dsa, bdf, bmy, 8/21/02)
- (7) Now reference T from "dao_mod.f". Now reference GEOS_CHEM_STOP from "error_mod.f" (bmy, 10/15/02)
- (8) Removed NTDT, NMIN from the arg list. Now uses functions GET_TS_DYN, GET_TS_CHEM, and GET_ELAPSED_MIN from "time_mod.f" (bmy, 3/27/03)
- (9) Remove reference to CMN, it's not needed (bmy, 7/20/04)
- 07 Mar 2012 M. Payer Added ProTeX headers
- 09 Nov 2012 M. Payer - Replaced all met field arrays with State_Met derived type object
- 17 Sep 2014 C. Keller Removed legacy code (unused variables).
- 26 Feb 2015 E. Lundgren Replace GET_PCENTER with State_Met%PMID and remove dependency on pressure_mod
- 01 Apr 2015 E. Lundgren Change State_Met%PMID to State_Met%PMID_DRY

10.4.1 emissch4

Subroutine EMISSCH4 places emissions of CH4 [kg] into the chemical species array.

INTERFACE:

```
SUBROUTINE EMISSCH4( am_I_Root, Input_Opt,
                     State_Met, RC )
```

USES:

USE CMN_DIAG_MOD USE CMN_SIZE_MOD

ONLY : AD58 USE DIAG_MOD,

USE HCO_INTERFACE_MOD, ONLY : HcoState, GetHcoDiagn

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP
USE GC_GRID_MOD, ONLY : GET_XOFFSET, GET_YOFFSET
USE HCO_STATE_MOD, ONLY : HCO_STATE
USE Input_Opt_Mod, ONLY : OptInput USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

LOGICAL. INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

WARNING: Soil absorption has to be the 11th field in CH4_EMIS

- (1) Created by Bryan Duncan (1/99). Adapted for CH4 chemistry by James Wang (7/00). Inserted into module "global_ch4_mod.f" by Bob Yantosca. (bmy, 1/16/01)
- (2) EMISSCH4 is independent of "CMN_OH", "CMN_CO", and "CMN_CO_BUDGET". (bmy, 1/16/01)
- (3) GLOBASEAEMIS, GLOBSEAEMIS are diagnostics by jsw.
- (4) Do not multiply CO emissions by 1.28 anymore (jsw, bmy, 2/12/01)
- (5) Renamed input files to CH4_monthly.geos.{RES} and CH4_aseasonal.geos.{RES}. (bmy, 2/12/01)
- (6) Add reference to "CMN_SETUP" for the DATA_DIR variable (bmy, 2/13/01)
- (7) Removed references to "biofuel_mod.f" and "biomass_mod.f"; these weren't necessary (bmy, 3/20/01)
- (8) Now reference IU_FILE and IOERROR from "file_mod.f". Now use IU_FILE instead of IUNIT as the file unit #. (bmy, 6/27/02)
- (9) Now reference BXHEIGHT and SUNCOS from "dao_mod.f". Remove reference to header file "comtrid.h" -- it's not used. Make FIRSTEMISS a local SAVEd variable. Also use MONTH from "CMN" instead of the variable LMN. (bmy, 11/15/02)
- (10) Now replace DXYP(JREF)*1d4 with routine GET_AREA_CM2 of "grid_mod.f". Now use function GET_MONTH and GET_TS_EMIS from "time_mod.f". Now use functions GET_XOFFSET and GET_YOFFSET from "grid_mod.f". IO and JO are now local variables. (bmy, 3/27/03)

```
(11) Now reference STT from "tracer_mod.f". Now reference DATA_DIR from
        "directory_mod.f". (bmy, 7/20/04)
(12) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
(13) Add non-local PBL capability (ccc, 8/31/09)
01 Mar 2012 - R. Yantosca - Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
07 Mar 2012 - M. Payer - Added ProTeX headers
25 Mar 2013 - R. Yantosca - Now accept am_I_Root, Input_Opt, State_Chm, RC
11 Apr 2014 - R. Yantosca - Remove call to INIT_GLOBAL_CH4
09 Sep 2014 - C. Keller - Implemented HEMCO
11 Sep 2015 - E. Lundgren - Remove area-dependency (except for global mass sums) by outputting diagnostics as kg/m2 not kg
11 Sep 2015 - E. Lundgren - Remove State_Chm from arg list since not used
```

10.4.2 chemch4

Subroutine CHEMCH4 computes the chemical loss of CH4 (sources - sinks). (jsw, bnd, bmy, 6/8/00, 10/3/05)

INTERFACE:

```
SUBROUTINE CHEMCH4( am_I_Root, Input_Opt, State_Met, State_Chm, RC )
```

USES:

```
USE CHEMGRID_MOD,
                       ONLY : ITS_IN_THE_CHEMGRID
USE CMN_DIAG_MOD
USE CMN_SIZE_MOD
USE DIAG_MOD,
                       ONLY: AD43
USE ErrCode_Mod
USE ERROR_MOD,
                       ONLY: GEOS_CHEM_STOP, ERROR_STOP
USE ERROR_MOD,
                       ONLY : IT_IS_NAN, IT_IS_FINITE
USE HCO_INTERFACE_MOD, ONLY : HcoState
USE HCO_EMISLIST_MOD,
                       ONLY : HCO_GetPtr
USE Input_Opt_Mod,
                       ONLY : OptInput
USE State_Chm_Mod,
                       ONLY : ChmState
USE State_Met_Mod,
                       ONLY : MetState
USE TIME_MOD,
                       ONLY : GET_DAY,
                                         GET_MONTH
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

CH4 SOURCES

- (1) Oxidation of methane, isoprene and monoterpenes (SRCO_fromHCs).
- (2) Direct emissions of CO from fossil fuel combustion, biomass burning and wood (for fuel) burning (SR SETEMIS).
- (3) Emissions.

CH4 SINKS:

- (1) Removal of CO by OH (SR OHparam & CO_decay).
- (2) CO uptake by soils (neglected).
- (3) Transport of CO to stratosphere from troposphere (in dynamical subroutines).
- (4) Removal by OH (Clarissa's OH--climatol_OH.f and CO_decay.f)
- (5) Transport of CH4 between troposphere and stratosphere, and destruction in strat (CH4_strat.f).

- (1) Created by Bryan Duncan (1/99). Adapted for CH4 chemistry by James Wang (6/8/00). Inserted into module "global_ch4_mod.f" by Bob Yantosca. (bmy, 1/16/01)
- (2) CHEMCH4 is independent of "CMN_OH", "CMN_CO", and "CMN_CO_BUDGET". (bmy, 1/16/01)
- (3) Updated comments (jsw, bmy, 2/12/01)
- (4) LD43 is already declared in CMN_DIAG; don't redefine it (bmy, 11/15/01)
- (5) Replaced all instances of IM with IIPAR and JM with JJPAR, in order to prevent namespace confusion for the new TPCORE (bmy, 6/25/02)
- (6) Now reference AD from "dao_mod.f". Now reference GEOS_CHEM_STOP from "error_mod.f" Now make FIRSTCHEM a local SAVEd variable. Now reference ALBD from "dao_mod.f". Now use MONTH and JDATE from "CMN" instead of LMN and LDY. (bmy, 11/15/02)
- (7) Remove NYMDb, NYMDe from the arg list. Now use functions GET_MONTH, GET_NYMDb, GET_NYMDe, GET_MONTH, GET_DAY from the new "time_mod.f" (bmy, 3/27/03)
- (8) Now reference DATA_DIR from "directory_mod.f" (bmy, 7/20/04)
- (9) Remove reference to BPCH2_MOD, it's not needed (bmy, 10/3/05)
- 07 Mar 2012 M. Payer Added ProTeX headers
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 25 Mar 2013 R. Yantosca Now accept am_I_Root, Input_Opt, State_Chm, RC
- 23 Oct 2013 R. Yantosca Now pass objects to GET_GLOBAL_OH routine
- 12 Feb 2014 K. Wecht Disable CH4 budget diagnostic (bracket the

```
code out with #ifdef blocks so it can be used)

23 Jul 2014 - R. Yantosca - Remove reference to obsolete CMN_mod.F

23 Jul 2014 - R. Yantosca - Reference ITS_IN_THE_CHEMGRID (chemgrid_mod.F)

24 Jul 2014 - R. Yantosca - Now compute BOXVL internally

17 Sep 2014 - C. Keller - Now use HEMCO to get CH4 loss and OH conc. field.

06 Jan 2016 - E. Lundgren - Use global physical parameters

30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

10 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code
```

10.4.3 ch4_decay

Subroutine CH4_DECAY calculates the decay rate of CH4 by OH. OH is the only sink for CH4 considered here. (jsw, bnd, bmy, 1/16/01, 7/20/04)

INTERFACE:

```
SUBROUTINE CH4_DECAY( State_Met, State_Chm )
```

USES:

```
USE CMN_DIAG_MOD

USE CMN_SIZE_MOD

USE CHEMGRID_MOD, ONLY : ITS_IN_THE_CHEMGRID

USE DIAG_MOD, ONLY : AD19

USE State_Chm_Mod, ONLY : ChmState

USE State_Met_Mod, ONLY : MetState

USE TIME_MOD, ONLY : GET_TS_CHEM, ITS_A_NEW_YEAR

USE TIME_MOD, ONLY : GET_MONTH
```

INPUT PARAMETERS:

```
TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

REMARKS:

We now use function ITS_IN_THE_CHEMGRID from chemgrid_mod.F to diagnose if box (I,J,L) is in the troposphere or stratosphere.

```
Monthly loss of CH4 is summed in TCH4(3)
TCH4(3) = CH4 sink by OH
```

- (1) Created by Bryan Duncan (1/99). Adapted for CH4 chemistry by James Wang (7/00). Inserted into module "global_ch4_mod.f" by Bob Yantosca. (bmy, 1/16/01) (2) CH4_DECAY is independent of "CMN_OH", "CMN_CO", and "CMN_CO_BUDGET". (bmy, 1/16/01)(3) Now use function GET_TS_CHEM from "time_mod.f" (bmy, 3/27/03) (4) Now references STT from "tracer_mod.f" (bmy, 7/20/04) 07 Mar 2012 - M. Payer - Added ProTeX headers
- 09 Nov 2012 M. Payer - Replaced all met field arrays with State_Met derived type object 12 Feb 2014 - K. Wecht - Disable CH4 budget diagnostic (bracket the
- code out with #ifdef blocks so it can be used)
- 24 Jul 2014 R. Yantosca Now compute BOXVL internally
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

10.4.4 ch4_ohsave

Subroutine CH4_OHSAVE archives the CH3CCl3 lifetime from the OH used in the CH4 simulation. (bnd, jsw, bmy, 1/16/01, 7/20/04)

INTERFACE:

SUBROUTINE CH4_OHSAVE(State_Met, State_Chm)

USES:

```
USE CHEMGRID_MOD,
                      ONLY : ITS_IN_THE_CHEMGRID
USE CMN_SIZE_MOD
USE DIAG_OH_MOD,
                      ONLY: DO_DIAG_OH_CH4
USE GC_GRID_MOD,
                      ONLY : GET_AREA_CM2
USE State_Chm_Mod,
                     ONLY : ChmState
USE State_Met_Mod,
                      ONLY : MetState
USE TIME_MOD,
                      ONLY : GET_MONTH
```

INPUT PARAMETERS:

```
TYPE(MetState), INTENT(IN) :: State_Met
                                         ! Meteorology State object
TYPE(ChmState), INTENT(IN) :: State_Chm
                                         ! Chemistry State object
```

REMARKS:

We now use function ITS_IN_THE_CHEMGRID from chemgrid_mod.F to diagnose if box (I,J,L) is in the troposphere or stratosphere.

```
(1 ) Created by Bryan Duncan (1/99). Adapted for CH4 chemistry by
James Wang (7/00). Inserted into module "global_ch4_mod.f"
by Bob Yantosca. (bmy, 1/16/01)
```

- (2) CH4_OHSAVE is independent of "CMN_OH", "CMN_CO", and "CMN_CO_BUDGET". (bmy, 1/16/01)
- (3) Now call DO_DIAG_OH_CH4 to pass OH diagnostic info to the "diag_oh_mod.f" (bmy, 7/20/04)
- 07 Mar 2012 M. Payer Added ProTeX headers
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 24 Jul 2014 R. Yantosca Now compute BOXVL internally
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

10.4.5 ch4_strat

Subroutine CH4_STRAT calculates uses production rates for CH4 to calculate loss of CH4 in above the tropopause. (jsw, bnd, bmy, 1/16/01, 7/20/04)

INTERFACE:

```
SUBROUTINE CH4_STRAT( am_I_Root, Input_Opt,
& State_Met, State_Chm, RC )
```

USES:

```
USE CMN_SIZE_MOD
USE CHEMGRID_MOD,
                       ONLY : GET_MIN_TPAUSE_LEVEL
USE CHEMGRID_MOD,
                       ONLY : ITS_IN_THE_NOCHEMGRID
USE ErrCode_Mod
USE ERROR_MOD,
                       ONLY : CHECK_SPC
USE Input_Opt_Mod,
                       ONLY : OptInput
USE State_Chm_Mod,
                       ONLY : ChmState
USE State_Met_Mod,
                       ONLY : MetState
USE TIME_MOD,
                       ONLY : GET_MONTH, GET_TS_CHEM
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input options

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

Production (mixing ratio/sec) rate provided by Dylan Jones. Only production by CH4 + OH is considered.

We now use function ITS_IN_THE_CHEMGRID from chemgrid_mod.F to diagnose if box (I,J,L) is in the troposphere or stratosphere.

REVISION HISTORY:

- (1) Created by Bryan Duncan (1/99). Adapted for CH4 chemistry by James Wang (7/00). Inserted into module "global_ch4_mod.f" by Bob Yantosca. (bmy, 1/16/01)
- (2) CH4_STRAT is independent of "CMN_OH", "CMN_CO", and "CMN_CO_BUDGET". (bmy, 1/16/01)
- (3) Removed LMN from the arg list and made it a local variable. Now use functions GET_MONTH and GET_TS_CHEM from "time_mod.f" (bmy, 3/27/03)
- (4) Now references STT from "tracer_mod.f" (bmy, 7/20/04)
- 07 Mar 2012 M. Payer Added ProTeX headers
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 23 Jun 2014 R. Yantosca Now accept am_I_Root and RC
- 24 Jul 2014 R. Yantosca Now compute BOXVL internally
- 24 Mar 2015 E. Lundgren Now pass Input_Opt to Check_STT
- 06 Jan 2016 E. Lundgren Use global physical parameters
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

10.4.6 ch4_budget

Subroutine CH4_BUDGET calculates the budget of CH4. This SR only works for monthly averages, so be sure to start on the first of the month and run to another first of the month! (jsw, bnd, bmy, 1/16/01, 10/3/05)

Disable CH4 Budget for SEAC4RS code to save memory kjw, 2/3/2014

INTERFACE:

SUBROUTINE CH4_BUDGET(State_Chm)

USES:

```
USE CMN_SIZE_MOD
```

USE GC_GRID_MOD, ONLY : GET_XOFFSET, GET_YOFFSET

USE State_Chm_Mod, ONLY : ChmState

USE TIME_MOD, ONLY : GET_MONTH, GET_YEAR
USE TIME_MOD, ONLY : GET_DIAGb, GET_CT_DYN

INPUT PARAMETERS:

TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object

REMARKS:

REVISION HISTORY:

- (1) Created by Bryan Duncan (1/99). Adapted for CH4 chemistry by James Wang (7/00). Inserted into module "global_ch4_mod.f" by Bob Yantosca. (bmy, 1/16/01)
- (2) CH4_BUDGET is independent of "CMN_OH", "CMN_CO", and "CMN_CO_BUDGET". (bmy, 1/16/01)
- (3) Updated comments (jsw, bmy, 2/13/01)
- (4) Renamed XLABEL to LABEL so as not to conflict w/ "CMN"
- (5) Now use functions GET_MONTH, GET_YEAR, GET_DIAGb, and GET_CT_DYN from "time_mod.f". Removed LMN from the arg list and made it a local variable. Use functions GET_XOFFSET and GET_YOFFSET from "grid_mod.f". (bmy, 3/27/03)
- (6) Now references STT from "tracer_mod.f" (bmy, 7/20/04)
- (7) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (8) Modified for the run with new emissions (j drevet, 03/06)
- 07 Mar 2012 M. Payer Added ProTeX headers
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.
- 10 Aug 2016 R. Yantosca Remove temporary tracer-removal code

10.4.7 sum_ch4

Function SUM_CH4 sums a section of the TCH4 array bounded by the input variables I1, I2, J1, J2, L1, L2, K1, K2. SUM_CH4 is called by module subroutine CH4_BUDGET. (jsw, bnd, bmy, 1/16/01)

Disable CH4 Budget for SEAC4RS code to save memory kjw, 2/3/2014

INTERFACE:

```
REAL(fp) FUNCTION SUM_CH4( I1, I2, J1, J2, L1, L2, K1, K2, UPDOWN,
                               State_Met )
USES:
      USE CHEMGRID_MOD,
                             ONLY : ITS_IN_THE_CHEMGRID
                             ONLY : ITS_IN_THE_NOCHEMGRID
      USE CHEMGRID_MOD,
      USE CMN_SIZE_MOD
      USE State_Met_Mod,
                             ONLY : State_Met
INPUT PARAMETERS:
       INTEGER, INTENT(IN) :: I1, I2 ! Min/max longitude indices of TCH4 to sum
       INTEGER, INTENT(IN) :: J1, J2 ! Min/max latitude indices of TCH4 to sum
       INTEGER, INTENT(IN) :: L1, L2 ! Min/max altitude indices of TCH4 to sum
       INTEGER, INTENT(IN) :: K1, K2 ! Min/max species indices of TCH4 to sum
       INTEGER, INTENT(IN) :: UPDOWN ! Sum in trop (=1) or in strat (=0)
       ! Also need to pass the State_Met for the CHEMGRID functions
       TYPE(MetState), INTENT(IN) :: State_Met
REMARKS:
    Store the sources/sinks of CH4 in TCH4 in total molecules
            (1) = Initial burden
            (2) = Final burden
   STNKS
            (3) = Tropospheric CH4 sink by OH
   SOURCES
            (4) = Total Source
             (5) = Industral
             (6) = Agriculture
             (7) = Biomass Burning
            (8) = Termites
             (9) = Wetland
             (10) = Soil absorption
             (11) = Interhemispheric Exchange (+ = northward)
            (12) = ...
   Levels
                     1 <= L <= LPAUSE(I,J) - 1 are tropospheric
           LPAUSE(I,J) <= L <= LLPAR
                                              are stratospheric (bmy, 4/17/00)
REVISION HISTORY:
    (1) Created by Bryan Duncan (1/99). Adapted for CH4 chemistry by
         James Wang (7/00). Inserted into module "global_ch4_mod.f"
         by Bob Yantosca. (bmy, 1/16/01)
    (2) CH4_BUDGET is independent of "CMN_OH", "CMN_CO", and "CMN_CO_BUDGET".
          (bmy, 1/16/01)
    (3) Updated comments (jsw, bmy, 2/12/01)
    07 Mar 2012 - M. Payer - Added ProTeX headers
   23 Jul 2014 - R. Yantosca - Now pass the State_Met for chemgrid functions
```

10.4.8 ch4_distrib

Subroutine CH4_DISTRIB allocates the chemistry sink to different emission species. (ccc, 10/2/09)

INTERFACE:

```
SUBROUTINE CH4_DISTRIB( PREVCH4, Input_Opt, State_Chm )
```

USES:

```
USE CMN_SIZE_MOD
```

USE ERROR_MOD, ONLY : SAFE_DIV
USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState

IMPLICIT NONE

INPUT PARAMETERS:

```
REAL(fp) :: PREVCH4(IIPAR, JJPAR, LLPAR)! CH4 bef chem TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

REVISION HISTORY:

```
07 Mar 2012 - M. Payer - Added ProTeX headers
```

25 Mar 2013 - R. Yantosca - Now accept Input_Opt, State_Chm args

20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete

30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

10.4.9 get_ch4_anthro

Function GET_CH4_ANTHRO returns the monthly average CH4 emissions at GEOS-Chem grid box (I,J). Data will be returned in units of [atoms C/cm2/s].

INTERFACE:

```
FUNCTION GET_CH4_ANTHRO( I, J, N, Input_Opt ) RESULT( CH4_ANTHRO )
```

USES:

INPUT PARAMETERS:

RETURN VALUE:

```
REAL(fp) :: CH4_ANTHRO ! Anthro CH4 emissions [molec/cm2/s]
```

REVISION HISTORY:

```
24 Jan 2012 - M. Payer - Initial version adapted from GET_RETRO_ANTHRO 25 Mar 2013 - S.D. Eastham- Adapted for unified simulations
```

$10.4.10 \quad \text{get_ch4_biog}$

Function GET_CH4_BIOG returns annual average biogenic CH4 emissions at GEOS-Chem grid-box (I,J). Data will be returned in units of [atoms C/cm2/s].

INTERFACE:

```
FUNCTION GET_CH4_BIOG( I, J, N, Input_Opt ) RESULT( CH4_BIOG )
```

USES:

INPUT PARAMETERS:

RETURN VALUE:

```
REAL(fp) :: CH4_BIOG ! Biogenic CH4 emissions [molec/cm2/s]
```

REVISION HISTORY:

```
24 Jan 2012 - M. Payer - Initial version adapted from GET_RETRO_ANTHRO 25 Mar 2013 - S.D. Eastham- Adapted for unified simulations
```

10.4.11 init_global_ch4

Subroutine INIT_GLOBAL_CH4 allocates and zeroes module arrays.

