# GEOS-Chem Reference

# 4. The Harvard-NASA Emissions Component (HEMCO)

## GEOS-CHEM SUPPORT TEAM

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|   |      |         | Calc_Ka                                     |
|   |      |         | Calc_Kl                                     |
|   |      |         | N_SW  |
|   |      | -       | P_SW  |
|   |      |         | V_SW  |
|   |      |         | D_WC  |
|   |      |         | D_HM  |
|   |      |         | Schmidt_W                                   |
|   |      |         | Schmidt_W                                   |
|   |      |         |   |
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|   |      |         | P_Air                                       |
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## 1 HEMCO "Core" modules

These contain routines that perform core HEMCO functions, such as establishing the data structures used to store the emissions data, etc.

#### 1.1 Fortran: Module Interface hco arr mod.F90

Module HCO\_Arr\_Mod contains routines and variables to initialize, validate, and cleanup HEMCO data arrays. HEMCO data arrays can be 2D or 3D. They can be organized as single arrays or as vector of arrays to represent an additional dimension (time).

The public data types Arr2D\_Hp and Arr3D\_Hp represent the 2D/3D arrays used by HEMCO. The HEMCO precision HP is defined in HCO\_Error\_Mod. There is also an integer 2D array (type Arr2D\_I) that can be used to store integer data. Additional data types can be added as needed.

Data values are stored in array 'Val'. Val can be self-allocated or a pointer to existing data, as denoted by the Alloc flag.

At the moment, the following HEMCO structures use HEMCO arrays:

- FileData: emission data (base emissions, scale factors, masks) stored in the FileData derived type. These data are read from disk as specified in the configuration file. See HCO\_FileData\_Mod.F90.
- FluxArr: the HEMCO flux arrays (emissions and deposition velocities) stored in the HEMCO state object. See HCO\_State\_Mod.F90.
- Grid: all grid information arrays (x midpoints, y midpoints, etc.) stored in the HEMCO state object.
- ExtDat: external data required by the extensions (primarily met fields). See HCOX\_State\_Mod.F90.

#### **INTERFACE:**

```
MODULE HCO_Arr_Mod
```

#### **USES:**

```
USE HCO_Error_Mod
```

IMPLICIT NONE

PRIVATE

### PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCO\_ArrInit
PUBLIC :: HCO\_ArrAssert
PUBLIC :: HCO\_ArrCleanup

#### PRIVATE MEMBER FUNCTIONS:

```
PRIVATE :: HCO_ArrInit_3D_Hp
  PRIVATE :: HCO_ArrInit_2D_Hp
  PRIVATE :: HCO_ArrInit_3D_Sp
  PRIVATE :: HCO_ArrInit_2D_Sp
  PRIVATE :: HCO_ArrInit_2D_I
  PRIVATE :: HCO_ArrVecInit_3D_Hp
  PRIVATE :: HCO_ArrVecInit_2D_Hp
  PRIVATE :: HCO_ArrVecInit_3D_Sp
  PRIVATE :: HCO_ArrVecInit_2D_Sp
  PRIVATE :: HCO_ValInit
  PRIVATE :: HCO_ValInit_3D_Sp
  PRIVATE :: HCO_ValInit_3D_Dp
  PRIVATE :: HCO_ValInit_2D_Sp
  PRIVATE :: HCO_ValInit_2D_Dp
  PRIVATE :: HCO_ValInit_2D_I
  PRIVATE :: HCO_ArrAssert_2D_Hp
  PRIVATE :: HCO_ArrAssert_3D_Hp
  PRIVATE :: HCO_ArrAssert_2D_Sp
  PRIVATE :: HCO_ArrAssert_3D_Sp
  PRIVATE :: HCO_ArrCleanup_3D_Hp
  PRIVATE :: HCO_ArrCleanup_2D_Hp
  PRIVATE :: HCO_ArrCleanup_3D_Sp
  PRIVATE :: HCO_ArrCleanup_2D_Sp
  PRIVATE :: HCO_ArrCleanup_2D_I
  PRIVATE :: HCO_ArrVecCleanup_3D_Hp
  PRIVATE :: HCO_ArrVecCleanup_2D_Hp
  PRIVATE :: HCO_ArrVecCleanup_3D_Sp
  PRIVATE :: HCO_ArrVecCleanup_2D_Sp
  PRIVATE :: HCO_ValCleanup_3D_Sp
  PRIVATE :: HCO_ValCleanup_3D_Dp
  PRIVATE :: HCO_ValCleanup_2D_Sp
  PRIVATE :: HCO_ValCleanup_2D_Dp
  PRIVATE :: HCO_ValCleanup_2D_I
PUBLIC DATA MEMBERS:
   ! 2D arrays
  TYPE, PUBLIC :: Arr2D_Hp
      REAL(hp), POINTER :: Val(:,:)
                                      ! x,y
      LOGICAL
                       :: Alloc
                                      ! Allocated?
  END TYPE Arr2D_Hp
  TYPE, PUBLIC :: Arr2D_I
      INTEGER, POINTER :: Val(:,:)
                                    ! x,y
      LOGICAL
                       :: Alloc
                                      ! Allocated?
  END TYPE Arr2D_I
  TYPE, PUBLIC :: Arr2D_Sp
     REAL(sp), POINTER :: Val(:,:) ! x,y
```

```
LOGICAL
                     :: Alloc ! Allocated?
  END TYPE Arr2D_Sp
   ! 3D arrays
  TYPE, PUBLIC :: Arr3D_Hp
     REAL(hp), POINTER :: Val(:,:,:) ! x,y,z
     LOGICAL
                 :: Alloc ! Allocated?
  END TYPE Arr3D_Hp
  TYPE, PUBLIC :: Arr3D_Sp
     REAL(sp), POINTER :: Val(:,:,:) ! x,y,z
                     :: Alloc ! Allocated?
     LOGICAL
  END TYPE Arr3D_Sp
PRIVATE TYPES:
  INTERFACE HCO_ArrInit
     MODULE PROCEDURE HCO_ArrInit_3D_Hp
     MODULE PROCEDURE HCO_ArrInit_2D_Hp
     MODULE PROCEDURE HCO_ArrInit_3D_Sp
     MODULE PROCEDURE HCO_ArrInit_2D_Sp
     MODULE PROCEDURE HCO_ArrInit_2D_I
     MODULE PROCEDURE HCO_ArrVecInit_3D_Hp
     MODULE PROCEDURE HCO_ArrVecInit_2D_Hp
     MODULE PROCEDURE HCO_ArrVecInit_3D_Sp
     MODULE PROCEDURE HCO_ArrVecInit_2D_Sp
  END INTERFACE HCO_ArrInit
  INTERFACE HCO_ValInit
     MODULE PROCEDURE HCO_ValInit_3D_Sp
     MODULE PROCEDURE HCO_ValInit_3D_Dp
     MODULE PROCEDURE HCO_ValInit_2D_Sp
     MODULE PROCEDURE HCO_ValInit_2D_Dp
     MODULE PROCEDURE HCO_ValInit_2D_I
  END INTERFACE HCO_ValInit
  INTERFACE HCO_ArrAssert
     MODULE PROCEDURE HCO_ArrAssert_2D_Hp
     MODULE PROCEDURE HCO_ArrAssert_3D_Hp
     MODULE PROCEDURE HCO_ArrAssert_2D_Sp
     MODULE PROCEDURE HCO_ArrAssert_3D_Sp
     MODULE PROCEDURE HCO_ArrAssert_2D_I
  END INTERFACE HCO_ArrAssert
  INTERFACE HCO_ArrCleanup
     MODULE PROCEDURE HCO_ArrCleanup_3D_Hp
     MODULE PROCEDURE HCO_ArrCleanup_2D_Hp
     MODULE PROCEDURE HCO_ArrCleanup_2D_I
     MODULE PROCEDURE HCO_ArrCleanup_3D_Sp
```

```
MODULE PROCEDURE HCO_ArrCleanup_2D_Sp
MODULE PROCEDURE HCO_ArrVecCleanup_3D_Hp
MODULE PROCEDURE HCO_ArrVecCleanup_2D_Hp
MODULE PROCEDURE HCO_ArrVecCleanup_3D_Sp
MODULE PROCEDURE HCO_ArrVecCleanup_2D_Sp
END INTERFACE HCO_ArrCleanup

INTERFACE HCO_ValCleanup

MODULE PROCEDURE HCO_ValCleanup_3D_Sp
MODULE PROCEDURE HCO_ValCleanup_3D_Dp
MODULE PROCEDURE HCO_ValCleanup_2D_Sp
MODULE PROCEDURE HCO_ValCleanup_2D_Dp
MODULE PROCEDURE HCO_ValCleanup_2D_Dp
MODULE PROCEDURE HCO_ValCleanup_2D_I
END INTERFACE HCO_ValCleanup_2D_I
```

#### REVISION HISTORY:

```
19 Dec 2013 - C. Keller - Initialization
01 Jul 2014 - R. Yantosca - Corrected errors in ProTeX headers
01 Jul 2014 - R. Yantosca - Now use F90 free-format indentation
01 Oct 2014 - C. Keller - Added Alloc flag
```

## 1.1.1 HCO\_ArrInit\_2D\_Hp

Subroutine HCO\_ArrInit\_2D\_Hp initializes the given data container 2D array. nx and ny denote the array size dimensions. If nx is set to 0, no data is allocated but Val is set to a (nullified) pointer instead.

#### **INTERFACE:**

```
SUBROUTINE HCO_ArrInit_2D_Hp( Arr, nx, ny, RC )
```

## **INPUT PARAMETERS:**

```
TYPE(Arr2D_Hp), POINTER :: Arr ! Array INTEGER, INTENT(IN) :: nx ! x-dim INTEGER, INTENT(IN) :: ny ! y-dim
```

## INPUT/OUTPUT PARAMETERS:

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

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

#### 1.1.2 HCO\_ArrInit\_2D\_Sp

Subroutine HCO\_ArrInit\_2D\_Sp initializes the given data container 2D array. nx and ny denote the array size dimensions. If nx is set to 0, no data is allocated but Val is set to a (nullified) pointer instead.

#### **INTERFACE:**

```
SUBROUTINE HCO_ArrInit_2D_Sp( Arr, nx, ny, RC )
```

#### INPUT PARAMETERS:

```
TYPE(Arr2D_Sp), POINTER :: Arr ! Array INTEGER, INTENT(IN) :: nx ! x-dim INTEGER, INTENT(IN) :: ny ! y-dim
```

## INPUT/OUTPUT PARAMETERS:

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

#### **REVISION HISTORY:**

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

#### 1.1.3 HCO\_ArrInit\_2D\_I

Subroutine HCO\_ArrInit\_2D\_I initializes the given data container integer 2D array. nx and ny denote the array size dimensions. If nx is set to 0, no data is allocated but Val is set to a (nullified) pointer instead.

#### INTERFACE:

```
SUBROUTINE HCO_ArrInit_2D_I(Arr, nx, ny, RC)
```

#### INPUT PARAMETERS:

```
TYPE(Arr2D_I), POINTER :: Arr ! Array
INTEGER, INTENT(IN) :: nx ! x-dim
INTEGER, INTENT(IN) :: ny ! y-dim
```

## INPUT/OUTPUT PARAMETERS:

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

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

#### 1.1.4 HCO\_ArrInit\_3D\_Hp

Subroutine HCO\_ArrInit\_3D\_Hp initializes the given data container 3D array. nx and ny denote the array size dimensions. If nx is set to 0, no data is allocated but Val is set to a (nullified) pointer instead.

#### **INTERFACE:**

```
SUBROUTINE HCO_ArrInit_3D_Hp( Arr, nx, ny, nz, RC )
```

#### INPUT PARAMETERS:

```
TYPE(Arr3D_Hp), POINTER :: Arr ! Array
INTEGER, INTENT(IN) :: nx ! x-dim
INTEGER, INTENT(IN) :: ny ! y-dim
INTEGER, INTENT(IN) :: nz ! z-dim
```

## INPUT/OUTPUT PARAMETERS:

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

#### REVISION HISTORY:

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

## 1.1.5 HCO\_ArrInit\_3D\_Sp

Subroutine HCO\_ArrInit\_3D\_Sp initializes the given data container 3D array. nx and ny denote the array size dimensions. If nx is set to 0, no data is allocated but Val is set to a (nullified) pointer instead.

#### **INTERFACE:**

```
SUBROUTINE HCO_ArrInit_3D_Sp( Arr, nx, ny, nz, RC )
```

#### INPUT PARAMETERS:

```
TYPE(Arr3D_Sp), POINTER :: Arr ! Array
INTEGER, INTENT(IN) :: nx ! x-dim
INTEGER, INTENT(IN) :: ny ! y-dim
INTEGER, INTENT(IN) :: nz ! z-dim
```

## INPUT/OUTPUT PARAMETERS:

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

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

#### 1.1.6 HCO\_ArrVecInit\_2D\_Hp

Subroutine HCO\_ArrVecInit\_2D\_Hp initializes the given data container 2D array vector. nn denotes the number of 2D arrays, and nx and ny denote the array size dimensions. If nx is set to 0, no data is allocated but Val is set to a (nullified) pointer instead.

#### **INTERFACE:**

```
SUBROUTINE HCO_ArrVecInit_2D_Hp( ArrVec, nn, nx, ny, RC )
```

#### INPUT PARAMETERS:

```
TYPE(Arr2D_Hp), POINTER :: ArrVec(:) ! Array vector INTEGER, INTENT(IN) :: nn ! vector length INTEGER, INTENT(IN) :: nx ! x-dim INTEGER, INTENT(IN) :: ny ! y-dim
```

## INPUT/OUTPUT PARAMETERS:

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

## **REVISION HISTORY:**

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

## 1.1.7 HCO\_ArrVecInit\_2D\_Sp

Subroutine HCO\_ArrVecInit\_2D\_Sp initializes the given data container 2D array vector. nn denotes the number of 2D arrays, and nx and ny denote the array size dimensions. If nx is set to 0, no data is allocated but Val is set to a (nullified) pointer instead.

#### **INTERFACE:**

```
SUBROUTINE HCO_ArrVecInit_2D_Sp( ArrVec, nn, nx, ny, RC )
```

#### **INPUT PARAMETERS:**

```
TYPE(Arr2D_Sp), POINTER :: ArrVec(:) ! Array vector
INTEGER, INTENT(IN) :: nn ! vector length
INTEGER, INTENT(IN) :: nx ! x-dim
INTEGER, INTENT(IN) :: ny ! y-dim
```

## INPUT/OUTPUT PARAMETERS:

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

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

#### 1.1.8 HCO\_ArrVecInit\_3D\_Hp

Subroutine HCO\_ArrVecInit\_3D\_Hp initializes the given data container 3D array vector. nn denotes the number of 2D arrays, and nx and ny denote the array size dimensions. If nx is set to 0, no data is allocated but Val is set to a (nullified) pointer instead.

#### **INTERFACE:**

```
SUBROUTINE HCO_ArrVecInit_3D_Hp( ArrVec, nn, nx, ny, nz, RC )
```

#### **INPUT PARAMETERS:**

```
TYPE(Arr3D_Hp),
                  POINTER
                                  :: ArrVec(:) ! Array vector
INTEGER,
                                               ! vector length
                  INTENT(IN)
                                 :: nn
INTEGER,
                  INTENT(IN)
                                 :: nx
                                               ! x-dim
                                               ! y-dim
INTEGER,
                  INTENT(IN)
                                 :: ny
                                               ! z-dim
INTEGER,
                  INTENT(IN)
                                  :: nz
```

#### INPUT/OUTPUT PARAMETERS:

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

## **REVISION HISTORY:**

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

## 1.1.9 HCO\_ArrVecInit\_3D\_Sp

Subroutine HCO\_ArrVecInit\_3D\_Sp initializes the given data container 3D array vector. nn denotes the number of 2D arrays, and nx and ny denote the array size dimensions. If nx is set to 0, no data is allocated but Val is set to a (nullified) pointer instead.

#### **INTERFACE:**

```
SUBROUTINE HCO_ArrVecInit_3D_Sp( ArrVec, nn, nx, ny, nz, RC )
```

#### INPUT PARAMETERS:

```
TYPE(Arr3D_Sp),
                  POINTER
                                 :: ArrVec(:) ! Array vector
INTEGER,
                  INTENT(IN)
                                               ! vector length
                                 :: nn
                                               ! x-dim
INTEGER,
                  INTENT(IN)
                                 :: nx
                                               ! y-dim
INTEGER,
                  INTENT(IN)
                                 :: ny
                                               ! z-dim
INTEGER,
                  INTENT(IN)
                                 :: nz
```

#### INPUT/OUTPUT PARAMETERS:

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

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

#### 1.1.10 HCO\_ValInit\_2D\_Sp

Subroutine HCO\_ValInit\_2D\_Sp initializes the given data container 2D single precision array. nx and ny denote the array size dimensions. If nx is set to 0, no data is allocated but Val is set to a (nullified) pointer instead.