INTERFACE:

SUBROUTINE INIT_GLOBAL_CH4(am_I_Root, Input_Opt, RC)

USES:

USE CMN_SIZE_MOD USE CMN_DIAG_MOD USE ErrCode_Mod

USE ERROR_MOD, ONLY : ALLOC_ERR ONLY : ERROR_STOP ONLY : OptInput USE ERROR_MOD, USE Input_Opt_Mod, USE State_Chm_Mod, ONLY : Ind_

INPUT PARAMETERS:

:: am_I_Root ! Are we on the root CPU? LOGICAL. INTENT(IN) TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

OUTPUT PARAMETERS:

INTEGER. INTENT(OUT) :: RC ! Success or failure?

REMARKS:

This routine is called from GC_INIT_EXTRA (in GeosCore/input_mod.f)

REVISION HISTORY:

(1) Now references ALLOC_ERR from "error_mod.f" (bmy, 10/15/02)

07 Mar 2012 - M. Payer - Added ProTeX headers

12 Feb 2014 - K. Wecht - Disable CH4 budget diagnostic (bracket the

code out with #ifdef blocks so it can be used

11 Apr 2014 - R. Yantosca - Now accept am_I_Root, Input_Opt, RC arguments

16 Jun 2016 - M. Sulprizio- Now define IDT_CH4 locally

20 Jun 2016 - R. Yantosca - Rename IDTCH4 to id_CH4 for consistency

20 Jun 2016 - R. Yantosca - Now stop run if id_CH4 is undefined

10.4.12 cleanup_global_ch4

Subroutine CLEANUP_GLOBAL_CH4 deallocates module arrays. (bmy, 1/16/01)

INTERFACE:

SUBROUTINE CLEANUP_GLOBAL_CH4

REVISION HISTORY:

```
(1 ) Now references ALLOC_ERR from "error_mod.f" (bmy, 10/15/02)
```

07 Mar 2012 - M. Payer - Added ProTeX headers

12 Feb 2014 - K. Wecht - Disable CH4 budget diagnostic (bracket the code out with #ifdef blocks so it can be used)

Fortran: Module Interface mercury_mod.F 10.5

Module MERCURY_MOD contains variables and routines for the GEOS-CHEM mercury simulation. Many choices of reaction mechanism and model processes can be selected with logical switches located in INIT_MERCURY.

INTERFACE:

MODULE MERCURY_MOD

USES:

```
USE DEPO_MERCURY_MOD, ONLY : ADD_HG2_SNOWPACK
USE DEPO_MERCURY_MOD,
                      ONLY : LHGSNOW
USE OCEAN_MERCURY_MOD, ONLY : LDYNSEASALT
USE OCEAN_MERCURY_MOD, ONLY : LGCAPEMIS
USE OCEAN_MERCURY_MOD, ONLY : LPOLARBR
USE OCEAN_MERCURY_MOD, ONLY: LGEIAO5
USE OCEAN_MERCURY_MOD, ONLY : LVEGEMIS
USE OCEAN_MERCURY_MOD, ONLY : LBRCHEM
USE OCEAN_MERCURY_MOD, ONLY : LRED_JNO2
USE OCEAN_MERCURY_MOD, ONLY : LHg2HalfAerosol
USE OCEAN_MERCURY_MOD, ONLY : STRAT_BR_FACTOR
USE OCEAN_MERCURY_MOD, ONLY : LAnthroHgOnly
USE OCEAN_MERCURY_MOD, ONLY : LOHO3CHEM
USE OCEAN_MERCURY_MOD, ONLY : LGCBROMINE
USE OCEAN_MERCURY_MOD, ONLY : LnoUSAemis
USE OCEAN_MERCURY_MOD, ONLY : LBROCHEM
USE OCEAN_MERCURY_MOD, ONLY : LNEI2005
USE OCEAN_MERCURY_MOD, ONLY : LInPlume
USE OCEAN_MERCURY_MOD, ONLY : LOCEANCOEF
USE PhysConstants
                          ! Physical constants
USE PRECISION_MOD ! For GEOS-Chem Precision (fp)
IMPLICIT NONE
```

PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: CHEMMERCURY PUBLIC :: CLEANUP_MERCURY PUBLIC :: INIT_MERCURY PUBLIC :: EMISSMERCURY PUBLIC :: PARTITIONHG2

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: EMITHG PRIVATE :: SRCHg0 PRIVATE :: SRCHg2 PRIVATE :: SRCHgP PRIVATE :: MERCURY_READYR

PRIVATE :: OHNOSTIME

PRIVATE :: CALC_HG2_SEASALT_LOSSRATE

PRIVATE :: RED_INPLUME_GRID PRIVATE :: DO_RED_INPLUME PRIVATE :: GET_HGBR_RATE

PRIVATE :: GET_LWC PRIVATE :: GET_VCLDF PRIVATE :: GET_03 PRIVATE :: GET_OH PRIVATE :: GET_BR PRIVATE :: GET_JNO2

REMARKS:

Nomenclature:

(1) Hg(0) a.k.a. Hg0 : Elemental mercury (2) Hg(II) a.k.a. Hg2 : Divalent mercury (3) HgP : Particulate mercury

Mercury Species (1-3 are always defined; 4-87 are defined for tagged runs)

(1) Hg(0): Hg(0) - total species (2) Hg(II) : Hg(II) - total species (3) HgP : HgP - total species

: Hg(0) - Canadian Anthropogenic (4) HgO_can

(5) HgO_usa : Hg(0) - USA Anthropogenic

: Hg(0) - Central American Anthropogenic (6) HgO_cam . ng(0) - South American Anthropogenic : Hg(0) - West African Anthropogenic : Hg(0) - Fort 10 (7) HgO_sam : Hg(0) - South American Anthropogenic (8) HgO_waf (9) HgO_eaf : Hg(0) - East African Anthropogenic (10) Hg0_saf : Hg(0) - South African Anthropogenic (11) HgO_naf : Hg(0) - North African Anthropogenic

: Hg(0) - OECD European Anthropogenic (12) Hg0_eur (13) HgO_eeu : Hg(0) - Eastern European Anthropogenic

: Hg(0) - Former USSR Anthropogenic (14) Hg0_sov : Hg(0) - Middle Eastern Anthropogenic (15) Hg0_mde : Hg(0) - South Asian Anthropogenic (16) Hg0_sas : Hg(0) - East Asian Anthropogenic (17) Hg0_eas

(18) HgO_sea : Hg(0) - Southeast Asian Anthropogenic

(19) HgO_jpn : Hg(0) - Japanese Anthropogenic : Hg(0) - Oceanian Anthropogenic (20) HgO_ocn

(21) HgO_so : Hg(0) - Biomass Burning : Hg(0) - Organic Soils (22) Hg0_bb

(23) HgO_geo : Hg(0) - Geogenic

(24) HgO_atl : Hg(0) - Middle Atlantic Subsurface Waters (25) HgO_nat : Hg(0) - North Atlantic Subsurface Waters

(26) HgO_sat : Hg(0) - South Atlantic Subsurface Waters
(27) HgO_npa : Hg(0) - North Pacific Subsurface Waters
(28) HgO_arc : Hg(0) - Arctic Subsurface Waters
(29) HgO_ant : Hg(0) - Antarctic Subsurface Waters
(30) HgO_oce : Hg(0) - Indo-Pacific Subsurface Waters
(31) HgO_str : Hg(0) - Stratospheric Hg from Intial Conditions
(32-59) Same as (4-31) but for Hg(II)
(60-87) Same as (4-31) but for Hg(P)

References:

- (1) Hall, B. (1995). "The gas phase oxidation of elemental mercury by ozone.", Water, Air, and Soil Pollution 80: 301-315.
- (2) Sommar, J., et al. (2001). "A kinetic study of the gas-phase reaction between the hydroxyl radical and atomic mercury." Atmospheric Environment 35: 3049-3054.
- (3) Selin, N., et al. (2007). "Chemical cycling and deposition of atmospheric mercury: Global constraints from observations." J. Geophys. Res. 112.
- (4) Selin, N., et al. (2008). "Global 3-D land-ocean-atmospehre model for mercury: present-day versus preindustrial cycles and anthropogenic enrichment factors for deposition." Global Biogeochemical Cycles 22: GB2011.
- (5) Allison, J.D. and T.L. Allison (2005) "Partition coefficients for metals in surface water, soil and waste." Rep. EPA/600/R-05/074, US EPA, Office of Research and Development, Washington, D.C.
- (6) Mintz, Y and G.K. Walker (1993). "Global fields of soil moisture and land surface evapotranspiration derived from observed precipitation and surface air temperature." J. Appl. Meteorol. 32 (8), 1305-1334.
- (7) Soerensen, A. et al. (2010), An improved global model for air-sea exchange of mercury: High concentrations over the North Atlantic, Environ. Sci. Technol., 44, 8574-8580.
- (8) Corbitt, E.S. et al. (2011), Global source-receptor relationships for mercury deposition under present-day and 2050 emissions scenarios, Environ. Sci. Technol., 45, 10477-10484.
- (9) Street, D.G. et al. (2009), Projections of global mercury emissions in 2050, Environ. Sci. Technol., 43, 2983-2988.
- (10) Holmes, C.D., et al. (2010) Global atmospheric model for mercury including oxidation by bromine atoms, AC&P, 10, 12,037-12,057.
- (11) Parrella, J. et al. (2012), Tropospheric bromine chemistry: implications for present and pre-industrial ozone and mercury, ACP.
- (12) Pohler, D. et al. (2010), Observation of halogen species in the Amundsen Gulf, Arctic, by active long-path differential optical absorption spectroscopy, Proc. Natl. Acad. Sci, 107(15): 6528-6587.
- (13) Prados-Roman, C. et al. (2011), Airborne DOAS limb measurements of tropospheric trace gas profiles: case studies on the profile retrieval of O4 and BrO, Atmos. Meas. Tech., 4: 1241-1260.

REVISION HISTORY:

- Updated for reduction rxn and online HgO ocean flux. Now use diagnostic arrays from "diagO3_mod.f". (eck, sas, bmy, 1/21/05)
 Now references "pbl_mix_mod.f". Remove FEMIS array and routine COMPUTE_FEMIS. (bmy, 2/15/05)
- (3) Now can read data for both GEOS and GCAP grids (bmy, 8/16/05)
- (4) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (5) Now references XNUMOL from "tracer_mod.f" (bmy, 10/25/05)
- (6) Various updates added for tagged Hg sim. (eck, sas, cdh, bmy, 4/6/06)
- (7) Now includes LPREINDHG logical switch for preindustrial simulation (eds 7/30/08)

```
13 Aug 2010 - R. Yantosca - Add modifications for MERRA (treat like GEOS-5)
```

- 01 Apr 2011 H. Amos added LVEGEMIS, distinct from LGCAPEMIS
- 27 Sep 2011 H. Amos Remove LHg_WETDasHNO3 logical, it's obsolete
- 01 Nov 2011 Y. Zhang Add subroutines to do in plume reduction of Hg
- 07 Feb 2012 E. Corbitt Imported tagged tracers; renamed nt to geo.
- 08 Feb 2012 R. Yantosca Add modifications for GEOS-5.7.x met
- 01 Mar 2012 R. Yantosca Now reference new grid_mod.F90
- 01 Mar 2012 R. Yantosca Use updated GET_LOCALTIME from time_mod.F
- 19 Apr 2012 E. Corbitt Added LGCBROMINE to use GEOS-Chem bromine.
- 03 Jun 2013 C. Holmes Extensively rewritten for simplicity
- 03 Jun 2013 R. Yantosca Added ProTeX headers
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 17 Nov 2014 M. Yannetti Added PRECISION_MOD
- 12 Mar 2015 R. Yantosca Now get JNO2 from the HEMCO data structure
- 12 Mar 2015 R. Yantosca Remove GET_GLOBAL_JNO2 routine
- 10 Aug 2015 J. Fisher Updated treatment of polar BrO chemistry (orig. 29/11/11)
- 05 Jan 2016 E. Lundgren Now use global dry air gas and Henry's Law consts
- 31 May 2016 E. Lundgren Replace Input_Opt%XNUMOL with AVO / (emMW_g*1e-3) where emMW_g is emitted MW from species database
- 29 Nov 2016 R. Yantosca grid_mod.F90 is now gc_grid_mod.F90

10.5.1 chemmercury

Subroutine CHEMMERCURY is the driver routine for mercury chemistry in the GEOS-CHEM module.

INTERFACE:

USES:

```
USE CMN_SIZE_MOD USE CMN_DIAG_MOD
```

```
USE DAO_MOD,
                              ONLY : IS_ICE
      USE DAO_MOD,
                              ONLY : IS_LAND
      USE DAO_MOD,
                              ONLY : IS_WATER
      USE DEPO_MERCURY_MOD,
                              ONLY : ADD_HG2_DD
      USE DEPO_MERCURY_MOD,
                              ONLY : ADD_HgP_DD
 #if defined( BPCH_DIAG )
      USE DIAG_MOD,
                              ONLY: AD44
 #endif
      USE DIAGO3_MOD,
                              ONLY: AD03_Hg2_Hg0, AD03_Hg2_03
      USE DIAGO3_MOD,
                              ONLY: ADO3_Hg2_Br, ADO3_Hg2_OH
      USE DIAGO3_MOD,
                              ONLY: ADO3_Hg2_SS, LDO3
                              ONLY: ADO3_Hg2_SSR, NDO3
      USE DIAGO3_MOD,
      USE DIAGO3_MOD,
                              ONLY : ADO3_Br
      USE ErrCode_Mod
      USE ERROR_MOD,
                              ONLY : DEBUG_MSG
      USE ERROR_MOD,
                              ONLY : ERROR_STOP
      USE ERROR_MOD,
                              ONLY : SAFE_DIV
      USE HCO_INTERFACE_MOD, ONLY : HcoState
      USE HCO_EmisList_Mod,
                              ONLY : HCO_GetPtr
      USE GLOBAL_BR_MOD,
                             ONLY : GET_GLOBAL_BR
      USE GC_GRID_MOD,
                             ONLY : GET_AREA_CM2
                             ONLY : OptInput
      USE Input_Opt_Mod,
      USE PBL_MIX_MOD,
                             ONLY : GET_FRAC_UNDER_PBLTOP
      USE Species_Mod,
                             ONLY : Species
      USE State_Chm_Mod,
                             ONLY : ChmState
      USE State_Met_Mod,
                             ONLY : MetState
      USE TIME_MOD,
                             ONLY : GET_MONTH
      USE TIME_MOD,
                             ONLY : GET_TS_CHEM
      USE TIME_MOD,
                             ONLY : ITS_A_NEW_MONTH
      USE TIME_MOD,
                              ONLY : ITS_TIME_FOR_A3
INPUT PARAMETERS:
      LOGICAL,
                      INTENT(IN)
                                    :: am_I_Root ! Are we on the root CPU?
      TYPE(OptInput), INTENT(IN)
                                    :: Input_Opt    ! Input Options object
                                    :: State_Met
      TYPE(MetState), INTENT(IN)
                                                  ! Meteorology State object
INPUT/OUTPUT PARAMETERS:
      TYPE(ChmState), INTENT(INOUT) :: State_Chm
                                                  ! Chemistry State object
OUTPUT PARAMETERS:
      INTEGER,
                      INTENT(OUT) :: RC
                                                 ! Success or failure?
```

REMARKS:

Description of the chemistry mechanism:

The comments and code below refer to 3 mercury species:

1. HgO or Hg(0) : gaseous elemental mercury

- 2. Hg2g or Hg(II)g : gaseous Hg(II) (comparable to RGM observations)
- 3. Hg2p or Hg(II)p : particle-bound Hg(II) (comparable to PBM observations)

Following Amos et al. (2012), the ${\rm Hg}({\rm II})$ partitioning between ${\rm Hg}2{\rm g}$ and ${\rm Hg}2{\rm p}$ is based on temperature and aerosol surface area. There is no refractory particulate ${\rm Hg}$.

In some legacy code below Hg2p is called HgP and Hg2g is called Hg2.

The differential equations for oxidation, reduction and deposition are:

 $d[Hg2p]/dt = -(k_Red_Hg2p + k_Dep_Hg2p) [Hg2p]$

The chemical mechanism currently assumes that the product of Hg(0) oxidation is in the gas phase. This can be easily changed.

Equilibrium partitioning between Hg2g and Hg2p is established at the beginning and end of CHEMMERCURY.

Notes on chemistry and deposition:

(1) Oxidation: Hg(0) --> Hg(II):

Oxidation by Br, BrO, OH, and O3 can be selectively enabled or disabled with switches (LBRCHEM, LBROCHEM, LOHO3CHEM) in INIT_MERCURY.

Hg(0)(g) + Br(g) --> + Br/OH --> Hg(II)g, rates are selected with
METHOD keyword below. Recommded kinetics are 'DonohoueYBBalabanov'
which use rates from Donohoue et al. (2006), Goodsite et al. (2004)
and Balabanov et al. (2005)

$$Hg(0)(g) + 03(g) --> Hg(II)$$
 , k = 3.0e-20 cm3 molec-1 s-1 Source: Hall, 1995

$$Hg(0)(g)+OH(g) \longrightarrow Hg(II)$$
, k = 8.7e-14 cm3 s-1 Source: Sommar et al. 2001

(2) Reduction:

Reduction rates can be scaled to NO2 photolysis rates or OH concentrations with the switch LRED_JNO2. In either case, aqueous-phase photochemical reduction of Hg(II) is included based on estimate of rate constant and scaled to NO2 photolysis or [OH]. The rate is tuned to match the global Hg(0) concentration and

seasonal cycle.

(3) Hg(0) dry deposition:

The dry deposition frequency is calculated by drydep_mod. If the non-local PBL mixing scheme is used, however, all dry deposition is done elsewhere. The ocean module separately cacluates Hg(0) dry deposition over ocean, so CHEMMERCURY only includes Hg(0) dry deposition over land.

(4) Hg(II)g and Hg(II)p dry deposition: The dry deposition frequencies are calculated by drydep_mod. If the non-local PBL mixing scheme is used, however, all dry deposition is done elsewhere.

(5) Sea-salt uptake of Hg(II)g
Hg(II)g is taken up into sea-salt aerosol and deposited to the ocean
surface at a rate based on wind speed and relative humidity. Hg(II)p
uptake into sea-salt aerosol may also occur at a slower rate, but is
not yet treated here.

- 01 Oct 1995 R. Yantosca Initial version
- 08 Dec 2009 R. Yantosca Added ProTeX headers
- 06 Dec 2004 N. (Eckley) Selin Initial version
- (1) Now references routine GET_PBL_MAX_L from "pbl_mix_mod.f". Now references AD44 from "diag_mod.f". Now sum the levels from T44 into the AD44 array. Now references N_TRACERS from "tracer_mod.f". (bmy, 2/24/05)
- (2) Bug fix: Set T44 to 0e0 for single precision. Now allow for zero dry deposition velocity. Now call INIT_MERCURY from "input_mod.f" (bmy, 4/6/06)
- 02 Apr 2013 C. Holmes CHEMMERCURY rewritten for clarity and easier maintainability. The chemistry and deposition for particle-bound mercury is now solved simultaneously with Hg(0) and gaseous Hg(II). The subroutine now uses a 4th-order Runge-Kutta method to solve the coupled chemistry. The subroutines CHEM_HGO_HG2 and CHEM_HGP are now obsolete.
- 04 Apr 2013 C. Holmes Use State_Met for met fields.
- 03 Jun 2013 R. Yantosca Now use fields from Input_OPt instead of from logical_mod.F and tracer_mod.F
- 26 Sep 2013 R. Yantosca Renamed GEOS_57 Cpp switch to GEOS_FP
- 23 Oct 2013 R. Yantosca Now pass objects to GET_GLOBAL_OH routine
- 06 Nov 2014 R. Yantosca Now use State_Met%AIRDEN(I,J,L)
- 06 Nov 2014 R. Yantosca Now use State_Met%CLDF(I,J,L)
- 26 Feb 2015 E. Lundgren Replace GET_PCENTER with State_Met%PMID_DRY.

 Remove dependency on pressure_mod.
- 12 Aug 2015 R. Yantosca Added support for MERRA2 meteorology
- 05 Jan 2016 E. Lundgren Use Henry's constant from species database and

```
calculate dry air gas constant from global params
25 Apr 2016 - R. Yantosca - Now pass Hg category # to ADD_Hg2_* routines
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.
01 Jul 2016 - R. Yantosca - Now rename species DB object ThisSpc to SpcInfo
11 Oct 2016 - R. Yantosca - Pass additional args to SET_OPTIONS_FROM_HEMCO
```

10.5.2 get_hgbr_rate

Function GET_HGBR_RATE computes the effective 1st order conversion rate of Hg(0) to Hg(II) via two-step recombination with Br and OH.

INTERFACE:

```
FUNCTION GET_HGBR_RATE( BR, T, P, OH, METHOD ) RESULT( K_HGBR )
```

INPUT PARAMETERS:

CHARACTER(LEN=*), INTENT(IN) :: METHOD

RETURN VALUE:

```
! K_HgBr : Effective 1st order loss rate of Hg(0) [1/s]
REAL(fp) :: K_HGBR
```

REMARKS:

This subroutine calculates the net rate of Hg(0) oxidation to Hg(II) through the following reactions. All are gas phase.

```
(1 ) Hg(0) + Br -> HgBr

(2 ) HgBr + M -> Hg(0) + Br

(2a ) HgBr -> Hg(0) + Br

(3Br) HgBr + Br -> HgBr2

(3OH) HgBr + OH -> HgBrOH
```

References:

1. Ariya, P. A., A. Khalizov, and A. Gidas (2002), Reaction of gaseous mercury with atomic and molecular halogens: kinetics, product studies, and atmospheric implications, Journal of Physical Chemistry A, 106,

7310-7320.