#### **INTERFACE:**

```
SUBROUTINE HCO_ValInit_2D_Sp( Val, nx, ny, Alloc, RC )
```

#### INPUT PARAMETERS:

```
REAL(sp), POINTER :: Val(:,:) ! Array INTEGER, INTENT(IN) :: nx ! x-dim INTEGER, INTENT(IN) :: ny ! y-dim
```

## INPUT/OUTPUT PARAMETERS:

```
LOGICAL, INTENT( OUT) :: Alloc ! allocated? INTEGER, INTENT(INOUT) :: RC ! Return code
```

#### REVISION HISTORY:

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

## 1.1.11 HCO\_ValInit\_2D\_Dp

Subroutine HCO\_ValInit\_2D\_Dp initializes the given data container 2D double precision array. nx and ny denote the array size dimensions. If nx is set to 0, no data is allocated but Val is set to a (nullified) pointer instead.

#### **INTERFACE:**

```
SUBROUTINE HCO_ValInit_2D_Dp( Val, nx, ny, Alloc, RC )
```

#### INPUT PARAMETERS:

```
REAL(dp), POINTER :: Val(:,:) ! Array INTEGER, INTENT(IN) :: nx ! x-dim INTEGER, INTENT(IN) :: ny ! y-dim
```

#### INPUT/OUTPUT PARAMETERS:

```
LOGICAL, INTENT( OUT) :: Alloc ! allocated? INTEGER, INTENT(INOUT) :: RC ! Return code
```

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

#### 1.1.12 HCO\_ValInit\_2D\_I

Subroutine HCO\_ValInit\_2D\_I initializes the given data container 2D integer array. nx and ny denote the array size dimensions. If nx is set to 0, no data is allocated but Val is set to a (nullified) pointer instead.

#### **INTERFACE:**

```
SUBROUTINE HCO_ValInit_2D_I( Val, nx, ny, Alloc, RC )
```

#### **INPUT PARAMETERS:**

```
INTEGER, POINTER :: Val(:,:) ! Array
INTEGER, INTENT(IN) :: nx ! x-dim
INTEGER, INTENT(IN) :: ny ! y-dim
```

## INPUT/OUTPUT PARAMETERS:

```
LOGICAL, INTENT( OUT) :: Alloc ! allocated?

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

#### REVISION HISTORY:

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

## 1.1.13 HCO\_ValInit\_3D\_Dp

Subroutine HCO\_ValInit\_3D\_Dp initializes the given data container 3D double precision array. nx and ny denote the array size dimensions. If nx is set to 0, no data is allocated but Val is set to a (nullified) pointer instead.

#### **INTERFACE:**

```
SUBROUTINE HCO_ValInit_3D_Dp( Val, nx, ny, nz, Alloc, RC )
```

## **INPUT PARAMETERS:**

```
REAL(dp), POINTER :: Val(:,:,:)! Array INTEGER, INTENT(IN) :: nx ! x-dim INTEGER, INTENT(IN) :: ny ! y-dim INTEGER, INTENT(IN) :: nz ! z-dim
```

## INPUT/OUTPUT PARAMETERS:

```
LOGICAL, INTENT( OUT) :: Alloc ! allocated? INTEGER, INTENT(INOUT) :: RC ! Return code
```

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

## 1.1.14 HCO\_ValInit\_3D\_Sp

Subroutine HCO\_ValInit\_3D\_Sp initializes the given data container 3D single precision array. nx and ny denote the array size dimensions. If nx is set to 0, no data is allocated but Val is set to a (nullified) pointer instead.

#### **INTERFACE:**

```
SUBROUTINE HCO_ValInit_3D_Sp( Val, nx, ny, nz, Alloc, RC )
```

#### **INPUT PARAMETERS:**

```
REAL(sp), POINTER :: Val(:,:,:)! Array INTEGER, INTENT(IN) :: nx ! x-dim INTEGER, INTENT(IN) :: ny ! y-dim INTEGER, INTENT(IN) :: nz ! z-dim
```

## INPUT/OUTPUT PARAMETERS:

```
LOGICAL, INTENT( OUT) :: Alloc ! allocated?
INTEGER, INTENT(INOUT) :: RC ! Return code
```

#### **REVISION HISTORY:**

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

## 1.1.15 HCO\_ArrAssert\_3D\_Hp

Routine HCO\_ArrAssert\_3D\_Hp makes sure that the passed 3D array is allocated.

#### **INTERFACE:**

```
SUBROUTINE HCO_ArrAssert_3D_Hp( ThisArr3D, I, J, L, RC )
```

#### INPUT PARAMETERS:

```
TYPE(Arr3D_Hp), POINTER :: ThisArr3D ! 3D array
INTEGER, INTENT(IN ) :: I, J, L ! Array dims
```

## INPUT/OUTPUT PARAMETERS:

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

#### **REMARKS:**

```
01 May 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

## 1.1.16 HCO\_ArrAssert\_3D\_Sp

Routine HCO\_ArrAssert\_3D\_Sp makes sure that the passed 3D array is allocated.

#### **INTERFACE:**

```
SUBROUTINE HCO_ArrAssert_3D_Sp( ThisArr3D, I, J, L, RC )
```

#### INPUT PARAMETERS:

## INPUT/OUTPUT PARAMETERS:

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

#### **REMARKS:**

#### REVISION HISTORY:

```
01 May 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

## 1.1.17 HCO\_ArrAssert\_2D\_Hp

Routine HCO\_ArrAssert\_2D\_Hp makes sure that the passed 2D array is allocated.

## **INTERFACE:**

```
SUBROUTINE HCO_ArrAssert_2D_Hp( ThisArr2D, I, J, RC )
```

## **INPUT PARAMETERS:**

```
TYPE(Arr2D_Hp), POINTER :: ThisArr2D ! 2D array INTEGER, INTENT(IN ) :: I, J ! Array dims
```

## INPUT/OUTPUT PARAMETERS:

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

#### **REMARKS:**

```
01 May 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

## 1.1.18 HCO\_ArrAssert\_2D\_Sp

Routine HCO\_ArrAssert\_2D\_Sp makes sure that the passed 2D array is allocated.

#### **INTERFACE:**

```
SUBROUTINE HCO_ArrAssert_2D_Sp( ThisArr2D, I, J, RC )
```

#### INPUT PARAMETERS:

```
TYPE(Arr2D_Sp), POINTER :: ThisArr2D ! 2D array INTEGER, INTENT(IN ) :: I, J ! Array dims
```

## INPUT/OUTPUT PARAMETERS:

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

#### **REMARKS:**

### **REVISION HISTORY:**

```
01 May 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

#### 1.1.19 HCO\_ArrAssert\_2D\_I

Routine HCO\_ArrAssert\_2D\_I makes sure that the passed 2D array is allocated.

## **INTERFACE:**

```
SUBROUTINE HCO_ArrAssert_2D_I( ThisArr2D, I, J, RC )
```

## INPUT PARAMETERS:

```
TYPE(Arr2D_I), POINTER :: ThisArr2D ! 2D array
INTEGER, INTENT(IN ) :: I, J ! Array dims
```

## INPUT/OUTPUT PARAMETERS:

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

## **REMARKS:**

```
01 May 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

## 1.1.20 HCO\_ArrCleanup\_2D\_Hp

Subroutine HCO\_ArrCleanup\_2D\_Hp cleans up the given container 2D array.

#### **INTERFACE:**

```
SUBROUTINE HCO_ArrCleanup_2D_Hp( Arr, DeepClean )
```

#### INPUT PARAMETERS:

#### **REVISION HISTORY:**

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

## $1.1.21 \quad HCO\_ArrCleanup\_2D\_Sp$

Subroutine HCO\_ArrCleanup\_2D\_Sp cleans up the given container 2D array.

#### **INTERFACE:**

```
SUBROUTINE HCO_ArrCleanup_2D_Sp( Arr, DeepClean )
```

#### INPUT PARAMETERS:

#### REVISION HISTORY:

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

#### 1.1.22 HCO\_ArrCleanup\_2D\_I

Subroutine HCO\_ArrCleanup\_2D\_I cleans up the given container 2D array.

#### **INTERFACE:**

```
SUBROUTINE HCO_ArrCleanup_2D_I( Arr, DeepClean )
```

#### INPUT PARAMETERS:

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

#### 1.1.23 HCO\_ArrCleanup\_3D\_Hp

Subroutine HCO\_ArrCleanup\_3D\_Hp cleans up the given container 3D array.

#### **INTERFACE:**

```
SUBROUTINE HCO_ArrCleanup_3D_Hp( Arr, DeepClean )
```

#### INPUT PARAMETERS:

```
TYPE(Arr3D_Hp),          POINTER :: Arr     ! Array
LOGICAL, INTENT(IN), OPTIONAL :: DeepClean ! Deallocate array?
```

#### **REVISION HISTORY:**

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

## 1.1.24 HCO\_ArrCleanup\_3D\_Sp

Subroutine HCO\_ArrCleanup\_3D\_Sp cleans up the given container 3D array.

#### INTERFACE:

```
SUBROUTINE HCO_ArrCleanup_3D_Sp( Arr, DeepClean )
```

#### INPUT PARAMETERS:

```
TYPE(Arr3D_Sp), POINTER :: Arr ! Array
LOGICAL, INTENT(IN), OPTIONAL :: DeepClean ! Deallocate array?
```

#### REVISION HISTORY:

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

#### 1.1.25 HCO\_ArrVecCleanup\_2D\_Hp

Subroutine HCO\_ArrVecCleanup\_2D\_Hp cleans up the given container 2D array vector.

#### **INTERFACE:**

```
SUBROUTINE HCO_ArrVecCleanup_2D_Hp( ArrVec, DeepClean )
```

#### INPUT PARAMETERS:

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

## 1.1.26 HCO\_ArrVecCleanup\_2D\_Sp

Subroutine HCO\_ArrVecCleanup\_2D\_Sp cleans up the given container 2D array vector.

#### **INTERFACE:**

```
SUBROUTINE HCO_ArrVecCleanup_2D_Sp( ArrVec, DeepClean )
```

#### INPUT PARAMETERS:

#### **REVISION HISTORY:**

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

## $1.1.27 \quad HCO\_ArrVecCleanup\_3D\_Hp$

Subroutine HCO\_ArrVecCleanup\_3D\_Hp cleans up the given container 3D array vector.

#### **INTERFACE:**

```
SUBROUTINE HCO_ArrVecCleanup_3D_Hp( ArrVec, DeepClean )
```

#### INPUT PARAMETERS:

#### REVISION HISTORY:

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

#### 1.1.28 HCO\_ArrVecCleanup\_3D\_Sp

Subroutine HCO\_ArrVecCleanup\_3D\_Sp cleans up the given container 3D array vector.

#### **INTERFACE:**

```
SUBROUTINE HCO_ArrVecCleanup_3D_Sp( ArrVec, DeepClean )
```

#### INPUT PARAMETERS:

```
TYPE(Arr3D_Sp), POINTER :: ArrVec(:) ! Array
LOGICAL, INTENT(IN), OPTIONAL :: DeepClean ! Deallocate array?
```

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

## 1.1.29 HCO\_ValCleanup\_2D\_Dp

Subroutine HCO\_ValCleanup\_2D\_Dp cleans up the given container 2D array. If DeepClean is set to TRUE and the array is indeed allocated (as determined by the Alloc flag), the array becomes deallocated. Otherwise, it is just nullified.

#### **INTERFACE:**

```
SUBROUTINE HCO_ValCleanup_2D_Dp( Val, Alloc, DeepClean )
```

#### INPUT PARAMETERS:

```
REAL(dp), POINTER :: Val(:,:) ! Array
LOGICAL, INTENT(IN) :: Alloc ! Allocated?
LOGICAL, INTENT(IN) :: DeepClean ! Deallocate array?
```

### **REVISION HISTORY:**

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

## 1.1.30 HCO\_ValCleanup\_2D\_Sp

Subroutine HCO\_ValCleanup\_2D\_Sp cleans up the given container 2D array. If DeepClean is set to TRUE and the array is indeed allocated (as determined by the Alloc flag), the array becomes deallocated. Otherwise, it is just nullified.

#### **INTERFACE:**

```
SUBROUTINE HCO_ValCleanup_2D_Sp( Val, Alloc, DeepClean )
```

#### INPUT PARAMETERS:

```
REAL(sp), POINTER :: Val(:,:) ! Array
LOGICAL, INTENT(IN) :: Alloc ! Allocated?
LOGICAL, INTENT(IN) :: DeepClean ! Deallocate array?
```

## **REVISION HISTORY:**

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

## 1.1.31 HCO\_ValCleanup\_2D\_I

Subroutine HCO\_ValCleanup\_2D\_I cleans up the given container 2D array. If DeepClean is set to TRUE and the array is indeed allocated (as determined by the Alloc flag), the array becomes deallocated. Otherwise, it is just nullified.

#### **INTERFACE:**

```
SUBROUTINE HCO_ValCleanup_2D_I( Val, Alloc, DeepClean )
```

### **INPUT PARAMETERS:**

```
INTEGER, POINTER :: Val(:,:) ! Array
LOGICAL, INTENT(IN) :: Alloc ! Allocated?
LOGICAL, INTENT(IN) :: DeepClean ! Deallocate array?
```

#### **REVISION HISTORY:**

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

## $1.1.32 \quad HCO\_ValCleanup\_3D\_Dp$

Subroutine HCO\_ValCleanup\_3D\_Dp cleans up the given container 3D array. If DeepClean is set to TRUE and the array is indeed allocated (as determined by the Alloc flag), the array becomes deallocated. Otherwise, it is just nullified.

#### **INTERFACE:**

```
SUBROUTINE HCO_ValCleanup_3D_Dp( Val, Alloc, DeepClean )
```

#### INPUT PARAMETERS:

```
REAL(dp), POINTER :: Val(:,:,:) ! Array
LOGICAL, INTENT(IN) :: Alloc ! Allocated?
LOGICAL, INTENT(IN) :: DeepClean ! Deallocate array?
```

#### **REVISION HISTORY:**

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

#### 1.1.33 HCO\_ValCleanup\_3D\_Sp

Subroutine HCO\_ValCleanup\_3D\_Sp cleans up the given container 3D array. If DeepClean is set to TRUE and the array is indeed allocated (as determined by the Alloc flag), the array becomes deallocated. Otherwise, it is just nullified.

#### **INTERFACE:**

```
SUBROUTINE HCO_ValCleanup_3D_Sp( Val, Alloc, DeepClean )
```

#### INPUT PARAMETERS:

```
REAL(sp), POINTER :: Val(:,:,:) ! Array
LOGICAL, INTENT(IN) :: Alloc ! Allocated?
LOGICAL, INTENT(IN) :: DeepClean ! Deallocate array?
```

```
20 Apr 2013 - C. Keller - Initial version
01 Oct 2014 - C. Keller - Added Alloc flag
```

## 1.2 Fortran: Module Interface hco\_calc\_mod.F90

Module HCO\_Calc\_Mod contains routines to calculate HEMCO core emissions based on the content of the HEMCO EmisList object. All emissions are in [kg/m2/s].

Emissions for the current datetime are calculated by multiplying base emissions fields with the associated scale factors. Different inventories are merged/overlayed based upon the category and hierarchy attributes assigned to the individual base fields. Within the same category, fields of higher hierarchy overwrite lower-hierarchy fields. Emissions of different categories are always added.

The assembled emission array is written into the corresponding emission rates array of the HEMCO state object: HcoStateHcoID denotes the corresponding species ID. Emis covers dimension lon, lat, lev on the HEMCO grid, i.e. unlike the emission arrays in EmisList that only cover the levels defined in the source files, Emis extends over all vertical model levels.

Negative emissions are not supported and are ignored. Surface deposition velocities are stored in HcoStatebe added therein.

In addition to emissions and surface deposition rates, HEMCO also supports concentrations (kg/m3). Data is automatically written into the concentration array HcoStateis marked as being concentration data (i.e. if DtaThe latter is automatically determined by HEMCO based upon the data units.

All emission calculation settings are passed through the HcoState options object (HcoState

- ExtNr: extension number to be considered.
- SpcMin: lower species ID (HEMCO ID) to be considered.
- SpcMax: upper species ID (HEMCO ID) to be considered. If set to -1, all species above or equal to SpcMin are considered.
- CatMin: lower emission category to be considered.
- CatMax: upper emission category to be considered. If set to -1, all categories above or equal to CatMin are considered.
- FillBuffer: if set to TRUE, the emissions will be written into buffer array HcoStateIf this option is enabled, only one species can be calculated at a time (by setting SpcMin/SpcMax, CatMin/CatMax and/or ExtNr accordingly). This option is useful for extensions, e.g. if additional scalings need to be done on some emission fields assembled by HEMCO (e.g. PARANOX extension).

#### **INTERFACE:**

MODULE HCO\_Calc\_Mod

**USES:** 

```
USE HCO_Diagn_Mod
USE HCO_Error_Mod
USE HCO_Types_Mod
USE HCO_DataCont_Mod, ONLY : Pnt2DataCont
IMPLICIT NONE
PRIVATE
```

#### PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCO\_CalcEmis
PUBLIC :: HCO\_CheckDepv
PUBLIC :: HCO\_EvalFld
PUBLIC :: HCO\_MaskFld

#### PRIVATE MEMBER FUNCTIONS:

PRIVATE :: GET\_CURRENT\_EMISSIONS

PRIVATE :: GetMaskVal
PRIVATE :: GetDilFact
PRIVATE :: GetVertIndx
PRIVATE :: GetIdx

! PARAMETER

! Mask threshold. All mask values below this value will be evaluated

! as zero (= outside of mask), and all values including and above this

! value as inside the mask. This is only of relevance if the MaskFractions

! option is false. If  ${\tt MaskFractions}$  is true, the fractional mask values are

! considered, e.g. a grid box can contribute 40% to a mask region, etc.

! The MaskFractions toggle can be set in the settings section of the HEMCO

! configuration file (Use mask fractions: true/false). It defaults to false.

REAL(sp), PARAMETER :: MASK\_THRESHOLD = 0.5\_sp

\_\_\_\_\_\_

## **REVISION HISTORY:**

```
25 Aug 2012 - C. Keller - Initial version.

06 Jun 2014 - R. Yantosca - Add cosmetic changes in ProTeX headers

08 Jul 2014 - R. Yantosca - Now use F90 free-format indentation

29 Dec 2014 - C. Keller - Added MASK_THRESHOLD parameter. Added option to apply scale factors only over masked area.

08 Apr 2015 - C. Keller - Added option for fractional masks.

11 May 2015 - C. Keller - Added HCO_EvalFld interface.
```

## 1.2.1 HCO\_CalcEmis

Subroutine HCO\_CalcEmis calculates the 3D emission fields at current datetime for the specified species, categories, and extension number.

#### **INTERFACE:**

```
SUBROUTINE HCO_CalcEmis( am_I_Root, HcoState, UseConc, RC )
```

#### **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_State

USE HCO_ARR_MOD, ONLY : HCO_ArrAssert

USE HCO_DATACONT_MOD, ONLY : ListCont_NextCont

USE HCO_FILEDATA_MOD, ONLY : FileData_ArrIsDefined
```

#### INPUT PARAMETERS:

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

LOGICAL, INTENT(IN ) :: UseConc ! Use concentration fields?
```

## INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object
INTEGER, INTENT(INOUT) :: RC ! Return code
```

#### REVISION HISTORY:

```
25 Aug 2012 - C. Keller - Initial Version

06 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX header

03 Aug 2014 - C. Keller - Bug fix for adding data to diagnostics. Now explicitly check for new species OR category.

21 Aug 2014 - C. Keller - Added concentration.

14 Apr 2016 - C. Keller - Bug fix: avoid double-counting if multiple regional inventories have the same hierarchy.

19 Sep 2016 - R. Yantosca - Use .neqv. for LOGICAL comparisons

26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

## 1.2.2 HCO\_CheckDepv

Subroutine HCO\_CheckDepv is a simple routine to check the dry deposition frequency value. This is to avoid unrealistically high deposition frequencies that may occur if grid box concentrations are very low. The deposition frequency is limited to a value that will make sure that the drydep exponent (exp(-depfreq \* dt )) is still small enough to remove all species mass. The maximum limit of depfreq \* dt can be defined as a HEMCO option (MaxDepExp). Its default value is 20.0.

#### INTERFACE:

```
SUBROUTINE HCO_CheckDepv( am_I_Root, HcoState, Depv, RC )
```

#### **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_State
```

### INPUT PARAMETERS:

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

## INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object REAL(hp), INTENT(INOUT) :: Depv ! Deposition velocity
```

#### 

#### **REVISION HISTORY:**

```
11 Mar 2015 - C. Keller - Initial Version
```

#### 1.2.3 Get Current Emissions

Subroutine Get\_Current\_Emissions calculates the current emissions for the specified emission container. This subroutine is only called by HCO\_CalcEmis and for base emission containers, i.e. containers of type 1.

## **INTERFACE:**

```
SUBROUTINE Get_Current_Emissions( am_I_Root, HcoState, BaseDct, & nI, nJ, nL, OUTARR_3D, MASK, RC, UseLL)
```

#### USES:

```
USE HCO_State_Mod, ONLY : HCO_State
USE HCO_tldx_MOD, ONLY : tlDx_GetIndx
```

USE HCO\_FileData\_Mod, ONLY : FileData\_ArrIsDefined

#### INPUT PARAMETERS:

```
:: am_I_Root
                                                     ! Root CPU?
LOGICAL,
                INTENT(IN )
INTEGER,
                 INTENT(IN)
                               :: nI
                                                      ! # of lons
                                                     ! # of lats
INTEGER,
                INTENT(IN)
                              :: nJ
                                                      ! # of levs
INTEGER,
                 INTENT(IN)
                              :: nL
```

## INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object
TYPE(DataCont), POINTER :: BaseDct ! base emission
! container
REAL(hp), INTENT(INOUT) :: OUTARR_3D(nI,nJ,nL) ! output array
REAL(hp), INTENT(INOUT) :: MASK (nI,nJ,nL) ! mask array
INTEGER, INTENT(INOUT) :: RC
```

### **OUTPUT PARAMETERS:**

```
INTEGER, INTENT( OUT), OPTIONAL :: UseLL
```

## **REMARKS:**

This routine uses multiple loops over all grid boxes (base emissions and scale factors use separate loops). In an OMP environment, this approach seems to be faster than using only one single loop (but repeated calls to point to containers, etc.). The alternative approach is used in routine Get\\_Current\\_Emissions\\_B at the end of this module and may be employed on request.

## **REVISION HISTORY:**

```
25 Aug 2012 - C. Keller - Initial Version

09 Nov 2012 - C. Keller - MASK update. Masks are now treated separately so that multiple masks can be added.

06 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers

07 Sep 2014 - C. Keller - Mask update. Now set mask to zero as soon as on of the applied masks is zero.

03 Dec 2014 - C. Keller - Now calculate time slice index on-the-fly.

29 Dec 2014 - C. Keller - Added scale factor masks.

02 Mar 2015 - C. Keller - Now check for missing values. Missing values are excluded from emission calculation.

26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

## 1.2.4 Get\_Current\_Emissions\_b (NOT USED!!)

Subroutine Get\_Current\_Emissions\_B calculates the current emissions for the specified emission field and passes the result to OUTARR\_3D.

This subroutine is only called by HCO\_CalcEmis and for fields with a valid species ID, i.e. for base emission fields.

!!! WARNING: this routine is not actively developed any more and may lag !!! behind Get\_Current\_Emissions

#### INTERFACE:

```
SUBROUTINE Get_Current_Emissions_B( am_I_Root, HcoState, BaseDct, & nI, nJ, nL, OUTARR_3D, MASK, RC)
```

#### **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_State
USE HCO_TIDX_MOD, ONLY : tIDx_GetIndx
```

USE HCO\_FILEDATA\_MOD, ONLY : FileData\_ArrIsDefined

#### INPUT PARAMETERS:

| LOGICAL, | <pre>INTENT(IN)</pre> | :: am_I_Root | ! Root CPU? |
|----------|-----------------------|--------------|-------------|
| INTEGER, | <pre>INTENT(IN)</pre> | :: nI        | ! # of lons |
| INTEGER, | <pre>INTENT(IN)</pre> | :: nJ        | ! # of lats |
| INTEGER, | <pre>INTENT(IN)</pre> | :: nL        | ! # of levs |

## INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object
TYPE(DataCont), POINTER :: BaseDct ! base emission
! container

REAL(hp), INTENT(INOUT) :: OUTARR_3D(nI,nJ,nL) ! output array

REAL(hp), INTENT(INOUT) :: MASK (nI,nJ,nL) ! mask array

INTEGER, INTENT(INOUT) :: RC
```

## **REVISION HISTORY:**

```
25 Aug 2012 - C. Keller - Initial Version

09 Nov 2012 - C. Keller - MASK update. Masks are now treated separately so that multiple masks can be added.

06 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX header

07 Sep 2014 - C. Keller - Mask update. Now set mask to zero as soon as on of the applied masks is zero.

02 Mar 2015 - C. Keller - Now check for missing values

26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

#### 1.2.5 HCO\_EvalFld\_3D

Subroutine HCO\_EvalFld\_3D returns the 3D data field belonging to the emissions list data container with field name 'cName'. The returned data field is the completely evaluated field, e.g. the base field multiplied by all scale factors and with all masking being applied (as specified in the HEMCO configuration file). This distinguished this routine from HCO\_GetPtr in hco\_emislist\_mod.F90, which returns a reference to the unevaluated data field.

## **INTERFACE:**

```
SUBROUTINE HCO_EvalFld_3D( am_I_Root, HcoState, cName, Arr3D, RC, FOUND )
USES:
```

```
USE HCO_STATE_MOD, ONLY : HCO_State
USE HCO_DATACONT_MOD, ONLY : ListCont_Find
```

## **INPUT PARAMETERS:**

```
LOGICAL, INTENT(IN ) :: am_I_Root ! Root CPU? CHARACTER(LEN=*), INTENT(IN ) :: cName
```

#### INPUT/OUTPUT PARAMETERS:

#### **OUTPUT PARAMETERS:**

```
LOGICAL, INTENT( OUT), OPTIONAL :: FOUND
```

```
11 May 2015 - C. Keller - Initial Version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

## 1.2.6 HCO\_EvalFld\_2D

Subroutine HCO\_EvalFld\_2D returns the 2D data field belonging to the emissions list data container with field name 'cName'. The returned data field is the completely evaluated field, e.g. the base field multiplied by all scale factors and with all masking being applied (as specified in the HEMCO configuration file). This distinguished this routine from HCO\_GetPtr in hco\_emislist\_mod.F90, which returns a reference to the unevaluated data field.

### **INTERFACE:**

```
SUBROUTINE HCO_EvalFld_2D( am_I_Root, HcoState, cName, Arr2D, RC, FOUND )
```

### **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_State
USE HCO_DATACONT_MOD, ONLY : ListCont_Find
```

#### INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root ! Root CPU? CHARACTER(LEN=*), INTENT(IN ) :: cName
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object REAL(hp), INTENT(INOUT) :: Arr2D(:,:) ! 2D array INTEGER, INTENT(INOUT) :: RC ! Return code
```

## **OUTPUT PARAMETERS:**

```
LOGICAL, INTENT( OUT), OPTIONAL :: FOUND
```

### REVISION HISTORY:

```
11 May 2015 - C. Keller - Initial Version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
01 Nov 2016 - C. Keller - Added error trap for UseLL
```

## 1.2.7 GetMaskVal

Subroutine GetMaskVal is a helper routine to get the mask value at a given location.

#### **INTERFACE:**

```
SUBROUTINE GetMaskVal (am_I_Root, Dct, I, J, MaskVal, Fractions, RC)

USES:
```

### **INPUT PARAMETERS:**

```
! Root CPU?
LOGICAL,
                  INTENT(IN
                              ) :: am_I_Root
INTEGER,
                 INTENT(IN
                              ) :: I
                                                         ! # of lons
                                                        ! # of lats
INTEGER,
                 INTENT(IN
                              ) :: J
                 INTENT(IN
                              ) :: Fractions
                                                        ! Use fractions?
LOGICAL,
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(DataCont), POINTER :: Dct ! Mask container
```

REAL(sp), INTENT(INOUT) :: MaskVal INTEGER, INTENT(INOUT) :: RC

#### REVISION HISTORY:

```
09 Apr 2015 - C. Keller - Initial Version
```

#### 1.2.8 HCO MaskFld

Subroutine HCO\_MaskFld is a helper routine to get the mask field with the given name. The returned mask field is fully evaluated, e.g. the data operation flag associated with this mask field is already taken into account. For instance, if the data operator of a mask field is set to 3, the returned array contains already the mirrored mask values.

#### **INTERFACE:**

```
SUBROUTINE HCO_MaskFld (am_I_Root, HcoState, MaskName, Mask, RC, FOUND)
```

### **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_State
USE HCO_DATACONT_MOD, ONLY : ListCont_Find
```

## INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root ! Root CPU? TYPE(HCO_STATE), POINTER :: HcoState CHARACTER(LEN=*), INTENT(IN ) :: MaskName
```

# INPUT/OUTPUT PARAMETERS:

```
REAL(sp), INTENT(INOUT) :: Mask(:,:)
INTEGER, INTENT(INOUT) :: RC
```

### **OUTPUT PARAMETERS:**

```
LOGICAL, INTENT( OUT), OPTIONAL :: FOUND
```

```
11 Jun 2015 - C. Keller - Initial Version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

### 1.2.9 GetVertIndx

Subroutine GetVertIndx is a helper routine to get the vertical index range of the given data field.

#### **INTERFACE:**

```
SUBROUTINE GetVertIndx ( am_I_Root, HcoState, Dct, I, J, LowLL, UppLL, RC )
```

## **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_State
```

#### INPUT PARAMETERS:

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

TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object

INTEGER, INTENT(IN ) :: I ! lon index

INTEGER, INTENT(IN ) :: J ! lat index
```

## INPUT/OUTPUT PARAMETERS:

```
TYPE(DataCont), POINTER :: Dct ! Mask container INTEGER, INTENT(INOUT) :: LowLL ! lower level index INTEGER, INTENT(INOUT) :: UppLL ! upper level index INTEGER, INTENT(INOUT) :: RC
```

## REVISION HISTORY:

```
06 May 2016 - C. Keller - Initial Version
```

## 1.2.10 GetIdx

Subroutine GetIdx is a helper routine to return the vertical level index for a given altitude. The altitude can be provided in level coordinates, in units of meters or as the 'PBL mixing height'.

## INTERFACE:

```
SUBROUTINE GetIdx( am_I_Root, HcoState, I, J, alt, altu, lidx, RC )
```

#### **USES:**

```
USE HCO_TYPES_MOD
USE HCO_STATE_MOD, ONLY : HCO_STATE
```

#### INPUT PARAMETERS:

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

TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object

INTEGER, INTENT(IN ) :: I, J ! horizontal index

INTEGER, INTENT(IN ) :: altu ! altitude unit
```

## **OUTPUT PARAMETERS:**

INTEGER, INTENT( OUT) :: lidx ! level index

# INPUT/OUTPUT PARAMETERS:

REAL(hp), INTENT(INOUT) :: alt ! altitude

INTEGER, INTENT(INOUT) :: RC

#### REVISION HISTORY:

09 May 2016 - C. Keller - Initial version

### 1.2.11 GetDilFact

Subroutine GetDilFact returns the vertical dilution factor, that is the factor that is to be applied to distribute emissions into multiple vertical levels. If grid box height information are available, these are used to compute the distribution factor. Otherwise, equal weight is given to all vertical levels.

!TODO: Dilution factors are currently only weighted by grid box heights (if these information are available) but any pressure information are ignored.