2. Balabanov, N. B., B. C. Shepler, and K. A. Peterson (2005), Accurate global potential energy surface and reaction dynamics for the ground state of HgBr2, Journal of Physical Chemistry A, 109(39), 8765-8773.

3. Donohoue, D. L., D. Bauer, B. Cossairt, and A. J. Hynes (2006), Temperature and Pressure Dependent Rate Coefficients for the Reaction of Hg with Br and the Reaction of Br with Br: A Pulsed Laser Photolysis-Pulsed Laser Induced Fluorescence Study, Journal of Physical Chemistry A, 110, 6623-6632.

- 4. Goodsite, M. E., J. M. C. Plane, and H. Skov (2004), A theoretical study of the oxidation of Hg-O to HgBr2 in the troposphere, Environmental Science & Technology, 38(6), 1772-1776.
- 5. Holmes, C. D., et al. (2006), Global lifetime of elemental mercury against oxidation by atomic bromine in the free troposphere, Geophys. Res. Lett., 33(20).
- 6. Khalizov, A. F., B. Viswanathan, P. Larregaray, and P. A. Ariya (2003), A theoretical study on the reactions of Hg with halogens: Atmospheric implications, Journal of Physical Chemistry A, 107(33), 6360-6365.

REVISION HISTORY:

```
06 Jul 2006 - C. Holmes - Initial version
05 Jan 2016 - E. Lundgren - Use global physical parameters
```

10.5.3 emissmercury

Subroutine EMISSMERCURY is the driver routine for mercury emissions.

NOTE/TODO: The mercury simulation is the only GEOS-Chem emission code that is not yet fully compatible with HEMCO. So far, only the anthropogenic emissions are included in HEMCO. For all other sources, the original mercury code is used.

For the non-local PBL mixing, all emissions are written into module array HG_EMIS (in kg m-2 s-1). These values are then used by vdiff_mod.F90. This is just a workaround to ensure backwards compatibility of the mercury code. Once we have added all mercury emissions to HEMCO, HG_EMIS is not used any more (ckeller, 10/21/2014).

INTERFACE:

```
SUBROUTINE EMISSMERCURY( am_I_Root, Input_Opt, & State_Met, State_Chm, RC )
```

USES:

```
785
      USE CMN_SIZE_MOD
      USE DEPO_MERCURY_MOD, ONLY : RESET_HG_DEP_ARRAYS
      USE ErrCode_Mod
      USE ERROR_MOD
      USE GC_GRID_MOD,
                           ONLY : GET_XMID, GET_YMID
                           ONLY : OptInput
      USE Input_Opt_Mod,
      USE LAND_MERCURY_MOD,
                           ONLY : LAND_MERCURY_FLUX, VEGEMIS
      USE LAND_MERCURY_MOD,
                           ONLY: SOILEMIS, BIOMASSHG
                           ONLY : SNOWPACK_MERCURY_FLUX
      USE LAND_MERCURY_MOD,
      USE OCEAN_MERCURY_MOD, ONLY : OCEAN_MERCURY_FLUX
                           ONLY : ChmState
      USE State_Chm_Mod,
      USE State_Met_Mod,
                           ONLY : MetState
      USE TIME_MOD,
                           ONLY : GET_MONTH, ITS_A_NEW_MONTH
      USE UnitConv_Mod
      ! Added for GTMM (ccc, 11/19/09)
      USE LAND_MERCURY_MOD, ONLY : GTMM_DR
INPUT PARAMETERS:
      LOGICAL,
                    INTENT(IN)
                                :: am_I_Root ! Are we on the root CPU?
      TYPE(OptInput), INTENT(IN)
                                 :: Input_Opt ! Input Options object
      TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
INPUT/OUTPUT PARAMETERS:
      OUTPUT PARAMETERS:
      INTEGER,
                    INTENT(OUT) :: RC
                                             ! Success or failure?
REMARKS:
REVISION HISTORY:
   03 Jun 2013 - N. (Eckley) Selin - Initial version
   (1 ) Now call OCEAN_MERCURY_FLUX from "ocean_mercury_mod.f" to compute
         the emissions of HgO from the ocean instead of reading it from disk.
         (sas, bmy, 1/20/05)
         from routine GET_FRAC_OF_PBL in "pbl_mix_mod.f" (bmy, 2/22/05)
   (3) Now modified for new ocean mercury module. (cdh, sas, bmy, 4/6/06)
```

- (2) Now no longer call COMPUTE_FEMIS, since we can get the same information
- 01 Mar 2012 R. Yantosca Now use GET_XMID(I,J,L) from grid_mod.F90
- 01 Mar 2012 R. Yantosca Now use GET_YMID(I,J,L) from grid_mod.F90
- 25 Mar 2013 R. Yantosca Now accept am_I_Root, Input_Opt, State_Chm, RC
- 08 Dec 2009 R. Yantosca Added ProTeX headers
- 20 Jun 2014 R. Yantosca Now pass Input_Opt to VEGEMIS
- 23 Jun 2014 R. Yantosca Now pass am_I_Root to OCEAN_MERCURY_FLUX
- 05 Oct 2015 E. Lundgren Now convert tracer units to kg locally

10.5.4 emithg

Subroutine EMITHG directs emission either to the chemical species array (State_Chmnon-local PBL mixing. This is a programming convenience.

INTERFACE:

```
SUBROUTINE EMITHG( I, J, L, ID, E_HG, Input_Opt, State_Chm )
```

USES:

```
USE ErrCode_Mod

USE GC_GRID_MOD, ONLY : GET_AREA_M2

USE Input_Opt_Mod, ONLY : OptInput

USE State_Chm_Mod, ONLY : ChmState

USE TIME_MOD, ONLY : GET_TS_EMIS
```

INPUT PARAMETERS:

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

REVISION HISTORY:

```
27 Aug 2009 - C. Holmes - Initial version
25 Mar 2013 - R. Yantosca - Now accept Input_Opt, State_Chm, arguments
```

$10.5.5 \quad \text{srcHg0}$

Subroutine SRCHg0 is the subroutine for Hg(0) emissions. Emissions of Hg(0) will be distributed throughout the boundary layer. (eck, cdh, bmy, 1/21/05, 4/6/06)

INTERFACE:

```
SUBROUTINE SRCHgO( am_I_Root, Input_Opt, State_Chm, RC )
```

USES:

```
USE CMN_SIZE_MOD

USE DIAGO3_MOD, ONLY : ADO3, NDO3, ADO3_nat

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP

USE Input_Opt_Mod, ONLY : OptInput

USE PBL_MIX_MOD, ONLY : GET_FRAC_OF_PBL, GET_PBL_MAX_L

USE State_Chm_Mod, ONLY : ChmState

USE TIME_MOD, ONLY : GET_TS_EMIS
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

- 21 Jan 2005 N. (Eckley) Selin, C. Holmes Initial version
- (1) Now use diagnostic arrays from "diag03_mod.f" (bmy, 1/21/05)
- (2) Now references GET_FRAC_OF_PBL and GET_PBL_MAX_L from "pbl_mix_mod.f". Remove reference to FEMIS. (bmy, 2/22/05)
- (3) EHgO_an is now a 2-D array. Modified for new ocean mercury module.

 Now use ID_HgO index array from "tracerid_mod.f". Now make sure

 STT does not underflow. (cdh, bmy, 4/6/06)
- 25 Mar 2013 R. Yantosca Now accept am_I_Root, Input_Opt, State_Chm, RC
- 30 Jun 2016 R. Yantosca Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

10.5.6 srcHg2

Subroutine SRCHg2 is the subroutine for Hg(II) emissions. Emissions of Hg(II) will be distributed throughout the boundary layer.

INTERFACE:

SUBROUTINE SRCHg2(am_I_Root, Input_Opt, State_Chm, RC)

USES:

```
USE CMN_SIZE_MOD
```

USE DIAGO3_MOD, ONLY : ADO3, NDO3

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP USE Input_Opt_Mod, ONLY : OptInput

USE PBL_MIX_MOD, ONLY : GET_FRAC_OF_PBL, GET_PBL_MAX_L

USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState
USE TIME_MOD, ONLY : GET_TS_EMIS

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

- 07 Dec 2004 N. (Eckley) Selin Initial version
- (1) Now use diagnostic arrays from "diag03_mod.f" (bmy, 1/21/05)
- (2) Now references GET_FRAC_OF_PBL and GET_PBL_MAX_L from "pbl_mix_mod.f". Remove reference to FEMIS. (bmy, 2/22/05)
- (3) EHg2_an is now a 2-D array. Now use ID_Hg2 index array from "tracerid_mod.f". Now make sure STT does not underflow. (eck, cdh, bmy, 4/6/06)
- 25 Mar 2013 R. Yantosca Now accept am_I_Root, Input_Opt, State_Chm, RC

10.5.7 srcHgp

Subroutine SRCHgP is the subroutine for HgP emissions. Emissions of HgP will be distributed throughout the boundary layer.

INTERFACE:

SUBROUTINE SRCHgP(am_I_Root, Input_Opt, State_Chm, RC)

USES:

```
USE CMN_SIZE_MOD
```

USE DIAGO3_MOD, ONLY: ADO3, NDO3

USE ErrCode_Mod

ONLY : ERROR_STOP USE ERROR_MOD, ONLY: OptInput
ONLY: GET_FRAC_OF_PBL, GET_PBL_MAX_L USE Input_Opt_Mod,

USE PBL_MIX_MOD,

USE State_Chm_Mod, ONLY : MetState USE State_Met_Mod, USE TIME_MOD, ONLY : GET_TS_EMIS

INPUT PARAMETERS:

:: am_I_Root ! Are we on the root CPU? LOGICAL. INTENT(IN) TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

- 07 Dec 2004 N. (Eckley) Selin Initial version
- (1) Now use diagnostic arrays from "diag03_mod.f" (bmy, 1/21/05)
- (2) Now references GET_FRAC_OF_PBL and GET_PBL_MAX_L from "pbl_mix_mod.f". Remove reference to FEMIS. (bmy, 2/22/05)
- (3) EHgP_an is now a 2-D array. Now use ID_HgP index array from "tracerid_mod.f". Now make sure STT does not underflow. (eck, cdh, bmy, 4/6/06)

10.5.8 mercury_readyr

Subroutine MERCURY_READYR reads the year-invariant emissions for Mercury from anthropogenic, ocean, and land sources.

INTERFACE:

```
SUBROUTINE MERCURY_READYR( am_I_Root, Input_Opt, RC )
```

USES:

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP

USE HCO_ERROR_MOD

USE HCO_INTERFACE_MOD, ONLY : HcoState
USE HCO_EMISLIST_MOD, ONLY : HCO_GetPtr
USE HCO_INTERFACE_MOD, ONLY : GetHcoDiagn
USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

```
06 Dec 2004 - N. (Eckley) Selin - Initial version
```

- (1) Now read data from mercury_200501 subdirectory. Now compute oceanic Hg(0) emissions w/ ocean flux module instead of reading them from disk. Now use 1985 TAU values. (sas, bmy, 1/20/05)
- (2) Now can read data for both GEOS and GCAP grids (bmy, 8/16/05)
- (3) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (4) Now read anthro emissions on GEOS 1x1 grid in DATA_1x1_DIR. Also

keep 2x25 and 4x5 files together in DATA_1x1_DIR. Also now use new land re-emissions files from Noelle Selin. (eck, bmy, 4/6/06)

- (5) Now reads anthro emissions for 17 world regions from David Streets for use in tagged simulations. (eds 2/7/12)
- (6) Bug fix: emissions are read on GENERIC grid (jaf, 2/8/12)
- 01 Mar 2012 R. Yantosca Now use GET_XMID(I,J,L) from grid_mod.F90
- 01 Mar 2012 R. Yantosca Now use GET_YMID(I,J,L) from grid_mod.F90
- 13 Mar 2012 M. Cooper Changed regrid algorithm to map_a2a
- 24 May 2012 R. Yantosca Fixed minor bugs in map_a2a algorithm
- 24 May 2012 H. Amos updated file paths for soil Hg files
- 28 Jun 2012 S. Kim Bug fix: you need to provide a location in the call to ERROR_STOP
- 24 Aug 2012 R. Yantosca DO_REGRID_A2A now reads netCDF input file
- 03 Jan 2013 M. Payer Renamed PERAREA to IS_MASS in DO_REGRID_A2A
- 13 Jan 2013 M. Payer Update soil Hg files for v9-02c (Y. Zhang)
- 06 Jun 2013 R. Yantosca Get ANTHRO_Hg_YEAR, Hg_SCENARIO from Input_Opt
- 06 Sep 2013 R. Yantosca Kludge: use MERRA soil file for GEOS-FP testing and debugging. Worry about this later.
- 06 Sep 2013 R. Yantosca Kludge: use GEOS-5 soil file for GEOS-4 testing and debugging. Worry about this later.
- 24 Sep 2014 C. Keller HEMCO update
- 29 Apr 2016 R. Yantosca Don't initialize pointers in declaration stmts

 $10.5.9 ext{ get_lwc}$

Function GET_LWC returns the cloud liquid water content [m3~H2O/m3~air] at a GEOSCHEM grid box as a function of temperature.

INTERFACE:

FUNCTION GET_LWC(T) RESULT(LWC)

USES:

INPUT PARAMETERS:

REAL(fp), INTENT(IN) :: T ! Temperature [K]

RETURN VALUE:

REAL(fp) :: LWC ! Liquid water content [m3 H2O/m3 air]

REVISION HISTORY:

31 Oct 2002 - R. Park - Initial version 18 Jan 2011 - R. Yantosca - Updated comments

$10.5.10 \text{ get_vcldf}$

Subroutine GET_VCLDF computes the volume cloud fraction for Hg0 and Hg2 chemistry.

INTERFACE:

```
FUNCTION GET_VCLDF( I, J, L, State_Met ) RESULT( VCLDF )
```

USES:

USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I ! Longitude index
INTEGER, INTENT(IN) :: J ! Latitude index
INTEGER, INTENT(IN) :: L ! Level index
```

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

RETURN VALUE:

REAL(fp) :: VCLDF ! Volume cloud fraction

REMARKS:

References:

```
(1 ) Sundqvist et al. [1989]
```

REVISION HISTORY:

```
06 Dec 2004 - N. (Eckley) Selin - Copied from "sulfate_mod.f" but was made into a function since we are already looping over (I,J,L) in CHEM_HgO_Hg2

09 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met derived type object

26 Feb 2015 - E. Lundgren - Replace GET_PCENTER and GET_PEDGE with State_Met%PMID and State_Met%PEDGE. Remove dependency on pressure_mod.
```

$10.5.11 \text{ get_o3}$

Function GET_O3 returns monthly mean O3 for the mercury simulation.

INTERFACE:

```
FUNCTION GET_03( I, J, L, State_Met ) RESULT( 03_MOLEC_CM3 )
```

USES:

```
USE CMN_SIZE_MOD
```

USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I ! Longitude index
INTEGER, INTENT(IN) :: J ! Latitude index
INTEGER, INTENT(IN) :: L ! Level index
```

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

RETURN VALUE:

REAL(fp) :: 03_MOLEC_CM3 ! 03 conc [molec/cm3]

REVISION HISTORY:

```
06 Dec 2002 - R. Yantosca - Initial version
```

- (1) We assume SETTRACE has been called to define IDO3. (bmy, 12/16/02)
- (2) Now reference inquiry functions from "tracer_mod.f" (bmy, 7/20/04)
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 24 Jul 2014 R. Yantosca Now compute BOXVL internally
- 11 Mar 2015 R. Yantosca Remove reference to GLOBAL_O3_MOD

10.5.12 get_oh

Function GET_OH returns monthly mean OH and imposes a diurnal variation.

INTERFACE:

```
FUNCTION GET_OH( I, J, L, State_Met ) RESULT( OH_MOLEC_CM3 )
```

USES:

```
USE CMN_SIZE_MOD
```

USE State_Met_Mod, ONLY : MetState
USE TIME_MOD, ONLY : GET_TS_CHEM

INPUT PARAMETERS:

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

RETURN VALUE:

REAL(fp) :: OH_MOLEC_CM3 ! OH conc [molec/cm3]

```
07 Dec 2004 - N. (Eckley) Selin - Initial version
```

- 28 Nov 2012 R. Yantosca Replace SUNCOS with State_Met%SUNCOS
- 28 Nov 2012 R. Yantosca Now pass State_Met via the argument list
- 11 Mar 2015 R. Yantosca Remove reference to GLOBAL_OH_MOD

$10.5.13 \text{ get_Br}$

Function GET_BR returns instantaneous Br concentration calculated from the monthly mean and an imposed diurnal variation.

INTERFACE:

```
FUNCTION GET_BR( I, J, L, BRO_MOLEC_CM3, State_Met )
& RESULT( BR_MOLEC_CM3 )
```

USES:

```
USE CHEMGRID_MOD,
                       ONLY : ITS_IN_THE_STRAT
USE CMN_SIZE_MOD
USE DAO_MOD,
                       ONLY : GET_OBK
USE DAO_MOD,
                      ONLY : IS_WATER
USE DIAGO3_MOD,
                     ONLY : ADO3_Br, LDO3,
                                                  ND03
                      ONLY : SAFE_DIV
USE ERROR_MOD,
                    ONLY : BR_MERGE, BR_TROP
USE GLOBAL_BR_MOD,
USE GLOBAL_BR_MOD,
                      ONLY : BR_STRAT, J_BRO
                       ONLY: BRO_MERGE, BRO_TROP, BRO_STRAT
USE GLOBAL_BR_MOD,
USE GC_GRID_MOD,
                       ONLY : GET_YMID
USE PBL_MIX_MOD,
                      ONLY : GET_FRAC_UNDER_PBLTOP
USE State_Met_Mod,
                      ONLY : MetState
USE TIME_MOD,
                      ONLY : GET_TS_CHEM, GET_LOCALTIME
USE TIME_MOD,
                      ONLY : ITS_A_NEW_DAY
USE TIME_MOD,
                      ONLY : GET_MONTH
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I ! Longitude index
INTEGER, INTENT(IN) :: J ! Latitude index
INTEGER, INTENT(IN) :: L ! Level index
REAL(fp), INTENT(OUT) :: BrO_MOLEC_CM3 ! BrO conc [molec/cm3]
TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

RETURN VALUE:

REAL(fp) :: BR_MOLEC_CM3 ! Br conc [molec/cm3]

```
06 Jul 2006 - C. Holmes - Initial version
01 Mar 2012 - R. Yantosca - Now use GET_YMID(I,J,L) from grid_mod.F90
01 Mar 2012 - R. Yantosca - Now use GET_LOCALTIME(I,J,L) from time_mod.F90
09 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met
derived type object
28 Nov 2012 - R. Yantosca - Replace SUNCOS with State_Met%SUNCOS
24 Jul 2014 - R. Yantosca - Now compute BOXVL internally
26 Feb 2015 - E. Lundgren - Remove dependency on pressure_mod (not used)
10 Aug 2015 - J. Fisher - implement variable polar BrO concentrations based
```

```
on temperature and incoming solar radiation

10 Aug 2015 - J. Fisher - only apply diurnal cycle to BrO from pTOMCAT daily means, NOT to polar BrO which represents instantaneous values

10 Aug 2015 - J. Fisher - add upper ice threshold to MERRA conditions for polar BrO release
```

10.5.14 ohno3time

Subroutine OHNO3TIME computes the sum of cosine of the solar zenith angle over a 24 hour day, as well as the total length of daylight. This is needed to scale the offline OH and NO3 concentrations.

INTERFACE:

SUBROUTINE OHNOSTIME

USES:

```
USE CMN_SIZE_MOD

USE GC_GRID_MOD, ONLY : GET_XMID, GET_YMID_R

USE TIME_MOD, ONLY : GET_NHMSb, GET_ELAPSED_SEC

USE TIME_MOD, ONLY : GET_TS_CHEM, GET_DAY_OF_YEAR, GET_GMT
```

REVISION HISTORY:

- 16 Dec 2002 R. Park & R. Yantosca Initial version
- (1) Copy code from COSSZA directly for now, so that we don't get NaN values. Figure this out later (rjp, bmy, 1/10/03)
- (2) Now replace XMID(I) with routine GET_XMID from "grid_mod.f". Now replace RLAT(J) with routine GET_YMID_R from "grid_mod.f". Removed NTIME, NHMSb from the arg list. Now use GET_NHMSb, GET_ELAPSED_SEC, GET_TS_CHEM, GET_DAY_OF_YEAR, GET_GMT from "time_mod.f". (bmy, 3/27/03)
- (3) Now store the peak SUNCOS value for each surface grid box (I,J) in the COSZM array. (rjp, bmy, 3/30/04)
- (4) Also added parallel loop over grid boxes (eck, bmy, 12/8/04)
- 01 Mar 2012 R. Yantosca Now use GET_XMID(I,J,L) from grid_mod.F90
- 01 Mar 2012 R. Yantosca Now use GET_YMID_R(I,J,L) from grid_mod.F90
- 16 May 2016 M. Sulprizio- Remove IJLOOP and change SUNTMP array dimensions from (MAXIJ) to (IIPAR,JJPAR)

10.5.15 calc_hg2_seasalt_lossrate

Subroutine CALC_HG2_SEASALT_LOSSRATE calculates the loss rate of RGM (/s) by uptake of RGM into sea salt aerosol for each model grid. Return value is a loss frequency

(/s)

INTERFACE:

SUBROUTINE CALC_HG2_SEASALT_LOSSRATE(State_Met)

USES:

USE CMN_SIZE_MOD ! Size parameters

USE DAO_MOD, ONLY : IS_WATER

USE PBL_MIX_MOD, ONLY : GET_PBL_TOP_M

USE State_Met_Mod, ONLY : MetState

INPUT PARAMETERS:

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

REMARKS:

The formula used here is a least-squares fit to the full-physics model of sea-salt aerosol emissions, hydroscopic growth, mass-transport limited uptake of Hg(II), and aerosol deposition presented by Holmes et al. (2009) See Holmes et al. 2010 for evaluation of this parameterization. (cdh, 11/25/09)

REVISION HISTORY:

```
25 Nov 2009 - C. Holmes - Initial version
25 Jul 2014 - R. Yantosca - Remove reference to function SFCWINDSQR
04 Dec 2014 - M. Yannetti - Remove reference to RNPBE_MOD
```

10.5.16 get_jno2

Function GET_JNO2 returns monthly mean JNO2 and imposes a diurnal variation.