#### **INTERFACE:**

### **USES:**

USE HCO\_STATE\_MOD, ONLY : HCO\_State

## INPUT PARAMETERS:

```
LOGICAL,
         INTENT(IN
                      )
                                   :: am_I_Root
                                                  ! Root CPU?
TYPE(HCO_State), POINTER
                                   :: HcoState
                                                  ! HEMCO state object
INTEGER, INTENT(IN
                                   :: I
                                                  ! lon index
                      )
INTEGER, INTENT(IN
                      )
                                   :: J
                                                  ! lat index
                                   :: L
                                                  ! lev index
INTEGER, INTENT(IN
                      )
                                                  ! lower level index
INTEGER,
          INTENT(IN
                      )
                                   :: LowLL
                                   :: UppLL
                                                  ! upper level index
INTEGER, INTENT(IN
                      )
```

## **OUTPUT PARAMETERS:**

REAL(hp), INTENT( OUT) :: DilFact ! Dilution factor

# INPUT/OUTPUT PARAMETERS:

```
REAL(hp), INTENT(INOUT) :: EmisL1
INTEGER, INTENT(INOUT) :: EmisL1Unit
REAL(hp), INTENT(INOUT) :: EmisL2
INTEGER, INTENT(INOUT) :: EmisL2Unit
INTEGER, INTENT(INOUT) :: RC
```

### **REVISION HISTORY:**

```
06 May 2016 - C. Keller - Initial Version
```

## 1.2.12 HCO\_CharSplit\_R8

Subroutine HCO\_CharSplit\_R8 splits the passed character string into N real8 values, using character SEP as separator. Wildcard values (WC) are set to -999.

### **INTERFACE:**

```
SUBROUTINE HCO_CharSplit_R8( CharStr, SEP, WC, Reals, N, RC)
```

#### **USES:**

```
USE CharPak_Mod, ONLY : StrSplit
```

### INPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(IN ) :: CharStr ! Character string CHARACTER(LEN=1), INTENT(IN ) :: SEP ! Separator CHARACTER(LEN=1), INTENT(IN ) :: WC ! Wildcard character
```

#### **OUTPUT PARAMETERS:**

```
REAL(dp), INTENT( OUT) :: Reals(:) ! Output values INTEGER, INTENT( OUT) :: N ! # of valid values
```

# INPUT/OUTPUT PARAMETERS:

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

## **REVISION HISTORY:**

```
18 Sep 2013 - C. Keller - Initial version (update)
```

## 1.2.13 HCO\_CharSplit\_R4

Subroutine HCO\_CharSplit\_R4 splits the passed character string into N real4 values, using character SEP as separator. Wildcard values (WC) are set to -999.

## **INTERFACE:**

```
SUBROUTINE HCO_CharSplit_R4( CharStr, SEP, WC, Reals, N, RC )
```

#### **USES:**

```
USE CharPak_Mod, ONLY : StrSplit
```

#### INPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(IN ) :: CharStr ! Character string CHARACTER(LEN=1), INTENT(IN ) :: SEP ! Separator CHARACTER(LEN=1), INTENT(IN ) :: WC ! Wildcard character
```

## **OUTPUT PARAMETERS:**

```
REAL(sp), INTENT( OUT) :: Reals(:) ! Output values INTEGER, INTENT( OUT) :: N ! # of valid values
```

## INPUT/OUTPUT PARAMETERS:

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

## **REVISION HISTORY:**

```
18 Sep 2013 - C. Keller - Initial version (update)
```

## 1.2.14 HCO\_CharSplit\_Int

Subroutine HCO\_CharSplit\_Int splits the passed character string into N integers, using character SEP as separator. Wildcard values (WC) are set to -999.

#### **INTERFACE:**

```
SUBROUTINE HCO_CharSplit_INT( CharStr, SEP, WC, Ints, N, RC )
```

### **USES:**

```
USE CharPak_Mod, ONLY : StrSplit
```

### INPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(IN ) :: CharStr ! Character string CHARACTER(LEN=1), INTENT(IN ) :: SEP ! Separator CHARACTER(LEN=1), INTENT(IN ) :: WC ! Wildcard character
```

## **OUTPUT PARAMETERS:**

```
INTEGER, INTENT( OUT) :: Ints(:) ! Output values
INTEGER, INTENT( OUT) :: N ! # of valid values
```

# INPUT/OUTPUT PARAMETERS:

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

```
18 Sep 2013 - C. Keller - Initial version (update)
```

### 1.2.15 HCO\_CharMatch

Subroutine HCO\_CharMatch returns the index of each vector element of vec1 in vec2. nn-match denotes the number of vec1 elements which have a matching counterpart in vec2. For example, if vec1 is (/ 'NO', 'CO', 'ALK4', 'HBr' /), and vec2 is (/ 'CO', 'NO', 'CH3Br' /), then matchidx becomes (/ 2, 1, -1, -1 /) and nnmatch is 2.

#### **INTERFACE:**

```
SUBROUTINE HCO_CharMatch( vec1, n1, vec2, n2, matchidx, nnmatch)
```

#### INPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(IN ) :: vec1(n1) ! char. vector 1
INTEGER, INTENT(IN ) :: n1 ! len of vec1
CHARACTER(LEN=*), INTENT(IN ) :: vec2(n2) ! char. vector 2
INTEGER, INTENT(IN ) :: n2 ! len of vec2
```

### **OUTPUT PARAMETERS:**

```
INTEGER, INTENT( OUT) :: matchidx(n1) ! index of vec2 in vec1
INTEGER, INTENT( OUT) :: nnmatch ! # of matches
```

### **REVISION HISTORY:**

```
18 Sep 2013 - C. Keller - Initial version (update)
```

## 1.2.16 HCO\_CharParse

Routine HCO\_CharParse parses the provided character string by searching for tokens such as \$ROOT, \$YYYY, etc., within the string and replacing those values by the intendend characters.

The following list shows the 'default' HEMCO tokens. These are available in any HEMCO simulation. Tokens \$ROOT, \$MET, and \$RES are internally stored as a HEMCO option in module hco\_extlist\_mod.F90 (see subroutine HCO\_SetDefaultToken).

- \$ROOT: will be replaced by the root path specified in the settings section of the configuration file.
- \$MET: will be replaced by the met-field token.
- \$RES: will be replaced by the resolution token.
- \$YYYY: will be replaced by the (4-digit) year according to the source time settings set in the configuration file.
- \$MM: will be replaced by the (2-digit) month according to the source time settings set in the configuration file.
- \$DD: will be replaced by the (2-digit) day according to the source time settings set in the configuration file.

- \$HH: will be replaced by the (2-digit) hour according to the source time settings set in the configuration file.
- \$MN: will be replaced by the (2-digit) minute.

## **INTERFACE:**

```
SUBROUTINE HCO_CharParse ( HcoConfig, str, yyyy, mm, dd, hh, mn, RC )
```

## **USES:**

```
USE HCO_ExtList_Mod, ONLY : HCO_GetOpt, HCO_Root
USE HCO_Types_Mod, ONLY : ConfigObj
```

#### INPUT PARAMETERS:

```
TYPE(ConfigObj), POINTER
                               :: HcoConfig
INTEGER,
                INTENT(IN
                                       ! replace $YYYY with this value
                               :: уууу
INTEGER,
                INTENT(IN )
                              :: mm
                                        ! replace $MM with this value
                                       ! replace $DD with this value
                            ) :: dd
INTEGER,
                INTENT(IN
                                       ! replace $HH with this value
INTEGER,
                INTENT(IN
                            ) :: hh
                                       ! replace $MN with this value
INTEGER,
                INTENT(IN ) :: mn
```

### **OUTPUT PARAMETERS:**

```
CHARACTER(LEN=*), INTENT( OUT) :: str ! string to be parsed
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC ! return code
```

### **REVISION HISTORY:**

```
01 Oct 2014 - C. Keller - Initial version
20 Sep 2015 - C. Keller - Tokens can now be any option setting set in the HEMCO configuration file.
```

## 1.2.17 HCO\_GetBase

Routine HCO\_GetBase returns the base location of the given file. This is the entire file path up to the last forward slash, e.g. for file '/home/dir/Config.rc', the base is '/home/dir/' **INTERFACE:** 

```
SUBROUTINE HCO_GetBase ( str, base, RC )
```

#### **USES:**

```
USE CharPak_Mod, ONLY : StrSplit
```

#### INPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(IN ) :: str ! string to be checked
```

### **OUTPUT PARAMETERS:**

```
CHARACTER(LEN=*), INTENT( OUT) :: base ! base
```

## INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC ! return code
```

#### REVISION HISTORY:

```
16 Mar 2015 - C. Keller - Initial version
```

#### 1.2.18 IsInWord

Function IsInWord checks if the word InString contains the sequence of SearchString.  ${\bf INTERFACE}$ :

```
FUNCTION IsInWord( InString, SearchString ) RESULT ( Cnt )
```

### INPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(IN ) :: InString
CHARACTER(LEN=*), INTENT(IN ) :: SearchString
```

## RETURN VALUE:

LOGICAL :: Cnt

#### REVISION HISTORY:

```
23 Oct 2012 - C. Keller - Initial Version
```

## 1.2.19 NextCharPos

Function NextCharPos returns the position of the next occurrence of character CHR in word WORD, starting from position START. Returns -1 if the word does not contain CHR at all (after position START).

## **INTERFACE:**

```
FUNCTION NextCharPos ( WORD, CHR, START ) RESULT ( POS )
```

## **USES:**

```
!INPUT ARGUMENTS:
```

```
CHARACTER(LEN=*), INTENT(IN) :: WORD
CHARACTER(LEN=1), INTENT(IN) :: CHR
INTEGER, OPTIONAL, INTENT(IN) :: START
!RETURN ARGUMENT:
```

INTEGER :: POS

```
09 Jul 2014 - C. Keller - Initial Version
```

### 1.2.20 GetNextLine

Subroutine GetNextLine returns the next line.

## **INTERFACE:**

```
SUBROUTINE GetNextLine( am_I_Root, LUN, LINE, EOF, RC )
```

#### **USES:**

#### INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root ! Are we on the root CPU?
INTEGER, INTENT(IN ) :: LUN ! Stream to read from
!OUTPUT PARAMETERS
CHARACTER(LEN=*), INTENT( OUT) :: LINE ! Next (valid) line in stream
!INPUT/OUTPUT PARAMETERS
LOGICAL, INTENT(INOUT) :: EOF ! End of file encountered?
```

LOGICAL, INTENT(INOUT) :: EOF ! End of file encountered? INTEGER, INTENT(INOUT) :: RC ! Success or failure?

#### REVISION HISTORY:

```
10 Apr 2015 - C. Keller - Initial Version
```

### 1.2.21 HCO\_ReadLine

Subroutine HCO\_Line reads a line from the provided stream.

### **INTERFACE:**

```
SUBROUTINE HCO_ReadLine( LUN, LINE, EOF, RC )
```

## INPUT PARAMETERS:

```
INTEGER, INTENT(IN ) :: LUN ! Stream LUN
```

### **OUTPUT PARAMETERS:**

```
CHARACTER(LEN=*), INTENT(INOUT) :: LINE ! Line LOGICAL, INTENT(INOUT) :: EOF ! End of file? INTEGER, INTENT(INOUT) :: RC ! Return code
```

```
18 Sep 2013 - C. Keller - Initial version (adapted from B. Yantosca's code)
15 Jul 2014 - R. Yantosca - Remove dependency on routine IOERROR
```

## 1.3 Fortran: Module Interface hco\_clock\_mod.F90

Module HCO\_Clock\_Mod contains routines and variables to handle the HEMCO time and calendar settings through the HEMCO clock object. The HEMCO clock carries information of the current UTC/local time as well as the UTC times from the previous time step. These values should be updated on every time step (-; HcoClock\_Set). It also contains separate variables for the current and previous emission datetime (year, month, day, hour, min, sec). This allows us to keep track of emission time steps even if the emission time steps are less frequent than the regular time step.

Subroutine HcoClock\_EmissionsDone indicates that emissions have been completely calculated for the current time step. Any calls to HcoClock\_Get will return IsEmisTime FALSE until the clock has been advanced to the next emission time step (via HcoClock\_Set).

The HEMCO clock object HcoClock is a private object and cannot be accessed directly from outside of this module. The HcoClock\_Get routine should be used instead. There are also some wrapper routines for frequently used checks, i.e. if this is a new year, month, etc.

Local times are calculated for 26 time zones, ranging from UTC-12 hours to UTC+13 hours. The time zone to be used at a given grid point is based on its geographical position. By default, the time zone is picked according to the longitude, with each time zone spanning 15 degrees. More detailed time zones can be provided through an external input file, specified in the HEMCO configuration file. The field name must be 'TIMEZONES', and the file must contain UTC offsets in hours. If such a file is provided, the time zones are determined based on these values. Minute offsets are ignored, e.g. UTC+9hr30min is treated as UTC+9hr. If the input field contains any invalid values (e.g. outside the range of UTC-12 - UTC+13 hours), the default algorithm is applied.

The HEMCO clock object also controls cases where the emission dates shall be held constant, e.g. for simulations where emission year 2000 shall be used irrespective of the simulation date. Fixed simulation dates can be set in the settings section of the HEMCO configuration file via settings 'Emission year', 'Emission month', 'Emission day', and 'Emission hour'. Only a subset of those settings can be provided, in which case all other time attributes will be taken from the simulation datetime.

### **INTERFACE:**

PRIVATE

MODULE HCO\_CLOCK\_MOD

## **USES:**

USE HCO\_Error\_Mod
USE Julday\_Mod
USE HCO\_TYPES\_MOD, ONLY : HcoClock
IMPLICIT NONE

### PUBLIC MEMBER FUNCTIONS:

! HEMCO Clock object:

```
PUBLIC :: HcoClock_Init
PUBLIC :: HcoClock_InitTzPtr
PUBLIC :: HcoClock_Set
PUBLIC :: HcoClock_Get
PUBLIC :: HcoClock_GetLocal
PUBLIC :: HcoClock_Cleanup
PUBLIC :: HcoClock_NewYear
PUBLIC :: HcoClock_NewMonth
PUBLIC :: HcoClock_NewDay
PUBLIC :: HcoClock_NewHour
PUBLIC :: HcoClock_First
PUBLIC :: HcoClock_Rewind
PUBLIC :: HcoClock_CalcDOY
PUBLIC :: HcoClock_Increase
PUBLIC :: HcoClock_EmissionsDone
PUBLIC :: HcoClock_SetLast
PUBLIC :: Get_LastDayOfMonth
```

## **REMARKS:**

The current local time implementation assumes a regular grid, i.e. local time does not change with latitude

## **REVISION HISTORY:**

```
29 Dec 2012 - C. Keller - Initialization

12 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers

12 Jun 2014 - R. Yantosca - Now use F90 freeform indentation

08 Oct 2014 - C. Keller - Added mid-month day calculation

03 Dec 2014 - C. Keller - Now use fixed number of time zones (24)

12 Jan 2015 - C. Keller - Added emission time variables.

02 Feb 2015 - C. Keller - Added option to get time zones from file

23 Feb 2015 - R. Yantosca - Added routine HcoClock_InitTzPtr

11 Jun 2015 - C. Keller - Added simulation times and option to fix emission year, month, day, and/or hour.
```

## 1.3.1 HcoClock\_Init

Subroutine HcoClock\_Init initializes the HEMCO clock.

### **INTERFACE:**

```
SUBROUTINE HcoClock_Init ( am_I_Root, HcoState, RC )
```

## **USES:**

```
USE HCO_ARR_MOD, ONLY : HCO_ArrInit
USE HCO_STATE_MOD, ONLY : HCO_State
```

#### INPUT PARAMETERS:

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

## INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state obj
INTEGER, INTENT(INOUT) :: RC ! Success or failure?
```

## REVISION HISTORY:

```
10 Sep 2013 - C. Keller - Initialization
12 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
12 Jun 2014 - R. Yantosca - Now use F90 freeform indentation
```

#### 1.3.2 HcoClock InitTzPtr

Subroutine HcoClock\_InitTzPtr initializes the TIMEZONES module variable. TIMEZONES points to the timezones data (i.e. offsets from UTC in hours) as read from disk. If the timezones data file is not being used, then the TIMEZONES pointer will be left unassociated.

### INTERFACE:

```
SUBROUTINE HcoClock_InitTzPtr( am_I_Root, HcoState, RC )
```

#### **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_State USE HCO_EMISLIST_MOD, ONLY : HCO_GetPtr
```

### INPUT PARAMETERS:

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

TYPE(HCO_State), POINTER :: HcoState ! HcoState object
```

# INPUT/OUTPUT PARAMETERS:

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

## **REMARKS:**

This routine has to be called in the HCO\_Run routine, immediately after the call to ReadList\_Read. The HEMCO configuration file has to be read first in order to determine if we are getting our timezone information from a file, or if we are computing it just based on longitude in the default manner.

```
23 Feb 2015 - R. Yantosca - Initial version
10 Mar 2015 - C. Keller - Packed message into am_I_Root statement
```

### 1.3.3 HcoClock\_Set

Subroutine HcoClock\_Set updates the HEMCO clock. These routine should be called at the beginning of every emission time step! If the current day of year (cDoy) is not provided, it is automatically calculated from the current date.

#### **INTERFACE:**

```
SUBROUTINE HcoClock_Set (am_I_Root, HcoState, cYr, cMt, cDy, cHr, & cMin, cSec, cDOY, IsEmisTime, RC
```

#### **USES:**

```
USE HCO_TYPES_MOD, ONLY : ConfigObj, Ext
USE HCO_STATE_MOD, ONLY : HCO_State
```

USE HCO\_EXTLIST\_MOD, ONLY : GetExtOpt, CoreNr

## INPUT PARAMETERS:

```
LOGICAL,
                INTENT(IN
                                        :: am_I_Root ! Root CPU?
                            )
INTEGER,
                INTENT(IN
                            )
                                         :: cYr
                                                      ! Current year
                                                      ! Current month
INTEGER,
                INTENT(IN
                            )
                                         :: cMt
INTEGER,
                INTENT(IN
                                                     ! Current day
                                         :: cDy
                                                      ! Current hour
INTEGER,
                INTENT(IN
                                        :: cHr
                                                     ! Current minute
INTEGER,
                INTENT(IN
                                         :: cMin
INTEGER,
                INTENT(IN
                                        :: cSec
                                                     ! Current second
INTEGER,
                INTENT(IN
                            ), OPTIONAL :: cDoy ! Current day of year
LOGICAL,
                INTENT(IN
                           ), OPTIONAL :: IsEmisTime! Is it time for emissions?
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HcoState object INTEGER, INTENT(INOUT) :: RC ! Success or failure?
```

#### REVISION HISTORY:

```
29 Dec 2012 - C. Keller - Initialization
12 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
12 Jun 2014 - R. Yantosca - Now use F90 freeform indentation
08 Jul 2014 - C. Keller - Now calculate DOY if not provided
12 Jan 2015 - C. Keller - Added IsEmisTime
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

## 1.3.4 HcoClock\_Get

Subroutine HcoClock\_Get returns the selected UTC variables from the HEMCO clock object.

#### **INTERFACE:**

```
SUBROUTINE HcoClock_Get (am_I_Root, Clock,
                                    cMM, cDD,
                           cYYYY,
                                               cH,
                                                          &
                                    cS, cDOY, cWEEKDAY, &
                           cM,
                          pYYYY,
                                    pMM, pDD, pH,
                                    pS, pDOY, pWEEKDAY, &
                          рM,
                                    sMM, sDD,
                          syyyy,
                                               sH,
                           sM,
                                    sS,
                                                          &
                          LMD,
                                    nSteps,
                                               cMidMon,
                                    dbtwmm,
                                               IsEmisTime, &
                           dslmm,
                           IsLast, RC)
```

**USES:** 

#### INPUT PARAMETERS:

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

TYPE(HcoClock), POINTER :: Clock ! HEMCO clock obj
```

#### **OUTPUT PARAMETERS:**

```
INTEGER, INTENT(
                  OUT), OPTIONAL
                                      :: cYYYY
                                                     ! Current year
                  OUT), OPTIONAL
INTEGER, INTENT(
                                      :: cMM
                                                     ! Current month
INTEGER, INTENT(
                  OUT), OPTIONAL
                                      :: cDD
                                                     ! Current day
INTEGER, INTENT(
                  OUT), OPTIONAL
                                      :: cH
                                                     ! Current hour
INTEGER, INTENT(
                  OUT), OPTIONAL
                                      :: cM
                                                     ! Current minute
INTEGER, INTENT(
                  OUT), OPTIONAL
                                                     ! Current second
                                      :: cS
INTEGER, INTENT(
                  OUT), OPTIONAL
                                      :: cDOY
                                                     ! Current day of year
INTEGER, INTENT(
                  OUT), OPTIONAL
                                      :: cWEEKDAY
                                                     ! Current weekday
INTEGER, INTENT(
                  OUT), OPTIONAL
                                                     ! Previous year
                                      :: pYYYY
INTEGER, INTENT(
                  OUT), OPTIONAL
                                      :: pMM
                                                     ! Previous month
INTEGER, INTENT(
                  OUT), OPTIONAL
                                      :: pDD
                                                     ! Previous day
INTEGER, INTENT(
                  OUT), OPTIONAL
                                      :: pH
                                                     ! Previous hour
INTEGER, INTENT(
                  OUT), OPTIONAL
                                      :: pM
                                                     ! Previous minute
INTEGER, INTENT(
                  OUT), OPTIONAL
                                      :: pS
                                                     ! Previous second
INTEGER, INTENT(
                  OUT), OPTIONAL
                                      :: sYYYY
                                                     ! Simulation year
                  OUT), OPTIONAL
INTEGER, INTENT(
                                      :: sMM
                                                     ! Simulation month
INTEGER, INTENT(
                  OUT), OPTIONAL
                                      :: sDD
                                                     ! Simulation day
INTEGER, INTENT(
                  OUT), OPTIONAL
                                                     ! Simulation hour
                                      :: sH
INTEGER, INTENT(
                  OUT), OPTIONAL
                                      :: sM
                                                     ! Simulation minute
INTEGER, INTENT(
                  OUT), OPTIONAL
                                      :: sS
                                                     ! Simulation second
INTEGER, INTENT(
                  OUT), OPTIONAL
                                                     ! Previous day of year
                                      :: pDOY
INTEGER, INTENT(
                  OUT), OPTIONAL
                                      :: pWEEKDAY
                                                     ! Previous weekday
INTEGER, INTENT(
                  OUT), OPTIONAL
                                      :: LMD
                                                     ! Last day of month
                  OUT), OPTIONAL
INTEGER, INTENT(
                                                     ! # of passed steps
                                      :: nSteps
INTEGER, INTENT(
                  OUT), OPTIONAL
                                      :: cMidMon
                                                     ! Mid-month day of curr. month
INTEGER, INTENT(
                  OUT), OPTIONAL
                                                     ! days since last mid-month
                                      :: dslmm
INTEGER, INTENT(
                  OUT), OPTIONAL
                                      :: dbtwmm
                                                     ! days between mid-month
LOGICAL, INTENT(
                  OUT), OPTIONAL
                                      :: IsEmisTime ! days between mid-month
LOGICAL, INTENT(
                  OUT), OPTIONAL
                                      :: IsLast
                                                     ! last time step?
```

## INPUT/OUTPUT PARAMETERS:

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

## **REVISION HISTORY:**

```
29 Dec 2012 - C. Keller - Initialization
12 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
12 Jun 2014 - R. Yantosca - Now use F90 freeform indentation
08 Oct 2014 - C. Keller - Added mid-month day arguments
12 Jan 2015 - C. Keller - Added IsEmisTime
```

### 1.3.5 HcoClock\_GetLocal

Subroutine HcoClock\_GetLocal returns the selected local time variables from the HEMCO clock object for the given longitude and latitude. At the moment, the time zone is selected purely on the given longitude and the passed latitude is not evaluated.

### **INTERFACE:**

```
SUBROUTINE HcoClock_GetLocal ( HcoState, I, J, cYYYY, cMM, & cDD, cH, CWEEKDAY, RC, verb )
```

## **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_State
```

### INPUT PARAMETERS:

### **OUTPUT PARAMETERS:**

```
INTEGER, INTENT( OUT), OPTIONAL :: cYYYY ! Current year INTEGER, INTENT( OUT), OPTIONAL :: cMM ! Current month INTEGER, INTENT( OUT), OPTIONAL :: cDD ! Current day REAL(hp), INTENT( OUT), OPTIONAL :: cH ! Current hour INTEGER, INTENT( OUT), OPTIONAL :: cWEEKDAY ! Current weekday INTEGER, INTENT(IN ), OPTIONAL :: verb ! verbose
```

## INPUT/OUTPUT PARAMETERS:

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

### **REMARKS:**

Module variable TIMEZONES points to the timezone data (i.e. offsets in hours from UTC) as read from disk. The data file containing UTC offsets is specified in the "NON-EMISSIONS DATA" section of the HEMCO configuration file, under the container name "TIMEZONES".

The TIMEZONES module variable is initialized by calling HcoClock\_InitTzPtr. in the HEMCO run method HCO\_Run (in module hco\_driver\_mod.F90). The call to HcoClock\_InitTzPtr immediately follows the call to ReadList\_Read, and is only done on the very first emissions timestep. The reason we have to initialize the TIMEZONES module variable in the run method (instead of in the init method) is because the HEMCO configuration file has to be read before the timezones data can be loaded into a HEMCO data container. If we are not reading timezone data from a file, then the TIMEZONES module variable will remain unassociated.

This fix was necessary in order to avoid segmentation faults when running with OpenMP parallelization turned on.

-- Bob Yantosca (23 Feb 2015)

### REVISION HISTORY:

```
29 Dec 2012 - C. Keller - Initialization
12 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
12 Jun 2014 - R. Yantosca - Now use F90 freeform indentation
23 Feb 2015 - R. Yantosca - Remove call to Hco_GetPtr: this was causing errors on runs with OpenMP parallelization
```

## 1.3.6 HcoClock\_First

Function HcoClock\_First returns TRUE on the first HEMCO time step, FALSE otherwise.

#### **INTERFACE:**

## RETURN VALUE:

LOGICAL :: First

# **REVISION HISTORY:**

```
29 Dec 2012 - C. Keller - Initialization
12 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
12 Jun 2014 - R. Yantosca - Now use F90 freeform indentation
06 Apr 2015 - C. Keller - Now use nEmisSteps and nSteps instead of previous years.
```

## 1.3.7 HcoClock\_Rewind

Function HcoClock\_Rewind returns TRUE if the last archived HEMCO time step is not in the past.

#### **INTERFACE:**

```
FUNCTION HcoClock_Rewind( Clock, EmisTime ) RESULT ( Rwnd )
!INPUT ARGUMENTS:
   TYPE(HcoClock), POINTER :: Clock
   LOGICAL, INTENT(IN) :: EmisTime
```

## RETURN VALUE:

LOGICAL :: Rwnd

## REVISION HISTORY:

08 May 2015 - C. Keller - Initial version

### 1.3.8 HcoClock\_NewYear

Function HcoClock\_NewYear returns TRUE if this is a new year (compared to the previous emission time step), FALSE otherwise.

### **INTERFACE:**

#### RETURN VALUE:

LOGICAL :: NewYear

## **REVISION HISTORY:**

```
29 Dec 2012 - C. Keller - Initialization
12 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
12 Jun 2014 - R. Yantosca - Now use F90 freeform indentation
```

#### 1.3.9 HcoClock\_NewMonth

Function HcoClock\_NewMonth returns TRUE if this is a new month (compared to the previous emission time step), FALSE otherwise.

#### **INTERFACE:**

```
FUNCTION HcoClock_NewMonth( Clock, EmisTime ) RESULT ( NewMonth )
!INPUT ARGUMENTS:
   TYPE(HcoClock), POINTER :: Clock
   LOGICAL,   INTENT(IN) :: EmisTime
```

#### RETURN VALUE:

LOGICAL :: NewMonth

## **REVISION HISTORY:**

```
29 Dec 2012 - C. Keller - Initialization
12 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
12 Jun 2014 - R. Yantosca - Now use F90 freeform indentation
```

## 1.3.10 HcoClock\_NewDay

Function HcoClock\_NewDay returns TRUE if this is a new day (compared to the previous emission time step), FALSE otherwise.

#### **INTERFACE:**

## RETURN VALUE:

```
LOGICAL :: NewDay
```

## **REVISION HISTORY:**

```
29 Dec 2012 - C. Keller - Initialization
12 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
12 Jun 2014 - R. Yantosca - Now use F90 freeform indentation
```

## 1.3.11 HcoClock\_NewHour

Function HcoClock\_NewHour returns TRUE if this is a new hour (compared to the previous emission time step), FALSE otherwise.

## **INTERFACE:**

```
FUNCTION HcoClock_NewHour( Clock, EmisTime ) RESULT ( NewHour )
!INPUT ARGUMENTS:
   TYPE(HcoClock), POINTER :: Clock
   LOGICAL, INTENT(IN) :: EmisTime
```

## RETURN VALUE:

```
LOGICAL :: NewHour
```

```
29 Dec 2012 - C. Keller - Initialization
12 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
12 Jun 2014 - R. Yantosca - Now use F90 freeform indentation
```

## 1.3.12 HcoClock\_Cleanup

Subroutine HcoClock\_Cleanup removes the given HcoHcoClock type.

### **INTERFACE:**

```
SUBROUTINE HcoClock_Cleanup ( Clock )
```

#### **USES:**

```
USE HCO_ARR_MOD, ONLY : HCO_ArrCleanup !INPUT ARGUMENTS:
    TYPE(HcoClock), POINTER :: Clock
```

### **REVISION HISTORY:**

```
29 Dec 2012 - C. Keller - Initialization
12 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
12 Jun 2014 - R. Yantosca - Now use F90 freeform indentation
```

## 1.3.13 HCO\_GetWeekday

Function HCO\_GetWeekday returns the weekday for the given date (year, month, day). 0 = Sunday, 1 = Monday, ..., 6 = Saturday.

## **INTERFACE:**

```
FUNCTION HCO_GetWeekday( year, month, day, gmt ) RESULT ( weekday )
```

## **INPUT PARAMETERS:**

```
INTEGER, INTENT(IN) :: year
INTEGER, INTENT(IN) :: month
INTEGER, INTENT(IN) :: day
REAL(sp), INTENT(IN) :: gmt
```

## RETURN VALUE:

```
INTEGER :: weekday
! NOTES: This function is largely based on the GEOS-Chem functions
in time_mod.F.
```

```
18 Dec 2013 - C. Keller - Initialization
12 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
12 Jun 2014 - R. Yantosca - Now use F90 freeform indentation
```

## 1.3.14 get\_lastdayofmonth

Function GET\_LASTDAYOFMONTH returns the last day of MONTH.

### **INTERFACE:**

```
FUNCTION Get_LastDayOfMonth( Month, Year ) RESULT ( LastDay )
```

### INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: Month
INTEGER, INTENT(IN) :: Year
```

## RETURN VALUE:

```
INTEGER :: LastDay
```

#### REVISION HISTORY:

```
13 Jan 2014 - C. Keller - Initial version
```

- 12 Jun 2014 R. Yantosca Cosmetic changes in ProTeX headers
- 12 Jun 2014 R. Yantosca Now use F90 freeform indentation

### 1.3.15 Set\_LocalTime

Subroutine Set\_LocalTime sets the local time vectors in the HEMCO clock object. Local time is calculated for each of the 24 defined time zones.

#### **INTERFACE:**

```
SUBROUTINE Set_LocalTime (am_I_Root, HcoState, Clock, UTC, RC)
```

## **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_State
```

### INPUT PARAMETERS:

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

TYPE(HCO\_STATE), POINTER :: HcoState

## INPUT/OUTPUT PARAMETERS:

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

```
13 Jan 2014 - C. Keller - Initial version
```

- 12 Jun 2014 R. Yantosca Cosmetic changes in ProTeX headers
- 12 Jun 2014 R. Yantosca Now use F90 freeform indentation
- 03 Dec 2014 C. Keller Now use fixed number of time zones (24)

## 1.3.16 HcoClock\_CalcDOY

FUNCTION HcoClock\_CalcDOY calculates the day of year for the given year, month, and day.

#### **INTERFACE:**

```
FUNCTION HcoClock_CalcDOY( YYYY, MM, DD ) RESULT ( DOY )
!INPUT ARGUMENTS:
   INTEGER, INTENT(IN) :: YYYYY ! Year
   INTEGER, INTENT(IN) :: MM ! Month
   INTEGER, INTENT(IN) :: DD ! Day
```

### **RETURN VALUE:**

```
INTEGER :: DOY ! Day of year
```

## **REVISION HISTORY:**

```
08 Jul 2014 - C. Keller - Initial version
```

## 1.3.17 HcoClock\_Increase

Subroutine HcoClock\_Increase increases the HEMCO clock by the specified time.