INTERFACE:

```
FUNCTION GET_JN02( I, J, L, State_Met ) RESULT( JN02_NOW )
```

USES:

```
USE CMN_SIZE_MOD
```

USE GC_GRID_MOD, ONLY : GET_YMID_R

USE PhysConstants

USE State_Met_Mod, ONLY : MetState

USE TIME_MOD, ONLY : GET_TS_CHEM, GET_DAY_OF_YEAR

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I ! Longitude index
INTEGER, INTENT(IN) :: J ! Latitude index
INTEGER, INTENT(IN) :: L ! Level index
```

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

RETURN VALUE:

```
REAL(fp) :: JNO2_NOW ! J(NO2) value [s-1]
```

REMARKS:

```
Impose the diurnal variation of JNO2 found by Parrish et al. (1983) under clear skies. J-NO2 \sim exp(-0.360 * sec(SZA))
```

REVISION HISTORY:

```
01 Mar 2012 - R. Yantosca - Now use GET_YMID_R(I,J,L) from grid_mod.F90 28 Nov 2012 - R. Yantosca - Now pass State_Met via the argument list 28 Nov 2012 - R. Yantosca - Replace SUNCOS with State_Met%SUNCOS
```

10.5.17 partitionhg2

Subroutine PARTITIONHG2 splits Hg(II) into gas and aerosol portions according to the thermodynamic equilibrium determined by temperature and aerosol surface area.

INTERFACE:

```
SUBROUTINE PARTITIONHG2( am_I_Root, Input_Opt, State_Chm, RC )
```

USES:

```
USE CMN_SIZE_MOD

USE ErrCode_Mod

USE ERROR_MOD, ONLY : SAFE_DIV , GEOS_CHEM_STOP

USE Input_Opt_Mod, ONLY : OptInput

USE OCEAN_MERCURY_MOD, ONLY : Fg

USE State_Chm_Mod, ONLY : ChmState

USE State_Met_Mod, ONLY : MetState
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER. INTENT(OUT) :: RC ! Success or failure?
```

```
12-Jul-2010 - H. Amos
                          - Add option to partition Hg2 according to Fg/Fp
02-Jan-2011 - H. Amos
                          - Add/clean up comments
                          - modify algorithms to reflect the fact that
04 Jan 2012 - H. Amos
                            anthropogenic Hg(p) is now emitted as Hg(II)
                            (i.e. it's no longer considered refractory).
28-Mar-2013 - C. Holmes
                          - Since we now assume that all HgP and Hg2
                            actively partition between gas and aerosol,
                            we no longer need to 'reverse' partition.
03 Jun 2013 - R. Yantosca - Now accept am_I_Root, Input_Opt, State_Chm, RC
18 Nov 2014 - M. Yannetti - Took out OCEAN_MERCURY_MOD calling Fp
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected
                            species ID from State_Chm%Map_Advect.
```

10.5.18 red_inplume_grid

Subroutine RED_INPLUME_GRID conducts in plume reduction of Hg2 for selected grids

INTERFACE:

```
SUBROUTINE RED_INPLUME_GRID( I, J, E_plant )
```

INPUT PARAMETERS:

```
INTEGER,INTENT(IN) :: I, J
REAL(fp), INTENT(IN) :: E_plant
```

REVISION HISTORY:

```
11 Jan 2011 - Y. Zhang - Initial version
```

10.5.19 do_red_inplume

USE CMN_SIZE_MOD

IMPLICIT NONE

Subroutine DO_RED_INPLUME conducts in plume reduction of Hg2 for selected grids.

INTERFACE:

```
SUBROUTINE DO_RED_INPLUME( am_I_Root, Input_Opt, RC )
```

USES:

```
USE ERROR_MOD, ONLY : ERROR_STOP
USE GC_GRID_MOD, ONLY : GET_AREA_M2
USE HCO_INTERFACE_MOD, ONLY : HcoState
USE HCO_EmisList_Mod, ONLY : HCO_GetPtr
USE Input_Opt_Mod, ONLY : OptInput
USE TIME_MOD, ONLY : EXPAND_DATE
```

INPUT PARAMETERS:

```
INTENT(IN) :: am_I_Root ! Are we on the root CPU?
LOGICAL,
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

OUTPUT PARAMETERS:

INTEGER. INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

```
11 Jan 2011 - Y. Zhang - Initial version
23 Jun 2014 - R. Yantosca - Now accept am_I_Root, Input_Opt, RC
06 Nov 2014 - R. Yantosca - Replace TRANSFER_2D with direct casts
17 Dec 2014 - R. Yantosca - Leave time/date variables as 8-byte
05 Mar 2015 - R. Yantosca - Add Input_Opt%RES_DIR to data path'
16 Mar 2015 - R. Yantosca - Remove bpch input
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
```

10.5.20 init_mercury

Subroutine INIT_MERCURY allocates and zeroes all module arrays.

INTERFACE:

```
SUBROUTINE INIT_MERCURY( am_I_Root, Input_Opt, State_Chm, RC )
```

USES:

```
USE CMN_DIAG_MOD
USE CMN_SIZE_MOD
USE ErrCode_Mod
```

USE ERROR_MOD, ONLY : ALLOC_ERR, ERROR_STOP
USE Input_Opt_Mod, ONLY : OptInput
USE Species_Mod, ONLY : Species
USE State_Chm_Mod, ONLY : ChmState

INPUT PARAMETERS:

```
LOGICAL.
             INTENT(IN) :: am_I_Root ! Are we on the root CPU?
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

INTENT(OUT) :: RC ! Success or failure? INTEGER,

```
02 Dec 2004 - N. (Eckley) Selin - Initial version
(1) Removed reference to FEMIS array. Now also allocates and zeroes the T44 array. Added reference to CMN_DIAG. Now references N_TRACERS from "tracer_mod.f". (bmy, 2/24/05)
(2) EHgO_an, EHg2_an, EHgP_an are now 2-D arrays. Now modified for updated ocean mercury module. (eck, cdh, sas, bmy, 4/6/06)
27 Sep 2011 - H. Amos - remove LHg_WETDasHNO3 logical, it's obsolete
```

11 Apr 2012 - R. Yantosca - Now retire lai_mod.F; remove call to INIT_LAI

11 Apr 2012 - R. Yantosca - Now move LAI initialization to main.F

03 Jun 2013 - R. Yantosca - Now use fields from Input_Opt

12 Mar 2015 - R. Yantosca - Now test if HEMCO_Collections are defined

25 Apr 2016 - R. Yantosca - Now use species database for tagHg indexing

29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts

01 Jul 2016 - R. Yantosca - Now rename species DB object ThisSpc to SpcInfo

10.5.21 set_options_from_hemco

Overrides some of the Hg simulation settings depending on the inputs that are specified in the HEMCO configuration file.

INTERFACE:

```
SUBROUTINE SET_OPTIONS_FROM_HEMCO( am_I_Root, Input_Opt, RC )
```

USES:

```
USE ERROR_MOD, ONLY : ERROR_STOP
```

USE HCO_ERROR_MOD

USE HCO_INTERFACE_MOD, ONLY : HcoState
USE HCO_ExtList_Mod, ONLY : GetExtOpt
USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root
TYPE(OptInput), INTENT(IN) :: Input_Opt
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REMARKS:

```
06 Jan 2015 - R. Yantosca - Initial version
11 Oct 2016 - R. Yantosca - Move call to DO_RED_INPLUME here
```

10.5.22 cleanup_mercury

Subroutine CLEANUP_MERCURY deallocates all module arrays.

INTERFACE:

SUBROUTINE CLEANUP_MERCURY

REVISION HISTORY:

```
06 Dec 2004 - N. (Eckley) Selin - Initial version (1) Now deallocate MLD, NPP, RAD (sas, bmy, 1/18/05) (2) Now deallocate T44 (bmy, 2/24/05)
```

10.6 Fortran: Module Interface depo_mercury_mod.F

Module DEPO_MERCURY_MOD contains routines to handle deposition fluxes for mercury. **INTERFACE:**

MODULE DEPO_MERCURY_MOD

USES:

```
USE PRECISION_MOD ! For Geos-Chem Precision (fp)

IMPLICIT NONE

PRIVATE
```

PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: ADD_Hg2_DD
PUBLIC :: ADD_Hg2_WD
PUBLIC :: ADD_HgP_DD
PUBLIC :: ADD_HgP_WD
PUBLIC :: ADD_HG2_SNOWPACK
```

PUBLIC :: RESET_HG_DEP_ARRAYS
PUBLIC :: CHECK_DIMENSIONS
PUBLIC :: READ_GTMM_RESTART
PUBLIC :: MAKE_GTMM_RESTART

PUBLIC :: UPDATE_DEP

PUBLIC :: INIT_DEPO_MERCURY
PUBLIC :: CLEANUP_DEPO_MERCURY

PUBLIC DATA MEMBERS:

PUBLIC :: DD_HG2, DD_HGP, WD_HG2, WD_HGP
PUBLIC :: HG2mth_wd, HG0mth_dd, HG2mth_dd

PUBLIC :: SNOW_HG_OC
PUBLIC :: SNOW_HG_LN

PUBLIC :: SNOW_HG_STORED_OC

```
PUBLIC :: SNOW_HG_STORED_LN
   PUBLIC :: LHGSNOW
   REAL(fp), ALLOCATABLE :: DD_Hg2(:,:,:)
   REAL(fp), ALLOCATABLE :: DD_HgP(:,:,:)
   REAL(fp), ALLOCATABLE :: WD_Hg2(:,:,:)
   REAL(fp), ALLOCATABLE :: WD_HgP(:,:,:)
   REAL(fp), ALLOCATABLE :: HGOmth_dd(:,:)
   REAL(fp), ALLOCATABLE :: HG2mth_dd(:,:)
   REAL(fp), ALLOCATABLE :: HG2mth_wd(:,:)
   REAL(fp), ALLOCATABLE :: SNOW_HG_OC(:,:,:)
   REAL(fp), ALLOCATABLE :: SNOW_HG_LN(:,:,:)
   REAL(fp), ALLOCATABLE :: SNOW_HG_STORED_OC(:,:,:)
   REAL(fp), ALLOCATABLE :: SNOW_HG_STORED_LN(:,:,:)
   REAL(fp), ALLOCATABLE :: HgOdryGEOS(:,:), HgIIdryGEOS(:,:),
                             HgIIwetGEOS(:,:)
!PRIVATE DATA MEMBERS:
   CHARACTER(LEN=255) :: GTMM_RST_FILE
   LOGICAL
                       :: LHGSNOW
```

```
23 Apr 2010 - C. Carouge - Initial version

12 Apr 2011 - J. Fisher - Add missing code from Holmes 2010

08 Feb 2012 - R. Yantosca - Add modifications for GEOS-5.7.x met

20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete

07 Nov 2014 - M. Yannetti - Added PRECISION_MOD

30 May 2013 - J. Fisher - Add land snow Hg reservoirs

06 Aug 2015 - J. Fisher - Add stored snow Hg reservoirs (orig.

29/11/11)

26 Apr 2016 - R. Yantosca - Make N_Hg_CATS IDTHg0, IDTHg2 module variables

29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90
```

$10.6.1 \quad add_Hg2_dd$

Subroutine ADD_Hg2_DD computes the amount of Hg(II) dry deposited out of the atmosphere into the column array DD_Hg2.

INTERFACE:

```
SUBROUTINE ADD_Hg2_DD( I, J, HG_CAT, DRY_Hg2 )
```

INPUT PARAMETERS:

10.6.2 add_Hg2_wd

Subroutine ADD_Hg2_WD computes the amount of Hg(II) wet scavenged out of the atmosphere into the column array WD_Hg2.

INTERFACE:

```
SUBROUTINE ADD_Hg2_WD( I, J, Hg_Cat, WET_Hg2 )
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I, J    ! Grid box lon & lat indices
INTEGER, INTENT(IN) :: Hg_Cat    ! Hg category number
REAL(fp), INTENT(IN) :: WET_Hg2    ! Hg(II) scavenged out of the
! atmosphere [kg]
```

REVISION HISTORY:

10.6.3 add_HgP_dd

Subroutine ADD_HgP_DD computes the amount of HgP dry deposited out of the atmosphere into the column array DD_HgP.

INTERFACE:

```
SUBROUTINE ADD_HgP_DD( I, J, Hg_Cat, DRY_HgP )
```

INPUT PARAMETERS:

10.6.4 add_HgP_wd

Subroutine ADD_HgP_WD computes the amount of HgP wet scavenged out of the atmosphere into the column array WD_HgP.

INTERFACE:

```
SUBROUTINE ADD_HgP_WD( I, J, Hg_Cat, WET_HgP )
```

INPUT PARAMETERS:

REVISION HISTORY:

10.6.5 add_hg2_snowpack

Subroutine ADD_Hg2_SNOWPACKS adds Hg2 deposition to snowpack.

INTERFACE:

```
SUBROUTINE ADD_HG2_SNOWPACK( I, J, Hg_Cat, DEP_Hg2, State_Met )
```

USES:

```
USE DAO_MOD, ONLY : IS_ICE, IS_LAND
USE DIAGO3_MOD, ONLY : ADO3, NDO3
USE State_Met_Mod, ONLY : MetState
```

INTENT(IN) :: I, J

INTENT(IN) :: Hg_Cat

! Grid box lon & lat indices

! Hg category number

! Hg2 (or HgP) deposited

INPUT PARAMETERS:

INTEGER,

INTEGER,

REAL(fp),

! Arguments as input

```
INTENT(IN) :: Dep_Hg2
      TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
REVISION HISTORY:
   02 Sep 2008 - C. Holmes - Initial version
   23 Apr 2010 - C. Carouge - Moved from mercury_mod.f to depo_mercury_mod.f
   25 Aug 2010 - R. Yantosca - Treat MERRA in the same way as GEOS-5
   26 Apr 2011 - J. Fisher - Use MERRA land fraction information
   12 Apr 2011 - J. Fisher - Add missing code from Holmes 2010
   13 Apr 2011 - R. Yantosca - Bug fix: reference IS_LAND from dao_mod.f
    8 Feb 2012 - R. Yantosca - Treat GEOS-5.7.x in the same way as MERRA
   09 Nov 2012 - M. Payer
                             - Replaced all met field arrays with State_Met
                               derived type object
   20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
   26 Sep 2013 - R. Yantosca - Renamed GEOS_57 Cpp switch to GEOS_FP
   30 May 2013 - J. Fisher - Add land snow Hg reservoirs
                             - Store reservoir of non-reducible Hg in snowpack
   06 Aug 2015 - J. Fisher
                               (orig. 29/11/11)
   11 Aug 2015 - R. Yantosca - MERRA2 behaves the same way as GEOS_FP
```

10.6.6 reset_hg_dep_arrays

Subroutine RESET_Hg_DEP_ARRAYS resets the wet and dry deposition arrays for Hg(II) and Hg(p) to zero. This allows us to call OCEAN_MERCURY_FLUX and LAND_MERCURY_FLUX in any order in MERCURY_MOD.

25 Apr 2016 - R. Yantosca - Remove reference to routines GET_HG2_CAT and

Hg_Cat argument.

GET_HGP_CAT, these are now passed in as the

INTERFACE:

SUBROUTINE RESET_HG_DEP_ARRAYS

```
02 Sep 2008 - C. Holmes
                         - Initial version
23 Apr 2010 - C. Carouge - Moved from ocean_mercury_mod.f to
                           depo_mercury_mod.f
```

10.6.7 make_gtmm_restart

MAKE_GTMM_RESTART writes a GTMM restart file with deposition fluxes and store deposition fluxes for continuous runs.

INTERFACE:

```
SUBROUTINE MAKE_GTMM_RESTART( am_I_Root, Input_Opt, NYMD,
& NHMS, TAU, RC )
```

USES:

```
USE BPCH2_MOD

USE CMN_SIZE_MOD

! Size parameters

USE ErrCode_Mod

USE GC_GRID_MOD,

ONLY : GET_XOFFSET, GET_YOFFSET

USE Input_Opt_Mod,

ONLY : OptInput

USE inquireMod,

ONLY : findFreeLUN

USE TIME_MOD,

ONLY : EXPAND_DATE
```

INPUT PARAMETERS:

USE TIME_MOD,

```
INTEGER, INTENT(IN) :: NYMD ! Year-Month-Date
INTEGER, INTENT(IN) :: NHMS ! and Hour-Min-Sec
REAL(f8), INTENT(IN) :: TAU ! TAU value: hrs since 1/1/85
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

ONLY : GET_CT_DYN, GET_CT_CHEM

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REVISION HISTORY:

```
15 Sep 2009 - C. Carouge - Initial version
03 Aug 2012 - R. Yantosca - Move calls to findFreeLUN out of DEVEL block
07 Aug 2012 - R. Yantosca - Now print LUN used to open file
20 Jun 2014 - R. Yantosca - Remove reference to directory_mod.F
```

$10.6.8 \quad read_gtmm_restart$

Subroutine READ_GTMM_RESTART reads dry and wet deposition for mercury from GTMM restart.

INTERFACE:

```
SUBROUTINE READ_GTMM_RESTART( am_I_Root, Input_Opt, & YYYYMMDD, HHMMSS,
```

```
& HgOdryGEOS, HgIIdryGEOS,
& HgIIwetGEOS, RC )
```

USES:

```
USE BPCH2_MOD, ONLY : OPEN_BPCH2_FOR_READ

USE CMN_SIZE_MOD

USE ErrCode_Mod

USE ERROR_MOD, ONLY : DEBUG_MSG

USE FILE_MOD, ONLY : IOERROR

USE Input_Opt_Mod, ONLY : OptInput
```

USE inquireMod, ONLY : findFreeLun
USE State_Chm_Mod, ONLY : ChmState
USE TIME_MOD, ONLY : EXPAND_DATE

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: YYYYMMDD, HHMMSS

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?!
```

REAL(fp), DIMENSION(IIPAR, JJPAR) :: HgOdryGEOS
REAL(fp), DIMENSION(IIPAR, JJPAR) :: HgIIdryGEOS
REAL(fp), DIMENSION(IIPAR, JJPAR) :: HgIIwetGEOS

REVISION HISTORY:

```
15 Sep 2009 - C. Carouge - Initial version
```

25 Jun 2014 - R. Yantosca - Remove references to tracer_mod.F

29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts

10.6.9 update_dep

Subroutine UPDATE_DEP update the monthly average for wet and dry deposition of Hg0 and Hg2 for mercury from GTMM restart.

INTERFACE:

```
SUBROUTINE UPDATE_DEP( NN )
```

USES:

```
#if defined( BPCH_DIAG )
    USE DIAG_MOD, ONLY : AD38, AD39
    USE DIAG_MOD, ONLY : AD44
#endif
    USE TIME_MOD, ONLY : GET_CT_DYN, GET_CT_CHEM
```

INPUT PARAMETERS:

```
INTEGER :: NN    ! Hg2 ID for wet deposition
```

REVISION HISTORY:

```
04 June 2010 - C. Carouge - Initial version
```

10.6.10 check_dimensions

Subroutine CHECK_DIMENSIONS makes sure that the dimensions of the Hg restart file extend to cover the entire grid.

INTERFACE:

```
SUBROUTINE CHECK_DIMENSIONS( NI, NJ, NL )
```

USES:

```
USE ERROR_MOD, ONLY : GEOS_CHEM_STOP USE CMN_SIZE_MOD
```

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NI, NJ, NL
```

REVISION HISTORY:

```
30 Aug 2010 - S. Strode, C. Holmes - Initial version
```

10.6.11 init_depo_mercury

Subroutine INIT_DEPO_MERCURY initialize deposition arrays for mercury.

INTERFACE:

```
SUBROUTINE INIT_DEPO_MERCURY( am_I_Root, Input_Opt, & State_Chm, RC )

!USES

USE CMN_SIZE_MOD

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ALLOC_ERR

USE Input_Opt_Mod, ONLY : OptInput

USE Species_Mod, ONLY : Species

USE State_Chm_Mod, ONLY : ChmState
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REVISION HISTORY:

```
23 Apr 2010 - C. Carouge - Moved arrays allocation from ocean_mercury_mod.f
23 Jun 2014 - R. Yantosca - Now accept am_I_Root, Input_Opt, RC
30 May 2013 - J. Fisher - Add land snow Hg reservoirs
06 Aug 2015 - J. Fisher - Add stored snow Hg reservoirs (orig. 29/11/11)
25 Apr 2016 - R. Yantosca - Now handle all Hg indexing locally
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
01 Jul 2016 - R. Yantosca - Now rename species DB object ThisSpc to SpcInfo
```

10.6.12 cleanup_depo_mercury

Subroutine CLEANUP_DEPO_MERCURY deallocate all arrays

INTERFACE:

SUBROUTINE CLEANUP_DEPO_MERCURY

REVISION HISTORY:

```
23 Apr 2010 - C. Carouge - Moved from ocean_mercury_mod.f
30 May 2013 - J. Fisher - Add land snow Hg reservoirs
06 Aug 2015 - J. Fisher - Add stored snow Hg reservoirs (orig. 29/11/11)
```

10.7 Fortran: Module Interface land_mercury_mod.F

Module LAND_MERCURY_MOD contains variables and routines for the land emissions for the GEOS-Chem mercury simulation.