## INTERFACE:

```
{\tt SUBROUTINE\ HcoClock\_Increase\ (\ am\_I\_Root,\ HcoState,\ TimeStep,\ EmisTime,\ RC\ )}
```

#### **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_State
```

## INPUT PARAMETERS:

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

TYPE(HCO_State), POINTER :: HcoState ! Hemco state

REAL(sp), INTENT(IN ) :: TimeStep ! Time step increase [s]

LOGICAL, INTENT(IN ) :: EmisTime ! Is new time step emission time?
```

## INPUT/OUTPUT PARAMETERS:

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

```
29 Jul 2014 - C. Keller - Initial version
08 Sep 2014 - C. Keller - Bug fix: now calculate UTC as fraction of day.
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

## 1.3.18 HcoClock\_EmissionsDone

Subroutine HcoClock\_EmissionsDone marks the current (emission) time step as having emissions completed. This is useful if the HEMCO core routines are called multiple times on the same time step, e.g. if there are two run phases.

### **INTERFACE:**

```
SUBROUTINE HcoClock_EmissionsDone(am_I_Root, Clock, RC)
```

### **INPUT PARAMETERS:**

```
LOGICAL, INTENT(IN ) :: am_I_Root ! Root CPU
TYPE(HcoClock), POINTER :: Clock ! HEMCO clock obj
```

# INPUT/OUTPUT PARAMETERS:

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

#### **REVISION HISTORY:**

```
13 Jan 2015 - C. Keller - Initial version
```

## 1.3.19 HcoClock\_SetLast

Subroutine HcoClock\_SetLast sets the IsLast flag.

#### **INTERFACE:**

```
SUBROUTINE HcoClock_SetLast( am_I_Root, Clock, IsLast, RC )
```

## INPUT PARAMETERS:

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

TYPE(HcoClock), POINTER :: Clock ! HEMCO clock obj

LOGICAL, INTENT(IN ) :: IsLast ! Is last time step?
```

## INPUT/OUTPUT PARAMETERS:

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

## **REVISION HISTORY:**

```
01 Nov 2016 - C. Keller - Initial version
```

## 1.4 Fortran: Module Interface hco\_config\_mod.F90

Module HCO\_Config\_Mod contains routines related to the HEMCO configuration file. It reads the content of the configuration file, checks which entires therein are actually used for this simulation run, and stores these information. This occurs in two calls: Config\_ReadFile and SetReadList. Config\_ReadFile writes the entire content of the configuration file into

buffer except for the input data associated with a disabled extension. SetReadList does many more logical checks and adds all data used by HEMCO to ReadList. Scale factors not used by any of the base emissions and base emission fields (e.g. scale factors that won't be used ) are removed in this step.

All data fields are saved in individual data containers, which are organized in the ConfigList. Hence, ConfigList is a collection of all HEMCO data containers, with every container representing an entry of the configuration file. Each data container has its unique container ID for identification. All HEMCO lists (ConfigList, ReadList, EmisList) access the same containers.

The configuration file provides all source file information of the emission fields and scale factors to be used. It must be read at the beginning of a simulation run.

As of HEMCO v2.0, the ConfigList linked list sits within the HEMCO configuration object (HcoConfig). HcoConfig must be passed to all routines. This allows the parallel usage of multiple invocations of HEMCO that use different input data. HcoConfig is initialized upon reading the HEMCO configuration file (within subroutine Config\_ReadFile).

#### **INTERFACE:**

```
MODULE HCO_Config_Mod
```

## **USES:**

```
USE HCO_ERROR_MOD

USE HCO_DIAGN_MOD

USE HCO_CHARTOOLS_MOD

USE HCO_TYPES_MOD

USE HCO_STATE_MOD, ONLY : HCO_State

IMPLICIT NONE

PRIVATE
```

## PUBLIC MEMBER FUNCTIONS:

PUBLIC :: SetReadList

PUBLIC :: Config\_ReadFile

PUBLIC :: Config\_GetnSpecies

PUBLIC :: Config\_GetSpecNames

!PRIVATE:

PRIVATE :: ReadSettings

PRIVATE :: ExtSwitch2Buffer

PRIVATE :: ConfigList\_AddCont

PRIVATE :: Config\_ReadCont
PRIVATE :: RegisterPrepare
PRIVATE :: Get\_targetID
PRIVATE :: Calc\_Coverage
PRIVATE :: Register\_Base
PRIVATE :: Register\_Scal

```
PRIVATE :: ReadAndSplit_Line
PRIVATE :: Config_GetSpecAttr
```

PRIVATE :: BracketCheck
PRIVATE :: AddZeroScal
PRIVATE :: AddShadowFields
PRIVATE :: ConfigInit
PRIVATE :: ParseEmisL

### **REVISION HISTORY:**

```
18 Jun 2013 - C. Keller - Initialization
08 Jul 2014 - R. Yantosca - Now use F90 free-format indentation
08 Jul 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
15 Feb 2015 - C. Keller - Added BracketCheck, AddZeroScal, AddShadowFields
15 Feb 2016 - C. Keller - Update to v2.0: ConfigList now sits in HcoConfig
```

## 1.4.1 Config\_Readfile

Subroutine CONFIG\_READFILE reads the HEMCO configuration file, archives all HEMCO options and settings (including traceback/error setup), and creates a data container for every (used) emission field in the config. file. All containers become linked through the ConfigList linked list. Note that lists EmisList and ReadList (created lateron) will point to the same containers, but will order the containers in a manner that is most efficient for the respective purpose. Argument HcoConfig represents the HEMCO configuration object. It contains pointers to the HEMCO traceback and error information as well as a pointer to ConfigList. If undefined, HcoConfig becomes initialized as part of this routine.

#### **INTERFACE:**

```
SUBROUTINE Config_ReadFile( am_I_Root, HcoConfig, ConfigFile, Phase, RC, IsNest )
```

#### **USES:**

```
USE inquireMod, ONLY : findFreeLUN USE CharPak_Mod, ONLY : STRREPL
```

USE HCO\_EXTLIST\_MOD, ONLY: AddExt, CoreNr, ExtNrInUse

#### INPUT PARAMETERS:

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

TYPE(ConfigObj), POINTER :: HcoConfig ! HEMCO config obj

CHARACTER(LEN=*), INTENT(IN) :: ConfigFile ! Full file name
```

INTEGER, INTENT(IN) :: Phase ! 0: all

! 1: Settings and switches only

! 2: fields only

LOGICAL, INTENT(IN ), OPTIONAL :: IsNest ! Nested call?

## INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC ! Success?

## **REVISION HISTORY:**

```
    17 Sep 2012 - C. Keller - Initialization
    O3 Jan 2014 - C. Keller - Now use Config_ReadCont calls.
    30 Sep 2014 - R. Yantosca - Now declare LINE w/ 2047 characters. This lets us handle extra-long species lists
    13 Feb 2015 - C. Keller - Removed section extension data: these are now listed in section base emissions.
    11 Dec 2015 - C. Keller - Read settings and extension switches even for nested configuration files.
    15 Feb 2016 - C. Keller - Now pass HcoConfig argument.
```

## 1.4.2 SetReadList

Subroutine SetReadList writes data to the data reading lists (ReadList). This routine assumes that the configuration file has been read beforehand (via Config\_ReadFile).

## **INTERFACE:**

```
SUBROUTINE SetReadList( am_I_Root, HcoState, RC )
```

#### **USES:**

```
USE HCO_DATACONT_Mod, ONLY : cIDList_Create USE HCO_READLIST_Mod, ONLY : ReadList_Init
```

#### INPUT PARAMETERS:

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

TYPE(HCO_State), POINTER :: HcoState ! HEMCO state
```

## INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC ! Error stat
```

## REVISION HISTORY:

```
18 Jun 2013 - C. Keller: Initialization
17 Sep 2013 - C. Keller: Now get data from buffer
```

## 1.4.3 Config\_ReadCont

Subroutine CONFIG\_READCONT reads the given line into a list container. Depending on the specified data type, the line is assumed to hold base emissions, scale factors, or mask information.

#### **INTERFACE:**

```
SUBROUTINE Config_ReadCont( am_I_Root, HcoConfig, IU_HCO, & CFDIR, DctType, EOF, RC)
```

## **USES:**

```
USE HCO_EXTLIST_MOD, ONLY : ExtNrInUse, HCO_GetOpt
USE HCO_TIDX_Mod, ONLY : HCO_ExtractTime
USE HCO_FILEDATA_Mod, ONLY : FileData_Init
USE HCO_DATACONT_Mod, ONLY : CatMax, ZeroScalID
```

#### INPUT PARAMETERS:

```
) :: am_I_Root ! Root CPU?
LOGICAL,
                  INTENT(IN
TYPE(ConfigObj), POINTER
                                :: HcoConfig ! Config object
                                             ! Logfile LUN
                              ) :: IU_HCO
INTEGER,
                  INTENT(IN
                                             ! Configuration file directory
CHARACTER(LEN=*), INTENT(IN
                              ) :: CFDIR
INTEGER,
                  INTENT(IN
                              ) :: DctType
                                             ! 1=base; 2=scale; 3=mask
```

## INPUT/OUTPUT PARAMETERS:

```
LOGICAL, INTENT(INOUT) :: EOF ! end of file encountered?
```

### **OUTPUT PARAMETERS:**

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

#### **REVISION HISTORY:**

#### 1.4.4 BracketCheck

Subroutine BracketCheck checks if base emission data is within a bracket and if that field shall be ignored or not. Brackets can be used to lump entires of the HEMCO configuration file into collections that can be collectively enabled or disabled. The first entry of a collection is marked adding an 'opening bracket' to the HEMCO configuration file (on the line above the entry). Opening brackets must start with three opening brackets, e.g.: '(((TEST'. Similarly, the end of a collection is marked by placing a closing bracket after the last entry of the collection: '))))TEST'. Brackets can be enabled / disabled in the EXTENSION SWITCH section of the HEMCO configuration file: # ExtNr ExtName on/off Species 0 Base: on \* -; TEST: true

It is also possible to use 'opposite' brackets, e.g. to use a collection only if the given setting is \*disabled\*. This can be achieved by precede the collection word with '.not.', e.g. '(((.not.TEST' and '))).not.TEST'. Similarly, multiple collections can be combined to be evaluated together, e.g. NAME1.or.NAME2.

### **INTERFACE:**

```
SUBROUTINE BracketCheck( am_I_Root, HcoConfig, STAT, LINE, SKIP, RC )
```

### **USES:**

```
USE HCO_EXTLIST_MOD, ONLY : GetExtOpt, GetExtNr
```

## **INPUT PARAMETERS:**

```
LOGICAL, INTENT(IN) :: am_I_Root ! root CPU?
INTEGER, INTENT(IN) :: STAT !
CHARACTER(LEN=*), INTENT(IN) :: LINE !
```

## INPUT/OUTPUT PARAMETERS:

```
TYPE(ConfigObj), POINTER :: HcoConfig ! Config object
LOGICAL, INTENT(INOUT) :: SKIP ! Skip
INTEGER, INTENT(INOUT) :: RC ! Success/failure
```

#### **REVISION HISTORY:**

```
15 Feb 2015 - C. Keller - Initial version.

12 Mar 2015 - C. Keller - Added 'mirror' option.
```

## 1.4.5 AddShadowFields

Subroutine AddShadowFields adds a shadow container for every additional category of a base emission field. These container contain the same container as the 'mother' container, but an additional scale factor of zero will be applied to them. This makes sure that no additional emissions are created by the virtue of the shadow container.

#### **INTERFACE:**

```
SUBROUTINE AddShadowFields( am_I_Root, HcoConfig, Lct, Cats, nCat, RC )
USES:
```

```
USE HCO_DATACONT_MOD, ONLY : CatMax, ZeroScalID
```

## **INPUT PARAMETERS:**

```
:: am_I_Root
                                                ! root CPU?
LOGICAL,
                 INTENT(IN)
TYPE(ConfigObj), POINTER
                                                ! Config object
                                :: HcoConfig
                                                ! List container of interest
TYPE(ListCont), POINTER
INTEGER,
                INTENT(IN)
                                :: Cats(CatMax) ! Category numbers
                                                ! number of categories
INTEGER,
                INTENT(IN)
                               :: nCat
```

## INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC ! Success/failure
```

#### **REVISION HISTORY:**

```
15 Feb 2015 - C. Keller - Initial version.
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

### 1.4.6 AddZeroScal

Subroutine AddZeroScal adds a scale factor of zero to the configuration container list. This scale factor is an internal scale factor used in combination with the 'shadow' containers. Its scale factor ID is defined in Hco\_DataCont\_Mod and must not be used otherwise, e.g. there must not be another scale factor in the HEMCO configuration file with the same scale factor ID. Otherwise, HEMCO will create an error lateron.

#### **INTERFACE:**

```
SUBROUTINE AddZeroScal( am_I_Root, HcoConfig, RC )
```

#### **USES:**

```
USE HCO_DATACONT_MOD, ONLY : ZeroScalID
USE HCO_DATACONT_MOD, ONLY : ListCont_Find
USE HCO_FILEDATA_MOD, ONLY : FileData_Init
```

#### INPUT PARAMETERS:

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

TYPE(ConfigObj), POINTER :: HcoConfig ! Config object
```

## INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC ! Success/failure
```

### **REVISION HISTORY:**

```
15 Feb 2015 - C. Keller - Initial version.
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

## 1.4.7 ExtSwitch2Buffer

Subroutine ExtSwitch2Buffer reads the HEMCO extension switches and registers all enabled extensions.

#### **INTERFACE:**

```
{\tt SUBROUTINE~ExtSwitch2Buffer(~am\_I\_Root,~HcoConfig,~IU\_HCO,~EOF,~RC~)}
```

#### **USES:**

USE CHARPAK\_Mod, ONLY : STRREPL, STRSPLIT, TRANLC
USE HCO\_EXTLIST\_MOD, ONLY : AddExt, AddExtOpt, HCO\_GetOpt

USE HCO\_EXTLIST\_MOD, ONLY : GetExtNr

### INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am\_I\_Root ! root CPU?

TYPE(ConfigObj), POINTER :: HcoConfig ! Config object

INTEGER, INTENT(IN) :: IU\_HCO ! HEMCO configfile LUN

# INPUT/OUTPUT PARAMETERS:

LOGICAL, INTENT(INOUT) :: EOF ! End of file?

INTEGER, INTENT(INOUT) :: RC ! Success/failure

## **REVISION HISTORY:**

17 Sep 2013 - C. Keller - Initialization (update)

30 Sep 2014 - R. Yantosca - Declare SUBSTR and SPECS  $\mbox{w/}\ 2047$  characters,

which lets us handle extra-long species lists

21 Apr 2015 - R. Yantosca - Bug fix: now look for END\_SECTION before

testing if the line is a comment. This will allow for tags labeled "### END SECTION".

12 Dec 2015 - C. Keller - Added argument IgnoreIfExist to AddExtOpt to

make sure that nested configuration files do

use the settings set at highest level.

### 1.4.8 ReadSettings

Subroutine ReadSettings reads the HEMCO settings, stores them as HEMCO core extension options, and also evaluates some of the values (e.g. to initialize the HEMCO error module).

### **INTERFACE:**

SUBROUTINE ReadSettings(am\_I\_Root, HcoConfig, IU\_HCO, EOF, RC)

## **USES:**

USE HCO\_EXTLIST\_MOD, ONLY : AddExtOpt, GetExtOpt, CoreNr

USE HCO\_EXTLIST\_MOD, ONLY : HCO\_SetDefaultToken

USE HCO\_EXTLIST\_MOD, ONLY : HCO\_GetOpt

USE CHARPAK\_MOD, ONLY : STRREPL, STRSPLIT, TRANLC

### INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am\_I\_Root ! root CPU?
TYPE(ConfigObj), POINTER :: HcoConfig ! Config obj

INTEGER, INTENT(IN) :: IU\_HCO ! HEMCO configfile LUN

## INPUT/OUTPUT PARAMETERS:

```
LOGICAL, INTENT(INOUT) :: EOF ! End of file?

INTEGER, INTENT(INOUT) :: RC ! Success/failure
```

## **REVISION HISTORY:**

```
17 Sep 2013 - C. Keller - Initialization (update)
21 Apr 2015 - R. Yantosca - Bug fix: now look for END_SECTION before testing if the line is a comment. This will allow for tags labeled "### END SECTION".

12 Dec 2015 - C. Keller - Added argument IgnoreIfExist to AddExtOpt to make sure that nested configuration files do use the settings set at highest level.
```

## 1.4.9 RegisterPrepare

Subroutine RegisterPrepare extracts the spatial coverages of all mask fields as well as the HEMCO species IDs of all base emissions.

The species IDs are determined by matching the species name read from the configuration file (in ConfigList) and the species names defined in the HEMCO state object HcoState.

Mask coverages are defined based upon the passed horizontal grid extensions on this CPU (xrng and yrng).

### **INTERFACE:**

```
SUBROUTINE RegisterPrepare( am_I_Root, HcoState, RC )
```

## **USES:**

```
USE HCO_EXTLIST_MOD, ONLY : ExtNrInUse
USE HCO_STATE_Mod, ONLY : HCO_GetHcoID
USE HCO_DATACONT_MOD, ONLY : ListCont_NextCont
```

#### INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root ! Root CPU
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state obj.
```

#### **OUTPUT PARAMETERS:**

```
INTEGER, INTENT(INOUT) :: RC
```

```
18 Sep 2013 - C. Keller - Initial version (update)
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

### 1.4.10 Register\_Base

Subroutine Register\_Base registers all base emission data and writes out all associated scale factor IDs.

#### INTERFACE:

```
SUBROUTINE Register_Base ( am_I_Root, HcoState, RC )
```

## **USES:**

```
USE HCO_READLIST_Mod, ONLY : ReadList_Set
USE HCO_DATACONT_Mod, ONLY : DataCont_Cleanup
USE HCO_DATACONT_MOD, ONLY : ListCont_NextCont
```

# INPUT/OUTPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Are we on the root CPU? TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object
```

# INPUT/OUTPUT PARAMETERS:

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

#### REVISION HISTORY:

```
18 Jun 2013 - C. Keller: Initialization
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

## 1.4.11 Register\_Scal

Subroutine Register\_Scal registers all scale factors.

### INTERFACE:

```
SUBROUTINE Register_Scal( am_I_Root, HcoState, RC )
```

## **USES:**

# INPUT PARAMETERS:

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

TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object
```

## INPUT/OUTPUT PARAMETERS:

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

## **REVISION HISTORY:**

```
18 Jun 2013 - C. Keller - Initialization
```

```
29 Dec 2014 - C. Keller - Now check for masks assigned to scale factors.
```

26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts

## 1.4.12 Get\_targetID

Subroutine Get\_targetID returns the target ID of a container. The target ID can point to the container ID (cID) of another base field if multiple emissions shall be added together prior to emission calculation, e.g. sectoral emissions data with same species ID, category, hierarchy, extension number, scale factors, etc.

Target ID is set to -999 if there exists another inventory over the full spatial region covered by this CPU for this species but with higher hierarchy. In this case, we can ignore the current container from here onwards!

## **INTERFACE:**

```
SUBROUTINE Get_targetID( am_I_Root, HcoState, Lct, targetID, RC )
```

## **USES:**

```
USE HCO_DataCont_Mod, ONLY : ListCont_Find
USE HCO_DataCont_Mod, ONLY : ListCont_NextCont
```

### INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
TYPE(HCO_State), POINTER :: HcoState
TYPE(ListCont), POINTER :: Lct
```

### **OUTPUT PARAMETERS:**

## INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

!NOTE: If data from multiple containers are added, the target ID is always set to the lowest cID of all involved containers, i.e. data are added to the container with the lowest cID. This makes sure that data is not accidentally overwritten, e.g. when updating container contents!

## **REVISION HISTORY:**

```
11 Apr 2013 - C. Keller - Initialization
07 Dec 2015 - C. Keller - Make sure emissions with limited time range do
never erase lower hierarchy base emissions.
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

## 1.4.13 Calc\_Coverage

Function Calc\_Coverage calculates the coverage of the specified lon/lat box with the area covered by the inventory. Returns 0 if no overlap, 1 if complete overlap, and -1 for partial overlap.

#### INTERFACE:

## **INPUT PARAMETERS:**

```
INTEGER, INTENT(IN) :: msk_x1
INTEGER, INTENT(IN) :: msk_x2
INTEGER, INTENT(IN) :: msk_y1
INTEGER, INTENT(IN) :: msk_y2
INTEGER, INTENT(IN) :: cpu_x1
INTEGER, INTENT(IN) :: cpu_x2
INTEGER, INTENT(IN) :: cpu_y1
INTEGER, INTENT(IN) :: cpu_y2
```

### **RETURN VALUE:**

INTEGER :: COVERAGE

### **REVISION HISTORY:**

11 Apr 2013 - C. Keller: Initialization

## 1.4.14 ReadAndSplit\_Line

Subroutine ReadAndSplit\_Line reads a line from the HEMCO config file and parses the specified columns into the passed integer and character variables. If the optional argument inLine is provided, this line will be parsed, otherwise a new line will be read from the config file. If the optional argument outLine is provided, this variable will hold the parsed line.

This routine splits the input line (or the next line of an open file with ID IU\_HCO), using the HEMCO separator (default: space) as separator. The resulting elements are then passed to the specified output characters and integers. For example, to pass the 5th element of a line to variable int1, set int1cl to 5, etc. An error will be returned (STAT=100) if any of the output columns exceeds the number of line elements. The optional argument optcl can be used to denote an optional value, e.g. no error is returned if the value at position optcl cannot be read. Only one optional value can be specified.

#### **INTERFACE:**

```
SUBROUTINE ReadAndSplit_Line( AIR,
                                        HcoConfig,
                                        IU_HCO,
                                                 char1, chr1cl, &
                               char2,
                                        chr2cl, char3, chr3cl, &
                                                 char5, chr5cl, &
                               char4,
                                        chr4cl,
                               char6,
                                        chr6cl,
                                                 char7, chr7cl, &
                                        chr8cl,
                                                 char9, chr9cl, &
                               char8,
                               char10,
                                        chr10cl,
                               int1,
                                        int1cl,
                                                 int2,
                                                         int2cl, &
                                                  STAT,
                               int3,
                                        int3cl,
                                                         inLine, &
                               outLine, optcl
```

#### **USES:**

USE CHARPAK\_Mod, ONLY : STRREPL, STRSPLIT

## INPUT PARAMETERS:

```
LOGICAL,
                  INTENT(IN
                                         :: AIR
TYPE(ConfigObj),
                                         :: HcoConfig
                  POINTER
INTEGER,
                  INTENT(IN
                                         :: IU_HCO
                            )
                                         :: chr1cl
INTEGER,
                  INTENT(IN
INTEGER,
                              )
                                         :: chr2cl
                  INTENT(IN
INTEGER,
                  INTENT(IN
                              )
                                         :: chr3cl
INTEGER,
                                         :: chr4cl
                  INTENT(IN
INTEGER,
                  INTENT(IN
                              )
                                         :: chr5cl
INTEGER,
                  INTENT(IN
                                         :: chr6cl
                            )
                                         :: chr7cl
INTEGER,
                  INTENT(IN
                            )
INTEGER,
                  INTENT(IN
                            )
                                         :: chr8cl
                                        :: chr9cl
INTEGER,
                  INTENT(IN
                            )
INTEGER,
                  INTENT(IN
                            )
                                        :: chr10cl
INTEGER,
                  INTENT(IN )
                                        :: int1cl
INTEGER,
                            )
                                         :: int2cl
                  INTENT(IN
INTEGER,
                  INTENT(IN )
                                        :: int3cl
                            ), OPTIONAL :: inLINE
CHARACTER(LEN=255), INTENT(IN
INTEGER,
                  INTENT(IN
                            ), OPTIONAL :: optcl
```

## **OUTPUT PARAMETERS:**

```
CHARACTER(LEN=*),
                   INTENT(INOUT)
                                          :: char1
CHARACTER(LEN=*),
                   INTENT(INOUT)
                                          :: char2
CHARACTER(LEN=*),
                                          :: char3
                  INTENT(INOUT)
CHARACTER(LEN=*),
                   INTENT (INOUT)
                                          :: char4
                  INTENT(INOUT)
CHARACTER(LEN=*),
                                         :: char5
                                         :: char6
CHARACTER(LEN=*),
                  INTENT (INOUT)
CHARACTER(LEN=*),
                                         :: char7
                  INTENT(INOUT)
CHARACTER(LEN=*),
                  INTENT(INOUT)
                                         :: char8
CHARACTER(LEN=*),
                                          :: char9
                  INTENT(INOUT)
CHARACTER(LEN=*),
                                         :: char10
                  INTENT(INOUT)
                                          :: int1
INTEGER,
                   INTENT (INOUT)
INTEGER,
                   INTENT (INOUT)
                                         :: int2
                   INTENT(INOUT)
                                         :: int3
INTEGER,
CHARACTER(LEN=255), INTENT( OUT), OPTIONAL :: outLINE
```

## INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: STAT

## **REVISION HISTORY:**

```
28 Aug 2013 - C. Keller - Initial version
```

11 Dec 2013 - C. Keller - Added optional arguments inLine and outLine

29 Dec 2014 - C. Keller - Added optional argument optcl. Now use wrapper

routines READCHAR and READINT.

13 Mar 2015 - C. Keller - Added check for include files.

### 1.4.15 READCHAR

Subroutine READCHAR is a helper routine to read character values from the HEMCO configuration file.

#### **INTERFACE:**

```
SUBROUTINE READCHAR ( LINE, SUBSTR, N, chrcl, charout, OPT, STAT )
```

## **INPUT PARAMETERS:**

```
CHARACTER(LEN=255), INTENT(IN ) :: LINE
CHARACTER(LEN=255), INTENT(IN ) :: SUBSTR(255)
INTEGER, INTENT(IN ) :: N
INTEGER, INTENT(IN ) :: chrcl
INTEGER, INTENT(IN ) :: OPT
```

# INPUT/OUTPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(INOUT) :: charout INTEGER, INTENT(INOUT) :: STAT
```

#### REVISION HISTORY:

```
29 Dec 2014 - C. Keller - Initial version
```

#### 1.4.16 **READINT**

Subroutine READINT is a helper routine to read integer values from the HEMCO configuration file.

## **INTERFACE:**

```
SUBROUTINE READINT (ExtList, LINE, SUBSTR, N, intcl, intout, OPT, STAT)
USES:
```

```
USE HCO_EXTLIST_MOD, ONLY : HCO_GetOpt
```

## INPUT PARAMETERS:

```
TYPE(Ext),
                 POINTER
                                :: ExtList
CHARACTER(LEN=255), INTENT(IN )
                                :: LINE
CHARACTER(LEN=255), INTENT(IN )
                                :: SUBSTR(255)
INTEGER,
                 INTENT(IN
                           )
                                :: N
                 INTENT(IN ) :: intcl
INTEGER,
INTEGER,
                 INTENT(IN )
                                :: OPT
```

## INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: intout INTEGER, INTENT(INOUT) :: STAT
```

```
29 Dec 2014 - C. Keller - Initial version
```

## 1.4.17 Get\_cID

Subroutine Get\_cID searches the whole ConfigList for an entry with the given ScalID and returns the corresponding container ID cID.

### **INTERFACE:**

```
SUBROUTINE Get_cID( ScalID, HcoConfig, cID, RC )
```

### INPUT PARAMETERS:

```
INTEGER, INTENT(IN ) :: scalID
TYPE(ConfigObj), POINTER :: HcoConfig
```

### **OUTPUT PARAMETERS:**

```
INTEGER, INTENT( OUT) :: cID
!INPUT/OUTPUTP PARAMETERS:
```

INTEGER, INTENT(INOUT) :: RC

### **REVISION HISTORY:**

```
18 Sep 2013 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

## 1.4.18 ConfigList\_AddCont

Subroutine ConfigList\_AddCont adds a new (blank) container to the ConfigList list.

# **INTERFACE:**

```
SUBROUTINE ConfigList_AddCont( Lct, List )
```

### **USES:**

```
USE HCO_DATACONT_Mod, ONLY : DataCont_Init USE HCO_DATACONT_Mod, ONLY : ListCont_Length
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(ListCont), POINTER :: Lct
TYPE(ListCont), POINTER :: List
```

```
17 Sep 2013 - C. Keller: Initialization (update)
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

## 1.4.19 ScalID\_Register

Subroutine ScalID\_Register adds the scale factor IDs ScalIDs to the list of scale factor IDs.

### **INTERFACE:**

```
SUBROUTINE ScalID_Register( Dct, HcoConfig, RC )
```

#### INPUT PARAMETERS:

```
TYPE(DataCont), POINTER :: Dct
TYPE(ConfigObj), POINTER :: HcoConfig
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

### **REVISION HISTORY:**

```
10 Jan 2014 - C. Keller: Initialization (update)
29 Dec 2014 - C. Keller: Now add new container to end of list to allow
list being updated while calling Register_Scal.
```

### 1.4.20 ScalID2List

Subroutine ScalID2List adds the scale factor IDs ScalIDs to the list of scale factor IDs.

### **INTERFACE:**

```
SUBROUTINE ScalID2List( ScalIDList, ID, RC )
```

### INPUT PARAMETERS:

```
TYPE(ScalIDCont), POINTER :: ScalIDList INTEGER, INTENT(IN ) :: ID
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

## 1.4.21 ScalID\_Cleanup

Subroutine ScalID\_Cleanup cleans up the internal ScalID list.

### **INTERFACE:**

```
SUBROUTINE ScalID_Cleanup( ScalIDList )
!INPUT ARGUMENTS:
TYPE(ScalIDCont), POINTER :: ScalIDList
```

#### REVISION HISTORY:

```
10 Jan 2014 - C. Keller: Initialization (update)
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 1.4.22 SpecName\_Register

Subroutine SpecName\_Register adds the species name SpecName to the list of species names.

### **INTERFACE:**

```
SUBROUTINE SpecName_Register( HcoConfig, SpecName, RC )
```

#### **USES:**

```
USE HCO_EXTLIST_MOD, ONLY : HCO_GetOpt
```

#### INPUT PARAMETERS:

```
TYPE(ConfigObj), POINTER :: HcoConfig CHARACTER(LEN=*), INTENT(IN ) :: SpecName
```

## INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

#### REVISION HISTORY:

```
10 Jan 2014 - C. Keller: Initialization (update)
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

### 1.4.23 SpecName\_Cleanup

Subroutine SpecName\_Cleanup cleans up the internal SpecName list.

### INTERFACE:

```
SUBROUTINE SpecName_Cleanup ( SpecNameList )
!INPUT/OUTPUT ARGUMENT:
    TYPE(SpecNameCont), POINTER :: SpecNameList
```

```
10 Jan 2014 - C. Keller: Initialization (update)
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

## 1.4.24 Config\_GetnSpecies

Function Config\_GetnSpecies is a wrapper function to get the number of (unique) species names in SpecNameList.

#### INTERFACE:

```
FUNCTION Config_GetnSpecies( HcoConfig ) RESULT( nSpecies )
!INPUT ARGUMENT:
    TYPE(ConfigObj), POINTER :: HcoConfig
```

## RETURN VALUE:

INTEGER :: nSpecies

#### REVISION HISTORY:

```
10 Jan 2014 - C. Keller: Initialization (update)
```

## 1.4.25 Config\_GetSpecNames

Subroutine Config\_GetSpecNames is a wrapper routine to obtain the list of (unique) species names defined in SpecNameList.