INTERFACE:

```
MODULE LAND_MERCURY_MOD
```

USES:

```
USE HCO_ERROR_MOD ! For real precisions (hp)
USE PRECISION_MOD ! For GEOS-Chem Precision (fp, f4, f8)

IMPLICIT NONE
PRIVATE
```

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: BIOMASSHG
PUBLIC :: VEGEMIS
PUBLIC :: SOILEMIS

PUBLIC :: LAND_MERCURY_FLUX

PUBLIC :: GTMM_DR

PUBLIC :: SNOWPACK_MERCURY_FLUX
PUBLIC :: INIT_LAND_MERCURY
PUBLIC :: CLEANUP_LAND_MERCURY

REVISION HISTORY:

```
02 Jun 2010 - N. E. Selin, C. Carouge - Initial version
02 Jun 2010 - C. Carouge - Group all land emissions routine for mercury into this new module.
13 Aug 2010 - R. Yantosca - Added modifications for MERRA
25 Aug 2010 - R. Yantosca - Treat MERRA in same way as GEOS-5
30 Aug 2010 - R. Yantosca - Added more ProTeX headers
12 Apr 2011 - J. Fisher - Add missing code from Holmes 2010
08 Feb 2012 - R. Yantosca - Treat GEOS-5.7.x in the same way as MERRA
01 Mar 2012 - R. Yantosca - Now reference new grid_mod.F90
11 Apr 2012 - R. Yantosca - Now reference new modis_lai_mod.F90
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
17 Nov 2014 - M. Yannetti - Added PRECISION_MOD
29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90
```

10.7.1 land_mercury_flux

Subroutine LAND_MERCURY_FLUX calculates emissions of Hg(0) from prompt recycling of previously deposited mercury to land, in [kg/s].

INTERFACE:

SUBROUTINE LAND_MERCURY_FLUX(LFLUX, LHGSNOW, State_Met)

USES:

```
USE CMN_SIZE_MOD ! Size parameters
USE DAO_MOD, ONLY : IS_ICE, IS_LAND
```

USE DEPO_MERCURY_MOD, ONLY : WD_HGP, WD_HG2, DD_HGP, DD_HG2

USE State_Met_Mod, ONLY : MetState
USE TIME_MOD, ONLY : GET_TS_EMIS

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: LHGSNOW ! Use HgO from snow?

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT) :: LFLUX(IIPAR,JJPAR,N_Hg_CATS) ! HgO flux ! [kg/s]
```

```
30 Aug 2010 - N. E. Selin, C. Holmes, B. Corbitt - Initial version
```

- (1) Now uses SNOWMAS from DAO_MOD for compatibility with GEOS-5. (eds 7/30/08)
- (2) Now includes REEMFRAC in parallelization; previous versions may have overwritten variable. (cdh, eds 7/30/08)
- (3) Now also reemit Hg(0) from ice surfaces, including sea ice (cdh, 8/19/08)
- 13 Aug 2010 R. Yantosca Add modifications for MERRA
- 25 Aug 2010 R. Yantosca Treat MERRA in same way as GEOS-5
- 26 Apr 2011 J. Fisher Use MERRA land fraction information
- 12 Apr 2011 J. Fisher Add missing code from Holmes 2010
- 08 Feb 2012 R. Yantosca Treat GEOS-5.7.x in the same way as MERRA
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met derived type object
- 26 Sep 2013 R. Yantosca Renamed GEOS_57 Cpp switch to GEOS_FP
- 12 Aug 2015 R. Yantosca Add support for MERRA2 meteorology

10.7.2 biomasshg

Subroutine BIOMASSHG is the subroutine for Hg(0) emissions from biomass burning. These emissions are active only for present day simulations and not for preindustrial simulations.

INTERFACE:

```
SUBROUTINE BIOMASSHG( am_I_Root, Input_Opt, EHgO_bb, RC )
```

USES:

```
USE CMN_SIZE_MOD
```

USE CMN_DIAG_MOD

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP

USE HCO_ERROR_MOD

USE HCO_STATE_MOD, ONLY : HCO_STATE
USE HCO_INTERFACE_MOD, ONLY : GetHcoDiagn
USE HCO_INTERFACE_MOD, ONLY : HcoState
USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Root CPU
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options

OUTPUT PARAMETERS:

REAL(fp), DIMENSION(:,:),INTENT(OUT) :: EHgO_bb

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REMARKS:

Emissions are based on an inventory of CO emissions from biomass burning (Duncan et al. J Geophys Res 2003), multiplied by a Hg/CO ratio in BB plumes from Franz Slemr (Poster, EGU 2006).

Slemr surveyed emission factors from measurements worldwide. Although his best estimate was 1.5e-7 mol Hg/ mol CO, we chose the highest value (2.1e-7 mol Hg/ mol CO) in the range because the simulations shown in Selin et al. (GBC 2008) required large Hg(0) emissions to sustain reasonable atmospheric Hg(0) concentrations. (eck, 11/13/2008)

REVISION HISTORY:

```
30 Jul 2008 - N. E. Selin, C. Holmes, B. Corbitt - Initial version
12 Apr 2011 - J. Fisher - Add missing code from Holmes 2010
01 Mar 2012 - R. Yantosca - Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
15 Aug 2014 - R. Yantosca - Removed reference to IDBCO; now obsolete
23 Sep 2014 - C. Keller - Now use HEMCO diagnostics
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
```

10.7.3 vegemis

Subroutine VEGEMIS is the subroutine for Hg(0) emissions from vegetation by evapotranspiration.

INTERFACE:

```
! Bug fix: VEGEMIS shouldn't be tied to GCAP emissions
! (jaf, eds, 4/1/11)
SUBROUTINE VEGEMIS( am_I_Root, Input_Opt, State_Met,
LVEGEMIS, EHgO_dist, EHgO_vg, RC)
```

USES:

```
USE CMN_SIZE_MOD

USE DAO_MOD, ONLY : IS_LAND

USE ErrCode_Mod

USE GC_GRID_MOD, ONLY : GET_AREA_M2

USE Input_Opt_Mod, ONLY : OptInput

USE State_Met_Mod, ONLY : MetState

USE TIME_MOD, ONLY : GET_MONTH, ITS_A_NEW_MONTH

USE TIME_MOD, ONLY : GET_TS_EMIS
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Met State object

LOGICAL, INTENT(IN) :: LVEGEMIS !

REAL(fp), DIMENSION(:,:), INTENT(IN) :: EHgO_dist !
```

OUTPUT PARAMETERS:

```
REAL(fp), DIMENSION(:,:), INTENT(OUT) :: EHgO_vg
                       INTENT(OUT) :: RC
                                                   ! Success or failure?
```

REMARKS:

Vegetation emissions are proportional to the evapotranspiration rate and the soil water mercury content. We assume a constant concentration of mercury in soil matter, based on the preindustrial and present-day simulations described in Selin et al. (GBC 2008) and in SOILEMIS subroutine. From the soil matter Hg concentration, we calculate a soil water Hg concentration in equilibrium (Allison and Allison, 2005).

NASA provides a climatology of evapotranspiration based on a water budget model (Mintz and Walker, 1993).

Calculate vegetation emissions following Xu et al (1999)

Fc = Ec Cw

Fc is HgO flux (ng m-2 s-1)

Ec is canopy transpiration (m s-1)

Cw is conc of HgO in surface soil water (ng m-3)

Calculate Cw from the Allison and Allison (2005) equilibrium formula

Cw = Cs / Kd

Cs is the concentration of Hg is surface soil solids, ng/g

Kd is the equilibrium constant = [sorbed]/[dissolved]

 $log Kd = 3.8 L/kg \rightarrow Kd = 6310 L /kg = 6.31D-3 m3/g$

We assume a global mean Cs = 45 ng/g for the preindustrial period. In iterative simulations we redistribute this according to the deposition pattern while maintining the global mean. The scaling factor, EHgO_dist, also accounts for the anthropogenic enhancement of soil Hg in the present day.

REVISION HISTORY:

```
30 Aug 2010 - N. Eckley, C. Holmes, B. Corbitt - Initial version
```

01 Mar 2012 - R. Yantosca - Now use GET_AREA_M2(I,J,L) from grid_mod.F90

20 Jun 2014 - R. Yantosca - Now accept Input_Opt via the arg list

10.7.4 soilemis

Subroutine SOILEMIS is the subroutine for Hg(0) emissions from soils.

INTERFACE:

```
SUBROUTINE SOILEMIS( EHgO_dist, EHgO_so, State_Met )
```

USES:

```
USE CMN_SIZE_MOD
                        ! Size par
ONLY : IS_LAND
                                 ! Size parameters
```

USE DAO_MOD,

USE GC_GRID_MOD, ONLY : GET_AREA_M2

USE MODIS_LAI_MOD, ONLY : ISOLAI => GC_LAI
USE State_Met_Mod, ONLY : MetState
USE TIME MOD

USE TIME_MOD, ONLY : GET_MONTH, ITS_A_NEW_MONTH

USE TIME_MOD, ONLY : GET_TS_EMIS

INPUT PARAMETERS:

REAL(fp), DIMENSION(:,:), INTENT(IN) :: EHgO_dist

TYPE(MetState), INTENT(IN) :: State_Met ! Met State object

OUTPUT PARAMETERS:

REAL(fp), DIMENSION(:,:), INTENT(OUT) :: EHgO_so

REMARKS:

Soil emissions are a function of solar radiation at ground level (accounting for attenuation by leaf canopy) and surface temperature. The radiation dependence from Zhang et al. (2000) is multiplied by the temperature dependence from Poissant and Casimir (1998). Finally, this emission factor is multiplied by the soil mercury concentration and scaled to meet the global emission total. Comments on soil Hg concentration:

We chose the preindustrial value of 45 ng Hg/g dry soil as the mean of the range quoted in Selin et al. (GBC 2008): 20-70 ng/g (Andersson, 1967; Shacklette et al., 1971; Richardson et al., 2003; Frescholtz and Gustin, 2004). Present-day soil concentrations are thought to be 15% greater than preindustrial (Mason and Sheu 2002), but such a difference is much less than the range of concentrations found today, so not well constrained. We calculate the present-day soil Hg distribution by adding a global mean 6.75 ng/g (=0.15 * 45 ng/g) according to present-day Hg deposition. (eck, 11/13/08)

- 30 Aug 2010 N. Eckley, B. Corbitt Initial version
- (1) Added comments. (cdh, eds, 7/30/08)
- (2) Now include light attenuation by the canopy after sunset. Emissions change by < 1% in high-emission areas (cdh, 8/13/2008)
- (3) Removed FRCLND for consistency with other Hg emissions (cdh, 8/19/08)
- 2 June 2010 C. Carouge Solve
- 13 Aug 2010 R. Yantosca Added modifications for MERRA
- 25 Aug 2010 R. Yantosca Treat MERRA in same way as GEOS-5
- 26 Apr 2011 J. Fisher Use MERRA land fraction information
- 12 Apr 2011 J. Fisher Bug fixes, add missing code from Holmes 2010
- 08 Feb 2012 R. Yantosca Treat GEOS-5.7.x in the same way as MERRA
- 10 Feb 2012 R. Yantosca Extend #if statement for SOIL_EMIS_FAC in order to get the code to compile w/o error.
- 01 Mar 2012 R. Yantosca Now use GET_AREA_CM2(I,J,L) from grid_mod.F90

```
11 Apr 2012 - R. Yantosca - Replace lai_mod.F with modis_lai_mod.F90
09 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met
derived type object
28 Nov 2012 - R. Yantosca - Replace SUNCOS with State_Met%SUNCOS
26 Sep 2013 - R. Yantosca - Renamed GEOS_57 Cpp switch to GEOS_FP
12 Aug 2015 - R. Yantosca - Add support for MERRA2 meteorology
```

10.7.5 snowpack_mercury_flux

Subroutine SNOWPACK_MERCURY_FLUX calculates emission of $\mathrm{Hg}(0)$ from snow and ice.

INTERFACE:

SUBROUTINE SNOWPACK_MERCURY_FLUX(FLUX, LHGSNOW, State_Met)

USES:

```
USE CMN_SIZE_MOD ! Size parameters

USE DEPO_MERCURY_MOD, ONLY : SNOW_HG_OC, SNOW_HG_LN

USE State_Met_Mod, ONLY : MetState

USE TIME_MOD, ONLY : GET_TS_EMIS
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: LHGSNOW ! Use Hg from snow?

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT) :: FLUX(IIPAR, JJPAR, N_Hg_CATS) ! HgO flux ! [kg/s]
```

REMARKS:

Emissions are a linear function of Hg mass stored in the snowpack. The Hg lifetime in snow is assumed to be 180 d when T< 270K and 7 d when T>270K $E = k * SNOW_HG$: k = 6D-8 if T<270K, 1.6D-6 otherwise These time constants reflect the time scales of emission observed in the Arctic and in field studies. Holmes et al 2010

Formulation from Holmes et al. 2010 is now obsolete. Instead, emissions from snow are tied to solar radiation, not temperature. Effective rate constant is in the mid-range of values estimated by Durnford and Dastoor (2011) and consistent with surface air HgO observations, as described in Fisher et al. (2011, in review).

Note that only MERRA provides incident shortwave radiation; other met fields only provide *net* shortwave radiation. The parameterization was designed and tested using MERRA, and therefore may not work as well with other met fields

```
15 Sep 2009 - C. Holmes, S. Carouge - Initial version
30 Aug 2010 - R. Yantosca - Added ProTex headers
12 Apr 2011 - J. Fisher - Add missing code from Holmes 2010
18 Nov 2011 - J. Fisher - Update to radiation-dependent formulation
09 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met
derived type object
28 Nov 2012 - R. Yantosca - Replace SUNCOS with State_Met%SUNCOS
30 Mar 2015 - R. Yantosca - Remove obsolete variables
```

10.7.6 gtmm_dr

GTMM_DR is a driver to call GTMM from GEOS-Chem.

INTERFACE:

```
SUBROUTINE GTMM_DR( am_I_Root, Input_Opt, State_Met, HgOgtm, RC )
```

USES:

```
USE BPCH2_MOD

USE CMN_SIZE_MOD

! Size parameters

USE DAO_MOD, ONLY: IS_LAND

USE DEPO_MERCURY_MOD, ONLY: CHECK_DIMENSIONS

USE DEPO_MERCURY_MOD, ONLY: WD_Hg2, WD_HgP, DD_HgP, DD_Hg2

USE DEPO_MERCURY_MOD, ONLY: READ_GTMM_RESTART

USE ErrCode_Mod

USE FILE_MOD, ONLY: IOERROR

USE Input_Opt_Mod, ONLY: OptInput

USE inquireMod, ONLY: findFreeLun

USE State_Met_Mod, ONLY: MetState

USE TIME_MOD, ONLY: EXPAND_DATE, YMD_EXTRACT

USE TIME_MOD, ONLY: GET_NYMD, GET_NHMS
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

OUTPUT PARAMETERS:

REMARKS:

```
NOTE: BINARY PUNCH INPUT IS BEING PHASED OUT. THIS DATA
                                     #####
    WILL EVENTUALLY BE READ IN FROM netCDF FILES VIA HEMCO!
#####
                                     #####
#####
      -- Bob Yantosca (05 Mar 2015)
                                     #####
```

REVISION HISTORY:

```
15 Sep 2009 - C. Carouge - Initial version
03 Aug 2012 - R. Yantosca - Move calls to findFreeLUN out of DEVEL block
05 Mar 2015 - R. Yantosca - Now add Input_Opt%RES_DIR to data path
```

10.7.7 init_land_mercury

Subroutine INIT_LAND_MERCURY allocates and zeroes all module arrays.

INTERFACE:

```
SUBROUTINE INIT_LAND_MERCURY( am_I_Root, Input_Opt,
                               State_Chm, RC
&
```

USES:

```
USE ErrCode_Mod
                    ONLY : ALLOC_ERR
ONLY : OptInput
USE ERROR_MOD,
USE Input_Opt_Mod,
                        ONLY : ChmState
```

INPUT PARAMETERS:

USE CMN_SIZE_MOD

USE State_Chm_Mod,

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER,
           INTENT(OUT) :: RC ! Success or failure?
```

```
14 Sep 2009 - C. Carouge - Initial version
23 Jun 2014 - R. Yantosca - Now accept am_I_Root, Input_Opt, RC
```

10.7.8 cleanup_land_mercury

Subroutine CLEANUP_LAND_MERCURY deallocates all module arrays.

INTERFACE:

SUBROUTINE CLEANUP_LAND_MERCURY

REVISION HISTORY:

```
14 Sep 2009 - C. Carouge - Initial version
```

10.8 Fortran: Module Interface pops_mod.F

Module POPS_MOD contains variables and routines for the GEOS-Chem peristent organic pollutants (POPs) simulation.

INTERFACE:

```
MODULE POPS_MOD
```

USES:

```
USE PhysConstants ! For physical constants
USE PRECISION_MOD ! For GEOS-Chem Precision (fp, f4, f8)

IMPLICIT NONE
PRIVATE
```

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: CHEMPOPS
PUBLIC :: INIT_POPS

REMARKS:

POPs Tracers

```
(1 ) POPG : Gaseous POP - total tracer
(2 ) POPPOC : OC-sorbed POP - total tracer
(3 ) POPPBC : BC-sorbed POP - total tracer
```

```
20 Sep 2010 - N.E. Selin - Initial Version

04 Jan 2011 - C.L. Friedman - Expansion on initial version

21 Aug 2014 - M. Sulprizio - Removed emissions routines now handled by HEMCO

04 Mar 2015 - R. Yantosca - Use REAL(f4) for pointer args to HCO_GetPtr

23 Dec 2015 - E. Lundgren - Use global physical constants

22 Jun 2016 - R. Yantosca - Rename species ID flags from IDT* to id_*

22 Jun 2016 - R. Yantosca - Rename species drydep flags from DRY* to dd_*

29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90
```

10.8.1 chempops

Subroutine CHEMPOPS is the driver routine for POPs chemistry (eck, 9/20/10)

INTERFACE:

```
SUBROUTINE CHEMPOPS( am_I_Root, Input_Opt,
& State_Met, State_Chm, RC )
```

USES:

```
USE CMN_SIZE_MOD
USE DRYDEP_MOD,
                        ONLY : DEPSAV
USE ErrCode_Mod
USE ERROR_MOD,
                        ONLY : DEBUG_MSG
USE ERROR_MOD,
                        ONLY : ERROR_STOP
USE HCO_INTERFACE_MOD, ONLY : HcoState
USE HCO_EmisList_Mod,
                        ONLY : HCO_GetPtr
USE Input_Opt_Mod,
                        ONLY : OptInput
USE State_Chm_Mod,
                        ONLY : ChmState
USE State_Met_Mod,
                        ONLY : MetState
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

```
TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

```
INTEGER, INTENT(OUT) :: RC ! Success or failure?
```

REVISION HISTORY:

10.8.2 chem_popgp

Subroutine CHEM_POPGP is the chemistry subroutine for the oxidation, gas-particle partitioning, and deposition of POPs. (eck, clf, 1/4/2011)

INTERFACE:

```
SUBROUTINE CHEM_POPGP ( V_DEP_G,
                           V_DEP_P_OCPO, V_DEP_P_OCPI,
                           V_DEP_P_BCPO, V_DEP_P_BCPI,
     lг.
     &
                           am_I_Root, Input_Opt,
     &
                           State_Met,
                                        State_Chm,
     7
                           RC )
USES:
      USE CMN_DIAG_MOD
      USE CMN_SIZE_MOD
#if defined( BPCH_DIAG )
      USE DIAG_MOD,
                           ONLY: AD44
#endif
      USE DIAG53_MOD
      USE ErrCode_Mod
      USE ERROR_MOD,
                           ONLY : DEBUG_MSG
      USE ERROR_MOD,
                           ONLY : SAFE_DIV
                         ONLY : GET_AREA_CM2
      USE GC_GRID_MOD,
      USE Input_Opt_Mod,
                          ONLY : OptInput
      USE PBL_MIX_MOD,
                           ONLY : GET_FRAC_UNDER_PBLTOP
      USE State_Chm_Mod,
                           ONLY : ChmState
      USE State_Met_Mod,
                           ONLY : MetState
      USE TIME_MOD,
                           ONLY : GET_TS_CHEM
INPUT PARAMETERS:
      ! Dry deposition frequencies [/s]
      REAL(fp),
                   INTENT(IN)
                                 :: V_DEP_G(IIPAR, JJPAR)
      REAL(fp),
                                 :: V_DEP_P_OCPO(IIPAR,JJPAR)
                   INTENT(IN)
      REAL(fp),
                   INTENT(IN)
                                 :: V_DEP_P_BCPO(IIPAR, JJPAR)
      REAL(fp),
                   INTENT(IN) :: V_DEP_P_OCPI(IIPAR,JJPAR)
                                :: V_DEP_P_BCPI(IIPAR,JJPAR)
      REAL(fp),
                   INTENT(IN)
      LOGICAL,
                    INTENT(IN)
                                :: am_I_Root ! Is this the root CPU?
      TYPE(OptInput), INTENT(IN)
                                 :: Input_Opt   ! Input Options object
      TYPE(MetState), INTENT(IN)
                                 :: State_Met
                                              ! Meteorology State object
INPUT/OUTPUT PARAMETERS:
      OUTPUT PARAMETERS:
                                             ! Success or failure?
      INTEGER,
                    INTENT(OUT) :: RC
REMARKS:
```

References:

⁽¹⁾ For OH rate constant: Brubaker & Hites. 1998. OH reaction kinetics of PAHs and PCDD/Fs. J. Phys. Chem. A. 102:915-921.

```
20 Sep 2010 - N.E. Selin - Initial Version based on CHEM_HGO_HG2
29 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met
derived type object

14 Apr 2014 - R. Yantosca - Now prevent div-by-zero in computations below

17 Sep 2014 - C. Keller - Renamed EmisList_GetDataArr to HCO_GetPtr

31 May 2016 - E. Lundgren - Replace Input_Opt%XNUMOL with AVO/(emMW_g*1e-3)
where emMW_g is emitted MW from species database

30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected
species ID from State_Chm%Map_Advect.

10 Aug 2016 - R. Yantosca - Removed temporary tracer-removal code

06 Oct 2016 - R. Yantosca - Now zero C_NO3 to avoid floating-point error
```

$10.8.3 \text{ rxn_ox_nodep}$

Subroutine RXN_OX_NODEP calculates new mass of POPG for given oxidation rates, without any deposition. This is for the free troposphere, or simulations with deposition turned off. (clf, 1/27/11, based on RXN_REDOX_NODEP in mercury_mod.f).

INTERFACE:

```
SUBROUTINE RXN_OX_NODEP( OLD_POPG, K_OX, E_KOX_T, & NEW_POPG, GROSS_OX )
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: OLD_POPG
REAL(fp), INTENT(IN) :: K_OX
REAL(fp), INTENT(IN) :: E_KOX_T
```

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT) :: NEW_POPG
REAL(fp), INTENT(OUT) :: GROSS_OX
```

REVISION HISTORY:

```
27 January 2011 - CL Friedman - Initial Version
```

$10.8.4 \text{ rxn_ox_withdep}$

Subroutine RXN_OX_WITHDEP calculates new mass of POPG for given rates of oxidation and deposition. This is for the boundary layer. (clf, 1/27/11, based on RXN_REDOX_NODEP in mercury_mod.f).

INTERFACE:

```
SUBROUTINE RXN_OX_WITHDEP( OLD_POPG, K_OX, K_DEPG, DT, E_KOX_T, & NEW_POPG, GROSS_OX, DEP_POPG )
USES:
USE ERROR_MOD, ONLY: ERROR_STOP
```

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: OLD_POPG
REAL(fp), INTENT(IN) :: DT
REAL(fp), INTENT(IN) :: K_OX
REAL(fp), INTENT(IN) :: K_DEPG
REAL(fp), INTENT(IN) :: E_KOX_T
```

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT) :: NEW_POPG
REAL(fp), INTENT(OUT) :: GROSS_OX
REAL(fp), INTENT(OUT) :: DEP_POPG
```

REVISION HISTORY:

27 January 2011 - CL Friedman - Initial Version

10.8.5 no_rxn_withdep

Subroutine NO_RXN_WITHDEP calculates new mass of POPP for given rate of deposition. No oxidation of POPP. This is for the boundary layer. (clf, 2/9/11)

INTERFACE:

```
SUBROUTINE NO_RXN_WITHDEP( OLD_POPP, K_DEPP, DT, & NEW_POPP, DEP_POPP )
```

USES:

USE ERROR_MOD, ONLY : ERROR_STOP

INPUT PARAMETERS:

```
REAL(fp), INTENT(IN) :: OLD_POPP
REAL(fp), INTENT(IN) :: K_DEPP
REAL(fp), INTENT(IN) :: DT
```

OUTPUT PARAMETERS:

```
REAL(fp), INTENT(OUT) :: NEW_POPP
REAL(fp), INTENT(OUT) :: DEP_POPP
```

```
9 February 2011 - CL Friedman - Initial Version
```

$10.8.6 \text{ get_oh}$

Function GET_OH returns monthly mean OH and imposes a diurnal variation.

INTERFACE:

```
FUNCTION GET_OH( I, J, L, State_Met ) RESULT( OH_MOLEC_CM3 )
```

USES:

```
USE CMN_SIZE_MOD ! Size parameters
```

USE State_Met_Mod, ONLY : MetState
USE TIME_MOD, ONLY : GET_TS_CHEM

INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I, J, L
```

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

REMARKS:

Copied GET_OH function from mercury_mod.f - CLF

REVISION HISTORY:

```
03 Feb 2011 - CL Friedman - Initial Version
```

29 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met derived type object

23 Sep 2014 - M. Sulprizio- Now get OH for offline aerosol sim from HEMCO

10.8.7 ohno3time

Subroutine OHNO3TIME computes the sum of cosine of the solar zenith angle over a 24 hour day, as well as the total length of daylight. This is needed to scale the offline OH and NO3 concentrations. (rjp, bmy, 12/16/02, 12/8/04)

INTERFACE:

SUBROUTINE OHNOSTIME

USES:

```
USE CMN_SIZE_MOD    ! Size parameters
```

USE GC_GRID_MOD, ONLY : GET_XMID, GET_YMID_R

USE TIME_MOD, ONLY : GET_NHMSb, GET_ELAPSED_SEC

USE TIME_MOD, ONLY: GET_TS_CHEM, GET_DAY_OF_YEAR, GET_GMT

REVISION HISTORY:

```
20 Sep 2010 - N.E. Selin - Initial Version for POPS_MOD
```

16 May 2016 - M. Sulprizio- Remove IJLOOP and change SUNTMP array dimensions from (MAXIJ) to (IIPAR, JJPAR)

10.8.8 init_pops

Subroutine INIT_POPS allocates and zeroes all module arrays.

INTERFACE:

```
SUBROUTINE INIT_POPS( am_I_Root, Input_Opt, State_Chm, RC )
```

USES:

```
USE ErrCode_Mod

USE ERROR_MOD, ONLY : ALLOC_ERR

USE ERROR_MOD, ONLY : DEBUG_MSG

USE Input_Opt_Mod, ONLY : OptInput

USE State_Chm_Mod, ONLY : ChmState

USE State_Chm_Mod, ONLY : Ind_
```

INPUT PARAMETERS:

USE CMN_SIZE_MOD

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

REVISION HISTORY:

10.8.9 cleanup_pops

Subroutine CLEANUP_POPS deallocates all module arrays.

INTERFACE:

SUBROUTINE CLEANUP_POPS

```
20 September 2010 - N.E. Selin - Initial Version
```

10.9 Fortran: Module Interface RnPbBe_mod.F

Module RnPbBe_MOD contains variables and routines used for the 222Rn-210Pb-7Be simulation. (hyl, swu, bmy, 6/14/01, 8/4/06)

INTERFACE:

MODULE RnPbBe_MOD

USES:

USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

IMPLICIT NONE PRIVATE

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: CHEMRnPbBe

PRIVATE MEMBER FUNCTIONS:

#if defined(NC_DIAG)

PRIVATE :: Diagn_RnPbBe_Update

#endif

- ! NOTE: WE NEED TO KEEP THIS HERE FOR NOW SINCE IT IS USED
- ! BY CODE IN mercury_mod.F. REMOVE IT LATER. (bmy, 7/7/14)
- ! Removed. (mdy, 12/4/14)

PUBLIC :: SLQ

REMARKS:

References:

- (1) Liu, H., D. Jacob, I. Bey, and R. M. Yantosca, Constraints from 210Pb and 7Be on wet deposition and transport in a global three-dimensional chemical tracer model driven by assimilated meteorological fields, JGR, 106, D11, 12,109-12,128, 2001.
- (2) Jacob et al., Evaluation and intercomparison of global atmospheric transport models using Rn-222 and other short-lived tracers, JGR, 1997 (102):5953-5970
- (3) Dorothy Koch, JGR 101, D13, 18651, 1996.
- (4) Lal, D., and B. Peters, Cosmic ray produced radioactivity on the Earth. Handbuch der Physik, 46/2, 551-612, edited by K. Sitte, Springer-Verlag, New York, 1967.

- 14 Jun 2001 H. Liu Initial version
- (1) Added existing routines to this module (bmy, 6/14/01)

- (2) Updated comments (bmy, 9/4/01)
- (3) Eliminate AVGF; redimensioned XTRA2 (bmy, 9/25/01)
- (4) Replace references to PW(I,J) with P(I,J) (bmy, 10/3/01)
- (5) Remove obsolete code from 9/01 and 10/01 (bmy, 10/23/01)
- (6) Removed duplicate variable declarations (bmy, 11/15/01)
- (7) Now read files from DATA_DIR/RnPbBe_200203/ directory.
 Also updated comments. (bmy, 3/29/02)
- (8) Incorporated latest changes from Hongyu Liu. Also split off the code to read in the 7Be emissions into a separate routine. Add parallel DO-loops in several places. Cleaned up DRYFLXRnPbBe, and now make sure ND44 accurately represents the drydep fluxes of 210Pb and 7Be. (hyl, bmy, 8/7/02)
- (9) Now reference AD from "dao_mod.f". Now references "error_mod.f". Moved routine DRYFLXRnPbBe into "drydep_mod.f". (bmy, 1/27/03)
- (10) Now references the new "time_mod.f" (bmy, 2/11/03)
- (11) Bug fix in EMISSRnPbBe -- take abs(lat) for 7Be emiss. (bmy, 6/10/03)
- (12) Bug fix in EMISSRnPbBe -- shut off 222Rn emissions in polar regions (swu, bmy, 10/28/03)
- (13) Now references "directory_mod.f", "logical_mod.f", and "tracer_mod.f" (bmy, 7/20/04)
- (14) Now modified for GCAP and GEOS-5 met fields (swu, bmy, 5/24/05)
- (15) Now references "tropopause_mod.f"
- (16) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- 19 Nov 2010 R. Yantosca Added ProTeX headers
- 08 Nov 2011 R. Yantosca Prevent out-of-bounds errors in diagnostics
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 01 Mar 2012 R. Yantosca Now use routines from the new grid_mod.F90
- 01 Aug 2012 R. Yantosca Add reference to findFreeLUN from inqure_mod.F90
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 07 Jul 2014 R. Yantosca Removed routines now orphaned by HEMCO
- 22 Aug 2014 R. Yantosca Removed LATSOU, PRESOU, BESOU arrays, these are now defined in the HEMCO code.
- 22 Aug 2014 R. Yantosca Remove XNUMOL_* parameters; these are obsolete
- 04 Nov 2014 M. Yannetti Added PRECISION_MOD
- 30 Jan 2015 E. Lundgren Add new diagnostics stuctures for netCDF output.
- 02 May 2016 R. Yantosca Now define IDTRn, IDTPb, IDTBe locally

10.9.1 chemRnPbBe

Subroutine CHEMRnPbBe performs loss chemistry on 222Rn, 210Pb, and 7Be.

INTERFACE:

```
SUBROUTINE CHEMRnPbBe( am_I_Root, Input_Opt, & State_Met, State_Chm, RC )
```

USES:

USE CHEMGRID_MOD, ONLY : ITS_IN_THE_STRATMESO

USE CMN_DIAG_MOD

USE CMN_SIZE_MOD

#if defined(BPCH_DIAG)

USE DIAG_MOD, ONLY: ADO1
USE DIAG_MOD, ONLY: ADO2

#endif

USE ErrCode_Mod

USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Chm_Mod, ONLY : Ind_
USE State_Met_Mod, ONLY : MetState
USE TIME_MOD, ONLY : GET_TS_CHEM

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

- 31 Oct 1999 H. Liu Initial version
- (1) Now use F90 syntax (bmy, hyl, 3/22/99)
- (2) Add FIRSTCHEM as an argument. Only compute the exponential terms when FIRSTCHEM = .TRUE., and save the values for later use (bmy, 3/24/99)
- (3) Cosmetic changes (bmy, 10/13/99)
- (4) Eliminate obsolete code and ND63 diagnostic (bmy, 4/12/00)
- (5) Cosmetic changes (bmy, 7/12/00)
- (6) Added to module "RnPbBe_mod.f". Also updated comments and made cosmetic changes. (bmy, 6/14/01)
- (7) Add diagnostics for Rn/Be emissions. Also cleaned up some old code and added parallel DO-loops. Updated comments. (hyl, 8/6/02)
- (8) Now make FIRSTCHEM a local SAVEd variable. (bmy, 1/27/03)
- (9) Now use function GET_TS_CHEM from "time_mod.f" (bmy, 2/11/03)
- (10) Now references STT and N_TRACERS from "tracer_mod.f" (bmy, 7/20/04)
- (11) Remove reference to CMN; it's obsolete. Now use inquiry functions from "tropopause_mod.f" to diagnose strat boxes. (bmy, 8/15/05)
- 08 Dec 2009 R. Yantosca Added ProTeX headers
- 08 Nov 2011 R. Yantosca Prevent out-of-bounds errors in diagnostics
- 09 Nov 2012 M. Payer Replaced all met field arrays with State_Met

```
derived type object

25 Mar 2013 - R. Yantosca - Now accept am_I_Root, Input_Opt, State_Chm, RC

22 Aug 2014 - R. Yantosca - Copy emissions above the PBL to tracer array

22 Aug 2014 - R. Yantosca - Cosmetic changes, for clarity

04 Sep 2014 - R. Yantosca - Add minor changes for efficiency

04 Nov 2014 - M. Yannetti - Changed REAL*8 to REAL(fp)

12 Dec 2014 - M. Yannetti - Changed Hemco REAL*8 to REAL(hp)

2 May 2016 - R. Yantosca - Now define IDTRn, IDTPb, IDTBe locally

22 Jun 2016 - R. Yantosca - Now use Ind_() to define species ID's

22 Jun 2016 - R. Yantosca - Rename species ID's to id_Rn, id_Pb, id_Be7

30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected species ID from State_Chm%Map_Advect.

10 Aug 2016 - R. Yantosca - Remove temporary tracer-removal code
```

10.9.2 diagn_rnpbbe_update

Subroutine DIAGN_RNPBBE_UPDATE updates the Rn/Pb/Be7 diagnostics ND01 (emissions) and ND02 (loss due to decay) that are written to netCDF. ND01 Rn and Be7 emissions diagnostics are included in HEMCO emissions and are therefore not updated in this subroutine.

INTERFACE:

```
SUBROUTINE Diagn_RnPbBe_Update( am_I_Root, NDxx, SpeciesName, & DiagArray, ColNo )
```

USES:

```
USE HCO_INTERFACE_MOD, ONLY : HcoState
USE HCO_DIAGN_MOD, ONLY : Diagn_Update
USE HCO_Error_Mod
USE Error_Mod
```

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
CHARACTER(LEN=4), INTENT(IN) :: NDxx ! Diagnostic id
CHARACTER(LEN=*), INTENT(IN) :: SpeciesName ! Species name
REAL(fp), TARGET, INTENT(IN) :: DiagArray(:,:,:)
INTEGER, INTENT(IN) :: ColNo ! Diag collection #
```

REVISION HISTORY:

```
30 Jan 2015 - E. Lundgren - Initial version
```

REMARKS:

10.10 Fortran: Module Interface rrtmg_rad_transfer_mod.F

Module RRTMG_RAD_TRANSFER_MOD contains arrays and routines for performing online radiative transfer in GEOS-Chem.

INTERFACE:

```
MODULE RRTMG_RAD_TRANSFER_MOD
```

USES:

```
USE CMN_FJX_MOD,
                     ONLY: RTODAER, RTSSAER, RTASYMAER,
                            WVAA, SPECMASK, LSPECRADMENU,
                            NSPECRADMENU
   USE CMN_SIZE_MOD, ONLY : IIPAR, JJPAR, LLPAR, NDUST, NAER
   USE DIAG_MOD,
                     ONLY: AD72 !RAD OUTPUT DIAGNOSTIC ARRAY
   USE OMP_LIB
   USE PARRRTM,
                     ONLY: NBNDLW
   USE PARRRSW,
                     ONLY: NBNDSW
   IMPLICIT NONE
    PRIVATE
!PUBLIC MEMBER FUNCTIONS
   PUBLIC :: CLEANUP_SURFACE_RAD
   PUBLIC :: INIT_SURFACE_RAD
   PUBLIC :: READ_SURFACE_RAD
   PUBLIC :: CLEANUP_MCICA_CLOUDS
   PUBLIC :: INIT_MCICA_CLOUDS
```

PUBLIC DATA MEMBERS:

```
ALLOCATABLE, PUBLIC, TARGET :: ALBDIR(:,:,:)
REAL*8,
         ALLOCATABLE, PUBLIC, TARGET :: ALBDIF(:,:,:)
REAL*8,
REAL*8,
         ALLOCATABLE, PUBLIC, TARGET :: EMISS (:,:,:)
        ALLOCATABLE, PUBLIC, TARGET :: CH4CLIM(:,:,:)
REAL*8,
REAL*8,
        ALLOCATABLE, PUBLIC, TARGET :: N2OCLIM(:,:,:)
        ALLOCATABLE, PUBLIC, TARGET :: CFC11CLIM(:,:,:)
REAL*8,
         ALLOCATABLE, PUBLIC, TARGET :: CFC12CLIM(:,:,:)
REAL*8,
        ALLOCATABLE, PUBLIC, TARGET :: CCL4CLIM(:,:,:)
REAL*8,
         ALLOCATABLE, PUBLIC, TARGET :: CFC22CLIM(:,:,:)
REAL*8,
!MCICA cloud variables now stored for reuse
REAL*8,
         ALLOCATABLE, PUBLIC, TARGET :: CLDFMCL_LW(:,:,:,:)
         ALLOCATABLE, PUBLIC, TARGET :: CIWPMCL_LW(:,:,:,:)
REAL*8,
         ALLOCATABLE, PUBLIC, TARGET :: CLWPMCL_LW(:,:,:,:)
REAL*8,
REAL*8,
        ALLOCATABLE, PUBLIC, TARGET :: TAUCMCL_LW(:,:,:,:)
         ALLOCATABLE, PUBLIC, TARGET :: CLDFMCL_SW(:,:,:,:)
REAL*8,
REAL*8,
        ALLOCATABLE, PUBLIC, TARGET :: CIWPMCL_SW(:,:,:,:)
        ALLOCATABLE, PUBLIC, TARGET :: CLWPMCL_SW(:,:,:,:)
REAL*8,
```

```
REAL*8, ALLOCATABLE, PUBLIC, TARGET :: TAUCMCL_SW(:,:,:,:)
REAL*8, ALLOCATABLE, PUBLIC, TARGET :: SSACMCL(:,:,:,:)
REAL*8, ALLOCATABLE, PUBLIC, TARGET :: ASMCMCL(:,:,:,:)
REAL*8, ALLOCATABLE, PUBLIC, TARGET :: FSFCMCL(:,:,:,:)
REAL*8, ALLOCATABLE, PUBLIC, TARGET :: REICMCL(:,:,:)
REAL*8, ALLOCATABLE, PUBLIC, TARGET :: RELQMCL(:,:,:)
```

REVISION HISTORY:

10.10.1 do_rrtmg_rad_transfer

INTERNAL SUBROUTINE

INTERFACE:

```
SUBROUTINE DO_RRTMG_RAD_TRANSFER( am_I_Root, THISDAY, THISMONTH, & ICLD, ISPECMENU, ISEED, & Input_Opt, State_Met, State_Chm, & RC )
```

```
ļ-----
! Modules from GeosRad
!-----
USE MCICA_SUBCOL_GEN_LW, ONLY : MCICA_SUBCOL_LW
USE MCICA_SUBCOL_GEN_SW, ONLY : MCICA_SUBCOL_SW
USE PARKIND,
                  ONLY : IM=>KIND_IM, RB=>KIND_RB
USE RRLW_CON,
                 ONLY : GASCON, AVOGAD
                 ONLY : NBNDLW, NGPTLW
USE PARRRTM,
                 ONLY: NBNDSW, NGPTSW, NAEREC
USE PARRRSW,
USE RRTMG_LW_RAD,
                 ONLY : RRTMG_LW
USE RRTMG_SW_RAD,
                  ONLY : RRTMG_SW
! GEOS-Chem modules
I-----
USE CHEMGRID_MOD,
                  ONLY : ITS_IN_THE_TROP
USE CHEMGRID_MOD,
                 ONLY : GET_CHEMGRID_LEVEL
                 ONLY: NSPECRAD! NUMBER OF SPECIES FOR RT
USE CMN_FJX_MOD,
USE CMN_FJX_MOD, ONLY : NASPECRAD ! NUMBER OF AEROSOL SPECIES
```

USE CMN_FJX_MOD, ONLY : SPECMASK, IRTWVSELECT USE CMN_FJX_MOD, ONLY : NWVSELECT, WVSELECT

USE CMN_FJX_MOD, ONLY : ACOEF_RTWV, BCOEF_RTWV, CCOEF_RTWV

USE CMN_FJX_MOD, ONLY : WVAA, NWVAA

USE CMN_FJX_MOD, ONLY : NWVAAO USE DIAG_MOD, ONLY : AD72

USE ErrCode_Mod

USE ERROR_MOD

USE GC_GRID_MOD, ONLY : GET_YMID
USE Input_Opt_Mod, ONLY : OptInput

USE PhysConstants, ONLY : AIRMW, PI, AVO

USE PRESSURE_MOD, ONLY : GET_PCENTER, GET_PEDGE

USE State_Chm_Mod, ONLY : ChmState
USE State_Chm_Mod, ONLY : Ind_
USE State_Met_Mod, ONLY : MetState

USE TIME_MOD, ONLY : GET_DAY_OF_YEAR, GET_HOUR

USE TOMS_MOD, ONLY : GET_OVERHEAD_O3

USE UnitConv_Mod

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am_I_Root ! root CPU?

INTEGER, INTENT(IN) :: THISDAY ! CURRENT DAY

INTEGER, INTENT(IN) :: THISMONTH ! CURRENT MONTH

INTEGER, INTENT(IN) :: ISPECMENU ! THE SPECIES BEING INCLUDED

! NEEDED FOR OUTPUT PURPOSES

INTEGER, INTENT(IN) :: ISEED

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object INTEGER, INTENT(INOUT) :: ICLD ! CLOUD FLAG FOR RRTMG ! O-NOCLOUD, 1-GREY CLOUD

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Failure or success

REMARKS:

THIS ROUTINE PASSES INPUTS TO THE RRTMG DRIVER ROUTINE "RAD_DRIVER" VIA THE ARGUMENT LIST. THIS PREVENTS CIRCULAR REFERENCES.

REVISION HISTORY:

17 AUG 2012 - R. YANTOSCA - INITIAL VERSION

15 Dec 2014 - M. Sulprizio- Moved radiation diagnostic from ND71 to ND72 to avoid conflicts with hourly max ppbv diagnostic.

15 Jan 2015 - M. Sulprizio- Added T_CTM and P_CTM arrays and calculate them in the same manner that we do in fast_jx_mod.F.

```
Also moved and fixed calculation of O3_CTM.
15 Jan 2015 - M. Sulprizio- Added ProTeX headers
13 Apr 2015 - R. Yantosca - Fixed inefficient loop ordering (should be J,I)
13 Apr 2015 - R. Yantosca - Add error check for JLOOP > 0 in a few places
23 Apr 2015 - R. Yantosca - Bug fix: YLAT was undefined; now corrected
23 Apr 2015 - R. Yantosca - Bug fix: all members of State_Met now use
                            (I,J,L) ordering. This is for the NASA GCM.
02 Jun 2015 - R. Yantosca - Bug fix: Add missing variables to OMP PRIVATE
03 Jun 2015 - R. Yantosca - Now use pointers to avoid array temporaries
12 Aug 2015 - E. Lundgren - Incoming tracer units are now [kg/kg] and
                            are converted to [kg] for RRTMG
12 Aug 2015 - E. Lundgren - Now accept am_I_Root and RC as arguments
21 Dec 2015 - M. Sulprizio- Get air density directly from State_Met object
22 Dec 2015 - M. Sulprizio- Replace CSPEC with State_Chm%Species
19 Jan 2016 - E. Lundgren - Use global physical constants from physicants
                            rather than comode_loop_mod
17 May 2016 - M. Sulprizio- Remove NCOL, IJLOOP and change dimensions of
                            arrays from IIPAR*JJPAR to IIPAR, JJPAR
31 May 2016 - E. Lundgren - Replace Input_Opt%TRACER_MW_G with emMW_g from
                            species database (emitted species g/mol)
16 Jun 2016 - K. Yu
                          - Now define species ID's with the Ind_ function
17 Jun 2016 - R. Yantosca - Only define species ID's on the first call
27 Jun 2016 - R. Yantosca - Bug fix: replace a couple of leftover IDO3
                            variables with the new id_03 species ID
30 Jun 2016 - M. Sulprizio- Replace ICH4 with id_CH4 to remove dependence
                            on comode_loop_mod.F
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected
                            species ID from State_Chm%Map_Advect.
```

10.10.2 set_specmask

Subroutine SET_SPECMASK converts the species switches in the input.mod radiation section into the list of species that should be passed through to RRTMG. This must be done in a subtractive way, e.g. If we require the DRE of sulfate then the baseline will contain all species and the sulfate run will contain everything but sulfate, this way the contribution of sulfate can be inferred. Therefore, all species are initially set to 1 and their inclusion results in SPECMASK for the particular species being set to zero. (dar 10/2013)

INTERFACE:

SUBROUTINE SET_SPECMASK(ISPECRADMENU)

USES:

```
USE CMN_FJX_MOD, ONLY: SPECMASK,NSPECRAD,NASPECRAD, & LSPECRADMENU,NSPECRADMENU
```

INPUT PARAMETERS:

INTEGER, INTENT(IN) :: ISPECRADMENU

REVISION HISTORY:

```
18 Jun 2013 - D.A. Ridley - Initial version
15 Jan 2015 - M. Sulprizio- Added ProTeX headers
26 Jun 2015 - E. Lundgren - Fix typo in NXTRA definition
```

10.10.3 read_surface_rad

Subroutine READ_SURFACE_RAD gets the surface albedo and emissivity from data files processed from MODIS MCD43C3.5 and MOD11C2. Albedo is direct (black sky) and diffuse (white sky) and interpolated to the first 21 wavelengths of GADS, used in the RRTMG code. Emissivity has been interpolated to last 40 wavelengths of GADS.! This routine is called from main.F when ITS_TIME_FOR_SURFACE_RAD() is true (every 8 days) DAR (10/2012)

INTERFACE:

SUBROUTINE READ_SURFACE_RAD(Input_Opt, FORCEREAD)

USES:

```
USE BPCH2_MOD,
                    ONLY : GET_NAME_EXT_2D, GET_RES_EXT
USE BPCH2_MOD,
                     ONLY : GET_TAUO,
                                          READ_BPCH2
USE CMN_FJX_MOD
USE CMN_SIZE_MOD
                         ! SIZE PARAMETERS
USE JULDAY_MOD,
                    ONLY: JULDAY, CALDATE
                    ONLY: GET_YEAR, GET_MONTH
USE TIME_MOD,
                    ONLY: GET_DAY, GET_DAY_OF_YEAR
USE TIME_MOD,
USE TIME_MOD,
                    ONLY: YMD_EXTRACT
```

INPUT PARAMETERS:

```
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input options
LOGICAL, INTENT(IN), OPTIONAL :: FORCEREAD ! Reset first-time flag?
```

REMARKS:

```
18 Jun 2013 - D.A. Ridley - Initial version
15 Jan 2015 - M. Sulprizio- Added ProTeX headers
10 Apr 2015 - R. Yantosca - Read from ExtData/CHEM_INPUTS/modis_surf_201210
```

10.10.4 read_strat_clim

Subroutine READ_STRAT_CLIM gets the stored N2O and CH4 profiles created based on TES climatology. These are global July mean profiles from TES that are interpolated to the 3D GEOS-Chem grid as a simple solution to account for stratospheric contribution of these species to radiative balance. This routine is called from main. F once at the start of the model run. DAR (12/2012)

INTERFACE:

```
SUBROUTINE READ_STRAT_CLIM( Input_Opt )
```

USES:

```
USE BPCH2_MOD, ONLY : GET_NAME_EXT_2D, GET_RES_EXT
USE BPCH2_MOD, ONLY : GET_TAUO, READ_BPCH2
```

USE CMN_FJX_MOD

USE CMN_SIZE_MOD ! SIZE PARAMETERS

USE Input_Opt_Mod, ONLY : OptInput

USE TIME_MOD, ONLY : GET_YEAR, GET_MONTH

USE TIME_MOD, ONLY : GET_DAY, GET_DAY_OF_YEAR

USE TRANSFER_MOD, ONLY : TRANSFER_3D

INPUT PARAMETERS:

```
TYPE(OptInput), INTENT(IN) :: Input_Opt  ! Input options
```

REMARKS:

REVISION HISTORY:

```
18 Jun 2013 - D.A. Ridley - Initial version
15 Jan 2015 - M. Sulprizio- Added ProTeX headers
10 Apr 2015 - R. Yantosca - Now read from ExtData/CHEM_INPUTS/RRTMG_201104/
```

10.10.5 init_surface_rad

Subroutine INIT_SURFACE_RAD initializes all allocatable module arrays.

INTERFACE:

```
SUBROUTINE INIT_SURFACE_RAD()
```

```
USE CMN_FJX_MOD
USE CMN_SIZE_MOD
```

USE ERROR_MOD, ONLY : ALLOC_ERR

REVISION HISTORY:

```
18 Jun 2013 - D.A. Ridley - Initial version
15 Jan 2015 - M. Sulprizio- Added ProTeX headers
```

10.10.6 init_strat_clim

Subroutine INIT_STRAT_CLIM initializes all allocatable module arrays.

INTERFACE:

SUBROUTINE INIT_STRAT_CLIM

USES:

```
USE CMN_FJX_MOD
USE CMN_SIZE_MOD
```

USE ERROR_MOD, ONLY : ALLOC_ERR

REVISION HISTORY:

```
18 Jun 2013 - D.A. Ridley - Initial version
15 Jan 2015 - M. Sulprizio- Added ProTeX headers
```

10.10.7 init meica clouds

Subroutine INIT_MCICA_CLOUDS initializes all allocatable module arrays.

INTERFACE:

```
SUBROUTINE INIT_MCICA_CLOUDS()
```

USES:

```
USE CMN_FJX_MOD
USE CMN_SIZE_MOD
```

USE ERROR_MOD, ONLY : ALLOC_ERR
USE PARRRTM, ONLY : NGPTLW
USE PARRRSW, ONLY : NGPTSW

```
18 Jun 2013 - D.A. Ridley - Initial version
15 Jan 2015 - M. Sulprizio- Added ProTeX headers
17 May 2016 - M. Sulprizio- Change array dimensions from IIPAR*JJPAR to
IIPAR,JJPAR
```

10.10.8 cleanup_surface_rad

Subroutine CLEANUP_SURFACE_RAD deallocates all module arrays.

INTERFACE:

SUBROUTINE CLEANUP_SURFACE_RAD

REVISION HISTORY:

```
18 Jun 2013 - D.A. Ridley - Initial version
15 Jan 2015 - M. Sulprizio- Added ProTeX headers
```

10.10.9 cleanup_strat_clim

Subroutine CLEANUP_STRAT_CLIM deallocates all module arrays.

INTERFACE:

SUBROUTINE CLEANUP_STRAT_CLIM

REVISION HISTORY:

```
18 Jun 2013 - D.A. Ridley - Initial version
15 Jan 2015 - M. Sulprizio- Added ProTeX headers
```

10.10.10 cleanup_mcica_clouds

Subroutine CLEANUP_MCICA_CLOUDS deallocates all module arrays.

INTERFACE:

SUBROUTINE CLEANUP_MCICA_CLOUDS

REVISION HISTORY:

```
18 Jun 2013 - D.A. Ridley - Initial version
15 Jan 2015 - M. Sulprizio- Added ProTeX headers
```

10.11 Fortran: Module Interface tagged_co_mod.F

Module TAGGED_CO_MOD contains variables and routines used for the geographically tagged CO simulation.

INTERFACE:

MODULE TAGGED_CO_MOD

USE PhysConstants

USE PRECISION_MOD ! For GEOS-Chem Precision (fp)

IMPLICIT NONE

PRIVATE

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: CALC_DIURNAL

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: CHEM_TAGGED_CO
PUBLIC :: GET_ALPHA_ISOP
PUBLIC :: INIT_TAGGED_CO
PUBLIC :: CLEANUP_TAGGED_CO

REMARKS:

Tagged CO Species (you can modify these as needs be!)

- (1) Total CO
- (2) CO from North American fossil fuel
- (3) CO from European fossil fuel
- (4) CO from Asian fossil fuel
- (5) CO from fossil fuel from everywhere else
- (6) CO from South American biomass burning
- (7) CO from African biomass burning
- (8) CO from Southeast Asian biomass burning
- (9) CO from Oceania biomass burning
- (10) CO from European biomass burning
- (11) CO from North American biomass burning
- (12) CO chemically produced from Methane
- (13) CO from Biofuel burning (whole world)
- (14) CO chemically produced from Isoprene
- (15) CO chemically produced from Monoterpenes
- (16) CO chemically produced from Methanol (CH3OH)
- (17) CO chemically produced from Acetone

- 28 Jul 2000- R. Yantosca Initial version
- (1) Removed obsolete code from CHEM_TAGGED_CO (bmy, 12/21/00)
- (2) Added CO sources from oxidation of biofuel VOC's, biomass burning VOC's, fossil fuel VOC's, and natural VOC's (bnd, bmy, 1/2/01)
- (3) Added chemical P(CO) from CH3OH and MONOTERPENES (bnd, bmy, 1/2/01)
- (4) Now cap SCALEYEAR at 1997 in "emiss_tagged_co" (bnd, bmy, 4/6/01)
- (5) Removed obsolete commented-out code (bmy, 4/23/01)
- (6) Added new module variables SUMACETCO, EMACET, CO_PRODS, CO_LOSSS, ISOP96, MONO96, and MEOH96. Also added new module routines GET_ALPHA_ISOP, READ_PCO_LCO_STRAT, GET_PCO_LCO_STRAT,

- READ_ACETONE, and READ_BIOG_FOR_GEOS3. (bnd, bmy, 6/14/01)
- (7) Now read files from DATA_DIR/tagged_CO_200106/ (bmy, 6/19/01)
- (8) Removed ISOP96, MONO96, and CH3OH96 since we now use the new GEOS-3 fields and no longer have to correct for the surface temperature. (bmy, 8/21/01)
- (9) Bug fix: don't call GLOBAL_NOX_MOD in routine CHEM_TAGGED_CO unless a logical switch is set (bmy, 8/28/01)
- (10) Updated comments (bmy, 9/6/01)
- (11) Deleted obsolete code for 1998 GEOS-3 fix. Also now archive ND46 diagnostic as [atoms C/cm2/s] (bmy, 9/13/01)
- (12) Bug fix in CHEM_TAGGED_CO: now save CO sources/sinks into the Total CO tracer (N=1). (qli, bmy, 9/21/01)
- (13) Resize arrays of (IIPAR, JJPAR) to (IIPAR, JJPAR) (bmy, 9/28/01)
- (14) Removed obsolete code from 9/28/01 (bmy, 10/23/01)
- (15) Updated comments (bmy, 2/15/02)
- (16) Removed double definition of SUMCH3OHCO (bmy, 3/20/02)
- (17) Now use P(I,J) + PTOP instead of PS(I,J) (bmy, 4/11/02)
- (18) Now divide module header into MODULE PRIVATE, MODULE VARIABLES, and MODULE ROUTINES sections. Updated comments (bmy, 5/28/02)
- (19) Now references "pressure_mod.f" (dsa, bdf, bmy, 8/21/02)
- (20) Now reference AD, BXHEIGHT, T and SUNCOS from "dao_mod.f". Also removed obsolete code from various routines. Now references ERROR_STOP from "error_mod.f". (bmy, 10/15/02)
- (21) Now references "grid_mod.f" and the new "time_mod.f". (bmy, 2/3/03)
- (22) Bug fix for NTAU in EMISS_TAGGED_CO. Bug fix for FILENAME in routine READ_PCO_LCO_STRAT. (ave, bnd, bmy, 6/3/03)
- (23) Updated arg list in call to EMISOP in EMISS_TAGGED_CO (bmy, 12/9/03)
- (24) Now references "directory_mod.f", "logical_mod.f", "tracer_mod.f". Now remove IJLOOP_CO. (bmy, 7/20/04)
- (25) Fixed bug in CHEM_TAGGED_CO (bmy, 3/7/05)
- (26) Now reads data from both GEOS and GCAP grids. Now also references "tropopause_mod.f". (bmy, 8/16/05)
- (27) Now modified for new "biomass_mod.f" (bmy, 4/5/06)
- (28) BIOMASS(:,:,IDBCO) from "biomass_mod.f" is now in units of [molec CO/cm2/s]. Adjust unit conversion accordingly. (bmy, 9/27/06)
- (29) Routines GET_ALPHA_ISOP, GET_PCO_LCO_STRAT, READ_PCO_LCO_STRAT, READ_ACETONE and INIT_TAGGED_CO are public now. Variable EMACET is public now. (phs, 9/18/07)
- 13 Aug 2010 R. Yantosca Add modifications for MERRA (treat like GEOS-5)
- 08 Feb 2012 R. Yantosca Add modifications for GEOS-5.7.2 met
- 01 Mar 2012 R. Yantosca Now reference new grid_mod.F90
- 23 Oct 2012 R. Yantosca Update prod/loss for new GMI strat chem
- 20 Aug 2013 R. Yantosca Removed "define.h", this is now obsolete
- 10 Apr 2014 R. Yantosca Now change CO_PRODS and CO_LOSSS to REAL*4
- 11 Jun 2014 J.A. Fisher Replace SUNCOS with SUNCOSmid for MEGAN
- 11 Jun 2014 J.A. Fisher Treat monoterpenes as in full chemistry
- 12 Jun 2014 J.A. Fisher Add option for non-local PBL mixing
- 10 Jul 2014 J.A. Fisher Add diurnal cycle for OH

```
10 Jul 2014 - J.A. Fisher - Change FIRSTEMISS to FIRSTTIME to allow initialisation when emissions are off
20 Nov 2014 - M. Yannetti - Added PRECISION_MOD
11 Mar 2015 - R. Yantosca - Add OH pointer for HEMCO data input
12 Jun 2016 - E. Lundgren - Use global physical parameters
13 Jun 2016 - R. Yantosca - Removed CO_PRODS and CO_LOSSS, we now get
14 GMI strat P(CO) and L(CO) directly from HEMCO
15 Jun 2016 - R. Yantosca - Removed GET_PCO_LCO_STRAT, it was obsolete
16 Jun 2016 - R. Yantosca - Get rid of READ_PCO_LCO_STRAT, it's obsolete
17 Jun 2016 - R. Yantosca - Add extra error checks; remove EMACET array
18 Jun 2016 - R. Yantosca - Grid_mod.F90 is now gc_grid_mod.F90
```

10.11.1 chem_tagged_co

USE CHEMGRID_MOD,

Subroutine CHEM_TAGGED_CO performs CO chemistry on geographically "tagged" CO species. Loss is via reaction with OH.

INTERFACE:

```
SUBROUTINE CHEM_TAGGED_CO( am_I_Root, Input_Opt, & State_Met, State_Chm, RC )
```

USES:

```
USE CMN_SIZE_MOD
USE CMN_DIAG_MOD
USE DIAG_MOD,
                        ONLY: AD65
USE ErrCode_Mod
                       ONLY : CHECK_VALUE
USE ERROR_MOD,
USE ERROR_MOD,
                       ONLY : ERROR_STOP
USE GC_GRID_MOD,
                       ONLY : GET_YMID
USE HCO_EmisList_Mod,
                       ONLY : HCO_GetPtr
USE HCO_Error_Mod
USE HCO_Interface_Mod, ONLY : HcoState, GetHcoID
USE Input_Opt_Mod,
                       ONLY : OptInput
USE PhysConstants,
                       ONLY : AVO
USE State_Chm_Mod,
                       ONLY : ChmState
USE State_Met_Mod,
                       ONLY : MetState
USE TIME_MOD,
                       ONLY : GET_TS_CHEM,
                                                GET_TS_EMIS
USE TIME_MOD,
                       ONLY : GET_MONTH,
                                                GET_YEAR
                       ONLY : ITS_A_NEW_MONTH, ITS_A_NEW_YEAR
USE TIME_MOD,
```

ONLY : ITS_IN_THE_STRAT

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object
```

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

- 19 Oct 1999 Q. Li, B. Duncan, B. Field Initial version
- (1) Now do chemistry all the way to the model top.
- (2) Use monthly mean OH fields for oxidation.
- (3) Now reference the monthly mean OH array and the routine which reads it from disk in "global_oh_mod.f" (bmy, 7/28/00)
- (4) Removed obsolete code from 10/6/00 (bmy, 12/21/00)
- (5) Added P(CO) from CH3OH and MONOTERPENES. Also account for the variation of CH4 conc. w/ latitude and year (bnd, bmy, 1/2/01)
- (6) Removed obsolete commented-out code (bmy, 4/23/01)
- (7) Updated with new stuff from bnd. Also references module routines & arrays from "global_nox_mod.f" and "error_mod.f". Removed THISMONTH as an argument since we can use the MONTH value from the "CMN" include file. (bmy, 6/14/01)
- (8) Remove GEOS-3 fix for biogenic fields (ISOP96, MONO96, CH3OH96), since we now use updated met fields w/o the surface temperature problem (bmy, 8/21/01)
- (9) Now only call GLOBAL_NOX_MOD to define the BNOX array, if switch ALPHA_ISOP_FROM_NOX is set. The NOx concentrations used to compute the CO yield from isoprene are currently only at 4x5 (bmy, 8/28/01)
- (10) Bug fix: now make sure to add CO production and loss into the STT(:,:,:,1), which is the Total CO tracer. (qli, bmy, 9/21/01)
- (11) Updated comments. Bug fix: multiply CO_OH (after using it to update tagged tracers) by GCO (the initial value of STT in molec/cm3) to convert it to an amount of CO lost by OH [molec/cm3]. (bmy, 2/19/02)
- (12) Removed PS as an argument; use P(I,J) + PTOP instead of PS, in order to ensure that we use P and AD computed from the same preesure by AIRQNT. (bmy, 4/11/02)
- (13) Now use GET_PCENTER from "pressure_mod.f" to compute the pressure at the midpoint of box (I,J,L). Also deleted obsolete, commented-out code. (dsa, bdf, bmy, 8/21/02)
- (14) Now reference AD and T from "dao_mod.f". Now make FIRSTCHEM a local SAVEd variable. (bmy, 11/15/02)
- (15) Now replace YLMID(J) with routine GET_YMID of "grid_mod.f". Now uses functions GET_TS_CHEM, GET_MONTH, GET_YEAR from the new "time_mod.f". (bmy, 2/10/03)
- (16) Now reference STT & N_TRACERS from "tracer_mod.f". Now references LSPLIT from "logical_mod.f". Now references AD65 from "diag_pl_mod.f". Updated comments. (bmy, 7/20/04)
- (17) Bug fix: re-insert ELSE between (1a-1) and (1a-2); it appears to have

```
been mistakenly deleted. (bmy, 3/7/05)
(18) Now references ITS_IN_THE_STRAT from "tropopause_mod.f". Now remove
      reference to "CMN", it's obsolete. (bmy, 8/22/05)
(19) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
(20) Remove reference to "global_ch4_mod.f" (bmy, 5/31/06)
(21) Use newest JPL 2006 rate constant for CO+OH (jaf, jmao, 3/4/09)
01 Mar 2012 - R. Yantosca - Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
01 Mar 2012 - R. Yantosca - Now use GET_YMID(I,J,L) from grid_mod.F90
22 Oct 2012 - R. Yantosca - Now pass am_I_Root=.TRUE. to GET_GLOBAL_CH4
23 Oct 2012 - R. Yantosca - Added ProTeX headers
                          - Replaced all met field arrays with State_Met
09 Nov 2012 - M. Payer
                            derived type object
25 Mar 2013 - R. Yantosca - Now accept am_I_Root, Input_Opt, State_Chm, RC
11 Apr 2013 - R. Yantosca - Now pass Input_Opt to GET_GLOBAL_NOX
10 Jun 2013 - R. Yantosca - Avoid array temporaries in CHECK_VALUE
23 Oct 2013 - R. Yantosca - Now pass objects to GET_GLOBAL_OH routine
10 Apr 2014 - R. Yantosca - Now use pointers to fields in State_Met
10 Apr 2014 - R. Yantosca - Bug fix: DTSRCE should be DTCHEM
10 Jul 2014 - J.A. Fisher - Add diurnal cycle for OH
10 Jul 2014 - J.A. Fisher - Restore assignment of DTCHEM
10 Jul 2014 - J.A. Fisher - Remove unused DTSRCE, PCO, and AREA_CM2
10 Jul 2014 - J.A. Fisher - Moved ALPHA definitions out of code
27 Aug 2014 - R. Yantosca - Bug fix: pass Input_Opt to GET_GLOBAL_CH4
21 Oct 2014 - C. Keller - Now use GetHcoVal instead ot Trac_Tend array
26 Feb 2015 - E. Lundgren - Replace GET_PCENTER with State_Met%PMID.
11 Mar 2015 - R. Yantosca - Remove references to global_nox_mod.F
11 Mar 2015 - R. Yantosca - Now get OH via the HEMCO data structure
06 Jan 2016 - E. Lundgren - Use global physical parameters
21 Mar 2016 - R. Yantosca - Now define FMOL_CO from the species database
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
28 Jun 2016 - R. Yantosca - Add error traps to make sure that the ISOP,
                            ACET, MONX non-advected species are all found
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected
                            species ID from State_Chm%Map_Advect.
11 Oct 2016 - R. Yantosca - If emissions are turned off, do not update
                            the SUM*CO arrays, they will remain zeroed out.
12 Oct 2016 - R. Yantosca - Bug fix: convert OH from kg/m3 (which HEMCO
```

10.11.2 calc_diurnal

Subroutine CALC_DIRUNAL computes the sume of the cosine of the solar zenith angle over a 24 hour day as well as the total length of daylight to scale the offline OH concentrations.

brings in from disk) to molec/cm3.

INTERFACE:

SUBROUTINE CALC_DIURNAL

USES:

```
USE CMN_SIZE_MOD
```

USE GC_GRID_MOD, ONLY : GET_YMID_R

USE TIME_MOD, ONLY : ITS_A_NEW_DAY, GET_MINUTE, GET_HOUR

USE TIME_MOD, ONLY : GET_TS_CHEM, GET_DAY_OF_YEAR, GET_LOCALTIME

REVISION HISTORY:

12 Mar 2014 - J. Fisher - Copied from OHNO3TIME in carbon_mod and COSSZA in dao_mod

10.11.3 get_alpha_isop

Function GET_ALPHA_ISOP returns the CO yield from Isoprene (ALPHA_ISOP) either as a function of NOx or as a constant.

INTERFACE:

```
FUNCTION GET_ALPHA_ISOP( FROM_NOX, NOX ) RESULT( ALPHA_ISOP )
```

USES:

USE ERROR_MOD, ONLY : ERROR_STOP

INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: FROM_NOX ! If =T, will take ALPHA_ISOP

! as f(NOx). If =F, will set

! ALPHA_ISOP to a constant

REAL(fp), INTENT(IN), OPTIONAL :: NOX ! NOx concentration [ppbv]

RETURN VALUE:

REAL(fp) :: ALPHA_ISOP ! CO yield from ISOP

- 13 Jun 2001 B. Duncan Initial version
- 01 Oct 1995 R. Yantosca Initial version
- (1) Now make NOx an optional argument (bmy, 8/28/01)
- (2) Now reference ERROR_STOP from "error_mod.f" (bmy, 10/15/02)
- (3) Updated comments (bmy, 7/20/04)
- 23 Oct 2012 R. Yantosca Added ProTeX headers

10.11.4 init_tagged_co

Subroutine INIT_TAGGED_CO allocates memory to module arrays.

INTERFACE:

```
SUBROUTINE INIT_TAGGED_CO( am_I_Root, Input_Opt, RC )
```

USES:

```
USE CMN_SIZE_MOD
USE ErrCode_Mod
```

USE ERROR_MOD, ONLY : Alloc_Err
USE Input_Opt_Mod, ONLY : OptInput

INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
```

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

REVISION HISTORY:

- 19 Jul 2000 R. Yantosca Initial version
- (1) Added ISOP96, MONO96, CH30H96 for GEOS-3 (bnd, bmy, 6/14/01)
- (2) Removed ISOP96, MONO96, CH30H96 for GEOS-3, since the new GEOS-3 fields make these no longer necessary (bmy, 8/21/09)
- (3) Now allocate BB_REGION, FF_REGION as (IIPAR, JJPAR) (bmy, 9/28/01)
- (4) Removed obsolete code from 9/28/01 (bmy, 10/22/01)
- (5) Now references ALLOC_ERR from "error_mod.f" (bmy, 10/15/02)
- (6) Now remove IJLOOP_CO (bmy, 7/20/04)
- (7) Now public. Now references ITS_A_H2HD_SIM from "tracer_mod.f". Allocate needed variables if H2/HD simulation (phs, 9/18/07)
- 23 Oct 2012 R. Yantosca Added ProTeX headers
- 23 Oct 2012 J. Fisher $\,$ Dimension CO_PRODS and CO_LOSSS with

(IIPAR, JJPAR, LLPAR) for new GMI strat chem

- 10 Apr 2014 R. Yantosca Now call DEFINE* routines to define the fossil fuel and biofuel regions
- 10 Apr 2014 R. Yantosca Now accept am_I_Root, Input_Opt, RC arguments
- 21 Mar 2016 R. Yantosca Remove CO_PRODS, CO_LOSSS arrays
- 28 Jun 2016 R. Yantosca Remove EMACET array

10.11.5 cleanup_tagged_co

Subroutine CLEANUP_TAGGED_CO deallocates memory from previously allocated module arrays.

INTERFACE:

SUBROUTINE CLEANUP_TAGGED_CO

REVISION HISTORY:

```
19 Jul 2000 - R. Yantosca - Initial version
```

- (1) Added ISOP96, MONO96, CH3OH96 for GEOS-3 (bnd, bmy, 6/14/01)
- (2) Removed ISOP96, MONO96, CH3OH96 for GEOS-3, since the new GEOS-3 fields make these no longer necessary (bmy, 8/21/09)
- (3) Now remove IJLOOP_CO (bmy, 7/20/04)
- 23 Oct 2012 R. Yantosca Added ProTeX headers
- 11 Mar 2015 R. Yantosca Now free the OH pointer
- 21 Mar 2016 R. Yantosca Remove CO_PRODS, CO_LOSSS
- 21 Mar 2016 R. Yantosca Also nullify GMI_PROD_CO and GMI_LOSS_CO ptrs
- 28 Jun 2016 R. Yantosca Remove EMACET array

10.12 Fortran: Module Interface tagged_o3_mod.F

Module TAGGED_O3_MOD contains variables and routines to perform a tagged O3 simulation. P(O3) and L(O3) rates need to be archived from a full chemistry simulation before you can run w/ Tagged O3.

INTERFACE:

MODULE TAGGED_03_MOD

USES:

```
USE PRECISION_MOD ! For GEOS-Chem Precision (fp, f4, f8)
```

IMPLICIT NONE

PRIVATE

"" If you want to the EXTENDED SIMULATION with all 13 tagged 03 species,

%% then uncomment this #ifdef statement. (bmy, 4/11/14)

#define USE_ALL_TAGO3_SPECIES 1

%%%

PUBLIC MEMBER FUNCTIONS:

PUBLIC :: CHEM_TAGGED_03
PUBLIC :: CLEANUP_TAGGED_03
PUBLIC :: INIT_TAGGED_03

PRIVATE MEMBER FUNCTIONS:

PRIVATE :: GET_REGIONAL_PO3

REMARKS:

THE SIMPLE TAGGED 03 SIMULATION (default setting) HAS THESE ADVECTED SPECIES:

(1) 03 : Total 03

(2) O3Strt : Stratospheric O3

THE EXTENDED TAGGED 03 SIMULATION HAS THESE ADVECTED SPECIES:

(1) 03 : Total 03 (2) O3Strt : O3 from the Stratosphere (tropopause - atm top (3) O3Ut : O3 produced in Upper Trop (350 hPa - tropopause) (4) O3Mt : O3 produced in Middle Trop (PBL top - 350 hPa (5) O3Row : O3 produced in Rest of World (surface - PBL top (6) O3PcBl : O3 produced in Pacific BL (surface - PBL top (7) O3NaBl : O3 produced in N. American BL (surface - PBL top (8) O3AtBl : O3 produced in Atlantic BL (surface - PBL top (9) O3EuBl : O3 produced in European BL (surface - PBL top (10) O3AfBl : O3 produced in N. African BL (surface - PBL top) (11) O3AsBl : O3 produced in Asian (surface - PBL top) (12) O3Init : O3 initial conditions (all levels) (13) O3USA : O3 produced over the USA (all levels)

NOTES:

- (1) The stratospheric O3 species must be species #2. This is due to how the Linoz stratospheric O3 chemistry scheme is written. We have accordingly reorganized the species numbers below.
- (2) The name "tagged_ox_mod.F" is historical. The Ox species in GEOS-Chem has now been replaced with O3. O3 usually makes up about 95% of Ox. The nomenclature "tagged Ox" is interchangeable with "tagged O3".

 As of Aug 2016, most uses of "tagged Ox" have been replaced with "tagged O3".

- 20 Aug 2003 A. Fiore Initial version
- (1) Now accounts for GEOS-4 PBL being in meters (bmy, 1/15/04)
- (2) Bug fix: don't put function call in WRITE statement (bmy, 2/20/04)
- (3) Now bracket AD44 with an !\$OMP CRITICAL block (bmy, 3/24/04)
- (4) Now define regions w/levels in GET_REGIONAL_POX (amf,rch,bmy,5/27/04)
- (5) Bug fix-avoid seg fault if PBLFRAC isn't allocated (bdf, bmy, 10/12/04)
- (6) Now reference "pbl_mix_mod.f" (bmy, 2/17/05)
- (7) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (8) Now references XNUMOL from "tracer_mod.f" (bmy, 10/25/05)
- (9) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (10) Modified for variable tropopause (phs, bmy, 1/19/07)
- (11) Now use LLTROP instead of LLTROP_FIX everywhere (bmy, 12/4/07)
- (12) Now use LD65 instead of LLTROP everywhere (phs, 11/17/08)
- (13) Updates for LINOZ (dbj, jliu, bmy, 10/26/09)
- 19 Nov 2010 R. Yantosca Added ProTeX headers

```
28 Feb 2012 - R. Yantosca - Removed support for GEOS-3
01 Mar 2012 - R. Yantosca - Now reference new grid_mod.F90
14 Mar 2013 - M. Payer
                          - Replace Ox with O3 as part of removal of NOx-Ox
                            partitioning
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
23 Jan 2014 - M. Sulprizio- Now use LLTROP instead of LD65 or LLTROP_FIX
                            everywhere (hyl, bmy, 11/3/11)
11 Apr 2014 - R. Yantosca - Add #ifdef USE_ALL_TAGO3_SPECIES to select
                            between the simple and extended simulations
11 Apr 2014 - R. Yantosca - Updated comments
11 Apr 2014 - R. Yantosca - Now make the O3Strt tracer #2 for both the
                            simple and extended tagged 03 simulations
11 Apr 2014 - R. Yantosca - Now make INIT_TAGGED_OX a public routine
17 Sep 2014 - C. Keller - Now use HEMCO for prod./loss rates. This makes
                            subroutine READ_POX_LOX obsolete.
06 Nov 2014 - R. Yantosca - Removed code orphaned by HEMCO
21 Nov 2014 - M. Yannetti - Added PRECISION_MOD
04 Mar 2015 - R. Yantosca - Declare pointer args to HCO_GetPtr with REAL(f4)
16 Jun 2016 - M. Sulprizio- Replace IDT03Strt from tracerid_mod.F with
                            a local definition (module variable id_O3Strat)
12 Jul 2016 - R. Yantosca - Remove routine ADD_STRAT_POX, we now just
                            directly add into State_Chm%Species in
                            strat_chm_mod.F90
10 Aug 2016 - M. Sulprizio- Rename from tagged_ox_mod.F to tagged_o3_mod.F
29 Nov 2016 - R. Yantosca - grid_mod.F90 is now gc_grid_mod.F90
```

10.12.1 get_regional_po3

Subroutine GET_REGIONAL_PO3 returns the P(O3) for each of the tagged O3 species. Tagged O3 species are defined by both geographic location and altitude.

INTERFACE:

SUBROUTINE GET_REGIONAL_PO3(I, J, L, PP, State_Met)

USES:

INPUT PARAMETERS:

! GEOS-Chem grid box indices for lon, lat, alt

```
INTEGER, INTENT(IN) :: I, J, L
! Meteorology State object
TYPE(MetState), INTENT(IN) :: State_Met
```

OUTPUT PARAMETERS:

```
! Array containing P(O3) for each tagged species REAL(fp), INTENT(OUT) :: PP(IIPAR, JJPAR, LLTROP, N_TAGGED)
```

REVISION HISTORY:

```
19 Aug 2003 - A. Fiore - Initial version
```

- (1) Updated from the old routine "chemo3_split.f" (rch, bmy, 8/20/03)
- (2) For GEOS-4, convert PBL from [m] to [hPa] w/ the hydrostatic law. Now references SCALE_HEIGHT from "CMN_GCTM". (bmy, 1/15/04)
- (3) Now uses model levels instead of pressure in order to delineate between PBL, MT, and UT regions (amf, rch, bmy, 5/27/04)
- (4) Now references ITS_IN_THE_TROP from "tropopause_mod.f". Now remove reference to "CMN", it's obsolete. (bmy, 8/22/05)
- (5) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (6) Resize the PP array from LLTROP to LLTROP_FIX (phs, 1/19/07)
- (7) Now use LLTROP instead of LLTROP_FIX (bmy, 12/4/07)
- (8) Now use LD65 instead of LLTROP (phs, 11/17/08)
- 08 Dec 2009 R. Yantosca Added ProTeX headers
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 01 Mar 2012 R. Yantosca Now use GET_XMID(I,J,L) from grid_mod.F90
- 01 Mar 2012 R. Yantosca Now use GET_YMID(I,J,L) from grid_mod.F90
- 26 Sep 2013 R. Yantosca Renamed GEOS_57 Cpp switch to GEOS_FP
- 23 Jan 2014 M. Sulprizio- Now use LLTROP instead of LD65 (hyl,bmy,11/3/11)
- 24 Jul 2014 R. Yantosca Now compute BOXVL internally \backslash
- 11 Aug 2015 R. Yantosca MERRA2 behaves the same way as GEOS-FP
- 25 Sep 2015 E. Lundgren Fix bug in setting X upper bound for ITS_IN_EUR
- 22 Oct 2015 E. Lundgren Fix PBLTOP and MTTOP levels for 750 hPa and 350 hPa for GEOS-5, MERRA, GEOS-FP and MERRA2

10.12.2 chem_tagged_o3

Subroutine CHEM_TAGGED_O3 performs chemistry for several O3 species which are tagged by geographic and altitude regions.

INTERFACE:

```
SUBROUTINE CHEM_TAGGED_03( am_I_Root, Input_Opt,
& State_Met, State_Chm, RC )
```

USE CHEMGRID_MOD, ONLY : ITS_IN_THE_TROP

USE CMN_DIAG_MOD

USE CMN_SIZE_MOD

USE DIAG_MOD, ONLY : AD65

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ERROR_STOP
USE ERROR_MOD, ONLY : GEOS_CHEM_STOP
USE HCO_EMISLIST_MOD, ONLY : HCO_GetPtr
USE HCO_INTERFACE_MOD, ONLY : HcoState
USE Input_Opt_Mod, ONLY : OptInput
USE State_Chm_Mod, ONLY : ChmState
USE State_Met_Mod, ONLY : MetState

IMPLICIT NONE

INPUT PARAMETERS:

USE TIME_MOD,

LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?

TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object

TYPE(MetState), INTENT(IN) :: State_Met ! Meteorology State object

ONLY : GET_TS_CHEM

INPUT/OUTPUT PARAMETERS:

TYPE(ChmState), INTENT(INOUT) :: State_Chm ! Chemistry State object

OUTPUT PARAMETERS:

INTEGER, INTENT(OUT) :: RC ! Success or failure?

!REMAKRS:

Dry deposition is now applied in mixing_mod.F90. We have the application of 0x dry deposition from this routine, as well as the archival of the ND44 drydep diagnostic. (bmy, 6/15/15)

- 20 Aug 2003 R. Hudman Initial version
- (1) Updated from the old routine "chemo3_split.f" (rch, bmy, 8/20/03)
- (2) Bug fix: don't put function call in WRITE statement (bmy, 2/20/04)
- (3) Now use ND44_TMP array to store vertical levels of drydep flux, then sum into AD44 array. This prevents numerical differences when using multiple processors. (bmy, 3/24/04)
- (4) Now references LDRYD from "logical_mod.f". Now references STT and N_TRACERS from "tracer_mod.f". Now references AD65 from "diag_pl_mod.f". Now uses ITS_A_NEW_DAY from "time_mod.f". (bmy, 7/20/04)
- (5) Bug fix: Now avoid a SEG FAULT error if PBLFRAC isn't allocated. (bdf, bmy, 10/12/04)
- (6) Replace PBLFRAC from "drydep_mod.f" with GET_FRAC_UNDER_PBLTOP from "pbl_mix_mod.f". Now only sum ND44 diagnostic up to the

```
maximum tropopsheric level. (bmy, 2/17/05)
(7) Resize PP, N D44_TMP arrays from LLTROP to LLTROP_FIX. Now only loop
      up to LLTROP_FIX (phs, 1/19/07)
(8) Now use LLTROP instead of LLTROP_FIX (bmy, 12/4/07)
(9) Now use LD65 instead of LLTROP (phs, 11/17/08)
(10) Now only compute loss rate in troposphere (dbj, bmy, 10/26/09)
08 Dec 2009 - R. Yantosca - Added ProTeX headers
01 Mar 2012 - R. Yantosca - Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
14 Mar 2013 - M. Payer
                         - Replace Ox with O3 as part of removal of NOx-Ox
                            partitioning
25 Mar 2013 - R. Yantosca - Now accept am_I_Root, Input_Opt, State_Chm, RC
20 Aug 2013 - R. Yantosca - Removed "define.h", this is now obsolete
23 Jan 2014 - M. Sulprizio- Now use LLTROP instead of LD65 (hyl,bmy,11/3/11)
11 Apr 2014 - R. Yantosca - Remove call to INIT_TAGGED_OX
24 Jul 2014 - R. Yantosca - Now compute BOXVL internally
17 Sep 2014 - C. Keller - Now use HEMCO for prod. and loss arrays
12 Jun 2015 - R. Yantosca - Now remove orphaned ND44 variables
15 Jun 2015 - R. Yantosca - Bug fix: PP doesn't have to be held PRIVATE
15 Jun 2015 - R. Yantosca - Updated comments for removal of drydep
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
30 Jun 2016 - R. Yantosca - Remove instances of STT. Now get the advected
                            species ID from State_Chm%Map_Advect.
```

10.12.3 init_tagged_o3

Subroutine INIT_TAGGED_O3 allocates and zeroes all module arrays.

INTERFACE:

```
SUBROUTINE INIT_TAGGED_03( am_I_Root, Input_Opt, State_Chm, RC )
```

USES:

```
USE CMN_SIZE_MOD

USE ErrCode_Mod

USE ERROR_MOD, ONLY : ALLOC_ERR

USE ERROR_MOD, ONLY : ERROR_STOP

USE Input_Opt_Mod, ONLY : OptInput

USE State_Chm_Mod, ONLY : ChmState

USE State_Chm_Mod, ONLY : Ind_
```

INPUT PARAMETERS:

USE CMN_DIAG_MOD

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU?
TYPE(OptInput), INTENT(IN) :: Input_Opt ! Input Options object
TYPE(ChmState), INTENT(IN) :: State_Chm ! Chemistry State object
```

OUTPUT PARAMETERS:

REMARKS:

This routine is now called from GC_INIT_EXTRA in GeosCore/input_mod.F.

REVISION HISTORY:

- 20 Aug 2003 R. Yantosca Initial version
- (1) Now reference N_TRACERS from "tracer_mod.f" (bmy, 7/20/04)
- (2) Now use LD65 instead of LLTROP to dimension P24H, L24H (phs, 11/18/08)
- 08 Dec 2009 R. Yantosca Added ProTeX headers
- 25 Mar 2013 R. Yantosca Now accept am_I_Root, Input_Opt, RC args
- 23 Jan 2014 M. Sulprizio- Now use LLTROP instead of LD65 to dimension P24H, L24H (hyl, bmy, 11/3/11)
- 20 Jun 2016 R. Yantosca Now define species ID's in the init phase
- 20 Jun 2016 R. Yantosca Add check to prevent array OOB errors
- 21 Jun 2016 R. Yantosca Rename IDTO3Strt to id_O3Strat

10.12.4 cleanup_tagged_o3

CLEANUP_TAGGED_O3 deallocates all module arrays.

INTERFACE:

SUBROUTINE CLEANUP_TAGGED_03()

- 20 Aug 2003 R. Yantosca Initial version
- 08 Dec 2009 R. Yantosca Added ProTeX headers