#### **INTERFACE:**

```
SUBROUTINE Config_GetSpecNames( HcoConfig, SpecNames, nSpecies, RC )
!INPUT ARGUMENT:
   TYPE(ConfigObj), POINTER :: HcoConfig
!OUTPUT PARAMTERS:
   CHARACTER(LEN=*), POINTER :: SpecNames(:)
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: nSpecies
INTEGER, INTENT(INOUT) :: RC
```

#### REVISION HISTORY:

```
10 Jan 2014 - C. Keller: Initialization (update)
```

# 1.4.26 Config\_getSpecAttr

Subroutine Config\_GetSpecAttr returns the number of species names N and the vector of species names SpecNames. SpecNames must be of length nnSpecs, i.e. in order to obtain SpecNames, Config\_getSpecAttr has to be called twice: N=0 CALL Config\_getSpecAttr ( N=N, RC=RC ) ALLOCATE(SpecNames(N)) CALL Config\_getSpecAttr ( N=N, SpecNames=SpecNames, RC=RC )

```
SUBROUTINE Config_GetSpecAttr( HcoConfig, N, SpecNames, RC )
!INPUT ARGUMENT:
```

TYPE(ConfigObj), POINTER :: HcoConfig

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: N
INTEGER, INTENT(INOUT) :: RC

### **OUTPUT PARAMETERS:**

CHARACTER(LEN=\*), POINTER, OPTIONAL :: SpecNames(:)

#### REVISION HISTORY:

```
10 Jan 2014 - C. Keller: Initialization (update)
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

#### 1.4.27 Check ContNames

Function Check\_Contnames compares the container names of two containers, ignoring the name 'tags', i.e. ignoring everything that follows double underscore (\_\_). For example, two containers with names "EDGAR\_NOX\_PNT" and "EDGAR\_NOX\_MOB" are considered equal, while "EDGAR\_NOX\_PNT" and "EDGAR\_NOX\_MOB" are not.

### **INTERFACE:**

```
FUNCTION Check_ContNames( Lct1, Lct2 ) RESULT( SameName )
```

## INPUT/OUTPUT PARAMETERS:

```
TYPE(ListCont), POINTER :: Lct1
TYPE(ListCont), POINTER :: Lct2
```

#### RETURN VALUE:

LOGICAL :: SameName

#### **REVISION HISTORY:**

```
10 Jan 2014 - C. Keller: Initialization (update)
```

## 1.4.28 ExtractSrcDim

Subroutine ExtractSrcDim extracts the source dimension attribute. Specifically, it checks if the field is expected to be 2D (xy) or 3D. Default 3D data is xyz, but it is also possible to explicitly define the number of vertical levels to be read, as well as the reading direction (up or down). For example, 'xy1' will be interpreted as reading only the first level, and 'xy27' will only read the first 27 levels. To reverse the vertical axis, use e.g. 'xy-1' to read only the top level, or 'xy-27' to read the top 27 levels, with the topmost level being put into the surface level.

SUBROUTINE ExtractSrcDim( am\_I\_Root, HcoConfig, SrcDim, Dta, RC )

# INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
TYPE(ConfigObj), POINTER :: HcoConfig
CHARACTER(LEN=*), INTENT(IN ) :: SrcDim
TYPE(FileData), POINTER :: Dta
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

### REVISION HISTORY:

```
20 May 2015 - C. Keller - Initial version
22 Jan 2016 - R. Yantosca - Bug fix, removed & in the middle of the line since the PGI compiler chokes on it.
```

# 1.4.29 ConfigInit

Subroutine ConfigInit is a wrapper routine to initialize the HEMCO configuration object.

## **INTERFACE:**

```
SUBROUTINE ConfigInit ( HcoConfig )
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(ConfigObj), POINTER :: HcoConfig
```

## **REVISION HISTORY:**

```
16 Feb 2016 - C. Keller: Initialization (update)
```

## 1.4.30 ParseEmisL

parses the emission level.

## **INTERFACE:**

```
SUBROUTINE ParseEmisL ( str, EmisL, EmisUnit )
```

### INPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(IN ) :: str
```

# INPUT/OUTPUT PARAMETERS:

```
REAL(hp), INTENT(OUT) :: EmisL INTEGER, INTENT(OUT) :: EmisUnit
```

```
09 May 2016 - C. Keller: Intial version.
```

## 1.5 Fortran: Module Interface hco\_datacont\_mod.F90

Module HCO\_DATACONT\_MOD contains routines and variables to handle the HEMCO data-container (DataCont) and corresponding list-container (ListCont) derived type.

DataCont holds all information of an emission field, such as emission category, emission hierarchy, scale factors, etc. DataCont also contains a pointer to the source data (see HCO\_FILEDATA\_MOD) for more information on the file data object. A data-container will be created for every emission field specified in the HEMCO configuration file.

The ListCont object is a derived type used to create linked lists. It contains a pointer to one data container (Dta) and a pointer to the next element of the list (NextCont). All HEMCO lists (ConfigList, ReadList, ListCont) are built from ListCont elements.

DataCont consists of the following elements:

- cName: container name, as set in the configuration file.
- cID: container ID, defined by HEMCO.
- targetID: target ID of this container. If target ID differs from the container ID, the data will be added to the content of the container with cID = targetID (e.g. data of container 1 will be added to container 5 if it has a target ID of 5). Internal use only.
- DctType: container type. 1 for base emissions, 2 for scale factors, 3 for masks (set parameter in HCO\_ERROR\_MOD)
- SpcName: Species name associated with this data container, as read from the configuration file. Only relevant for base emission arrays.
- HcoID: HEMCO species ID corresponding to SpcName.
- ExtNr: Extension number. Extension number 0 is reserved for HEMCO core, other extensions can have freely defined extensions number, as specified in the configuration file. Only relevant for base emissions.
- Cat: emission category, as set in the configuration file. Only relevant for base emissions.
- Hier: emission hierarchy, as set in the configuration file. Only relevant for base emissions.
- ScalID: scale factor ID, as set in the configuration file. Only relevant for scale factors and masks.
- Oper: mathematical operator applied to scale factor. If 1, the field will be multiplied (E=BxS); if -1, division is applied (E=B/S); if 2, field will be squared (E=BxSxS). For masks, operator 3 can be used to mirror the mask data, i.e. E=Bx(1-S). Only relevant for scale factors and masks.
- Scal\_cID: vector of scale factor IDs associated to a base emission field, as specified in the configuration file. Only relevant for base emissions.

- Scal\_cID\_set: the Scal\_cID values read from the configuration file are translated to the corresponding container IDs values (the scale IDs are defined in the configuration file, container IDs are automatically set by HEMCO) to optimize container assignment operations. Scal\_cID\_set indicates whether or not the Scal\_cID holds the container IDs or still the original scale factor IDs. For internal use only.
- Dta: a file data object, holding information about the source file, update frequency, the data arrays, etc. See HCO\_FILEDATA\_MOD for more information.
- DtaHome: a data container only holds a pointer to a file data object, i.e. it is possible that multiple containers share the same file data object. the DtaHome flag is used to determine whether this is the home container of this file data object. For internal use only.

### **INTERFACE:**

```
MODULE HCO_DataCont_Mod
```

## **USES:**

```
USE HCO_TYPES_MOD
USE HCO_Error_Mod
USE HCO_Arr_Mod
IMPLICIT NONE
PRIVATE
```

#### PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: DataCont_Init

PUBLIC :: DataCont_Cleanup

PUBLIC :: cIDList_Create

PUBLIC :: cIDList_Cleanup

PUBLIC :: Pnt2DataCont

PUBLIC :: ListCont_NextCont

PUBLIC :: ListCont_Find

PUBLIC :: ListCont_Length

PUBLIC :: ListCont_Cleanup
```

#### REVISION HISTORY:

```
19 Dec 2013 - C. Keller: Initialization
01 Jul 2014 - R. Yantosca - Now use F90 free-format indentation
01 Jul 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
```

#### 1.5.1 DataCont\_Init

Subroutine DataCont\_Init initializes a new (blank) data container Dct.

```
SUBROUTINE DataCont_Init( Dct, cID )
```

#### INPUT PARAMETERS:

```
TYPE(DataCont), POINTER :: Dct INTEGER, INTENT(IN) :: cID
```

### **REVISION HISTORY:**

```
19 Dec 2013 - C. Keller: Initialization
```

# 1.5.2 DataCont\_Cleanup

Subroutine DataCont\_Cleanup cleans up data container Dct. If ArrOnly is set to True, this will only cleanup the data array of the container but keep all meta-data.

### INTERFACE:

```
SUBROUTINE DataCont_Cleanup( Dct, ArrOnly )
```

#### **USES:**

```
USE HCO_FILEDATA_MOD, ONLY : FileData_Cleanup
```

#### ARGUMENTS:

```
TYPE(DataCont), POINTER :: Dct
LOGICAL, INTENT(IN), OPTIONAL :: ArrOnly
```

### **REVISION HISTORY:**

```
19 Dec 2013 - C. Keller: Initialization
```

## 1.5.3 ListCont\_Cleanup

Subroutine ListCont\_Cleanup cleans up list List The corresponding data container (Lst-ContRemoveDct is set to true.

### INTERFACE:

```
SUBROUTINE ListCont_Cleanup( List, RemoveDct )
```

### INPUT PARAMETERS:

```
TYPE(ListCont), POINTER :: List
LOGICAL, INTENT(IN) :: RemoveDct
```

```
19 Dec 2013 - C. Keller: Initialization
25 Oct 2016 - R. Yantosca - Do not nullify pointers in declaration stmts
```

### 1.5.4 cIDList\_Create

Subroutine cIDList\_Create creates a vector of pointers (cIDList) pointing to all available containers of the passed List. The vector index of cIDList corresponds to the container cIDs, i.e. cIDList(3) will point to data container with cID = 3.

### **INTERFACE:**

```
SUBROUTINE cIDList_Create( am_I_Root, HcoState, List, RC )
```

#### **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_State
```

### **ARGUMENTS:**

```
LOGICAL, INTENT(IN) :: am_I_Root
TYPE(HCO_State), POINTER :: HcoState
TYPE(ListCont), POINTER :: List
INTEGER, INTENT(INOUT) :: RC
```

## **REVISION HISTORY:**

```
24 Aug 2012 - C. Keller - Initial Version
25 Oct 2016 - R. Yantosca - Do not nullify pointers in declaration stmts
```

## 1.5.5 cIDList\_Cleanup

Subroutine cIDList\_Cleanup cleans up cIDList.

### **INTERFACE:**

```
SUBROUTINE cIDList_Cleanup( HcoState )
```

### **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_State
```

### **ARGUMENTS:**

```
TYPE(HCO_State), POINTER :: HcoState
```

```
24 Aug 2012 - C. Keller - Initial Version
```

### 1.5.6 Pnt2DataCont

Subroutine Pnt2DataCont returns the data container Dct with container ID cID.

### **INTERFACE:**

```
SUBROUTINE Pnt2DataCont( am_I_Root, HcoState, cID, Dct, RC )
```

## **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_State
```

### INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root
TYPE(HCO_State), POINTER :: HcoState
INTEGER, INTENT(IN) :: cID
TYPE(DataCont), POINTER :: Dct
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

### **REVISION HISTORY:**

```
11 Apr 2012 - C. Keller - Initial version
```

### 1.5.7 ListCont\_NextCont

Routine ListCont\_NextCont returns container Lct from data list List. This is the generic routine for cycling through the data container lists.

If Lct is empty (i.e. NULL), the first container of List is returned. If Lct already points to a list container, the pointer is advanced to the next container in that list (LctFLAG is set to HCO\_SUCCESS if the return container Lct is defined, and to HCO\_FAIL otherwise.

### **INTERFACE:**

```
SUBROUTINE ListCont_NextCont( List, Lct, FLAG )
```

# **INPUT PARAMETERS:**

```
TYPE(ListCont), POINTER :: List
TYPE(ListCont), POINTER :: Lct
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: FLAG
```

```
11 Apr 2012 - C. Keller - Initial version
```

### 1.5.8 ListCont\_Find\_Name

Subroutine ListCont\_Find\_Name searches for (data) container name NME in list List and returns a pointer pointing to this container (Lct).

### **INTERFACE:**

```
SUBROUTINE ListCont_Find_Name( List, NME, FOUND, Lct )
```

### **ARGUMENTS:**

```
TYPE(ListCont), POINTER :: List ! List to be searched CHARACTER(LEN=*), INTENT(IN ) :: NME ! Container name LOGICAL, INTENT(OUT) :: FOUND ! Container found? TYPE(ListCont), POINTER, OPTIONAL :: Lct ! matched list container
```

### **REVISION HISTORY:**

```
04 Dec 2012 - C. Keller: Initialization
25 Oct 2016 - R. Yantosca - Do not nullify pointers in declaration stmts
```

### 1.5.9 ListCont\_Find\_ID

Subroutine ListCont\_Find\_ID searches for (data) container cID or ScalID (ID) in list List and returns a pointer pointing to this (list) container (Lct).

### **INTERFACE:**

```
SUBROUTINE ListCont_Find_ID( List, ID, IsScalID, FOUND, Lct )
```

#### INPUT PARAMETERS:

```
TYPE(ListCont), POINTER :: List ! List to be searched INTEGER, INTENT(IN ) :: ID ! cID or ScalID INTEGER, INTENT(IN ) :: IsScalID ! 1=ID is ScalID; ! else: ID is cID
```

## **OUTPUT PARAMETERS:**

```
LOGICAL, INTENT(OUT) :: FOUND ! Container found? TYPE(ListCont), POINTER, OPTIONAL :: Lct ! Container w/ ID
```

```
04 Dec 2012 - C. Keller: Initialization
25 Oct 2016 - R. Yantosca - Do not nullify pointers in declaration stmts
```

### 1.5.10 ListCont\_Length

Subroutine ListCont\_Length returns the length of the passed list.

#### **INTERFACE:**

```
FUNCTION ListCont_Length ( List ) RESULT ( nnCont )
```

## **INPUT PARAMETERS:**

TYPE(ListCont), POINTER :: List INTEGER :: nnCont

#### **REVISION HISTORY:**

15 Feb 2016 - C. Keller: Initial version

# 1.6 Fortran: Module Interface hco\_diagn\_mod.F90

Module HCO\_Diagn\_mod contains routines and variables to handle the HEMCO diagnostics. The HEMCO diagnostics consist of a flexible suite of diagnostics container organized in list DiagnList. Each diagnostics container contains information about the diagnostics type (extension number, emission category / hierarchy, species ID), data structure (Scalar, 2D, 3D), and output units (mass, area, time).

The HEMCO diagnostics module can store multiple, independent diagnostics 'collections', identifiable through the assigned collection number. Each collection has an output frequency assigned to it, as well as an output file name (prefix). All containers of the same collection will have the same output frequency. Currently, the following output frequencies are defined: 'Hourly', 'Daily', 'Monthly', 'Annually', 'End', 'Manual'.

HEMCO has three default built-in diagnostic collections: default, manual, and restart. These three collections become automatically defined during initialization of HEMCO, and diagnostic containers can be added to them anytime afterwards. The output frequency of the default collection can be specified in the HEMCO configuration file through argument 'DiagnFreq'. This can be a character indicating the output frequency (valid entries are 'Always', 'Hourly', 'Daily', 'Monthly', 'Annually', 'Manual', and 'End') or by two integer strings of format '00000000 000000' denoting the year-month-day and hour-minute- second output interval, respectively. For example, setting DiagnFreq to '00000001 000000' would be equivalent to setting it to 'Daily'. A value of '00000000 030000' indicates that the diagnostics shall be written out every 3 hours.

The restart collection always gets an output frequency of 'End', but writing its content to disk can be forced at any given time using routine HcoDiagn\_Write (see below). The manual diagnostics has an output frequency of 'Manual', which means that its content is never written to disk. Instead, its fields need to be fetched explicitly from other routines via routine Diagn\_Get.

The public module variables HcoDiagnIDDefault, HcoDiagnIDManual, and HcoDiagnRestart

can be used to refer to these collections. The user can also define its own collections. It is recommended to do this outside of this module, e.g. at the model - HEMCO interface.

Diagnostic collections are written to disk using the routines in module hcoio\_diagn\_mod.F90. Routine HcoDiagn\_Write will write out the three built-in HEMCO collections. Other collections need be written out explicitly using routine HCOIO\_Diagn\_WriteOut. The HEMCO option 'HcoWritesDiagn' determines if the three HEMCO collections are automatically written out by the HEMCO driver routines (hco\_driver\_mod.F90). If HcoWritesDiagn is set to FALSE, the user can freely decide when to write out the diagnostics. This is useful if the HEMCO diagnostics contain fields that are used/filled outside of HEMCO.

Diagnostics container are created at the beginning of a simulation using subroutine Diagn\_Create. During the simulation, content is added to the individual containers via Diagn\_Update. Diagnostics data is fetched using Diagn\_Get. All emissions are stored in units of [kg/m2] and only converted to desired output units when returning the data. The container variable IsOutFormat denotes whether data is currently stored in output units or internal units. Variable nnGetCalls counts the number of times a diagnostics is called through Diagn\_Get without updating its content. This is useful if you want to make sure that data is only written once per time step.

There are two types of emission diagnostics: automatic ('AutoFill') and manual diagnostics. AutoFill diagnostics become automatically filled during execution of HEMCO. AutoFill diagnostics can be at species level (level 1), ExtNr level (level 2), emission category level (level 3), or hierarchy level (level 4). Level 1 diagnostics write out the collected emissions of the specified species, level 2 diagnostics write out emissions for the given ExtNr only (ignoring emissions from all other ExtNr's), etc. Manual diagnostics can represent any content. They never become filled automatically and all update calls (Diagn\_Update) have to be set manually.

Individual diagnostics are identified by its name and/or container ID. Both are specified when creating the diagnostics (Diagn\_Create).

Before adding diagnostics to a collection, the collection needs to be created using subroutine DiagnCollection\_Create. The collection number argument (COL) should always be specified when creating, editing or obtaining a diagnostics. If this argument is omitted, the default HEMCO collection (HcoDiagnIDDefault) is taken.

#### **INTERFACE:**

```
MODULE HCO_Diagn_Mod
```

### **USES:**

!

```
USE HCO_Error_Mod

USE HCO_Types_Mod

USE HCO_Arr_Mod

USE HCO_Clock_Mod

USE HCO_State_Mod, ONLY : HCO_State
```

IMPLICIT NONE PRIVATE

#### PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HcoDiagn\_AutoUpdate

PUBLIC :: HcoDiagn\_Init
PUBLIC :: Diagn\_Create
PUBLIC :: Diagn\_Update
PUBLIC :: Diagn\_Get

PUBLIC :: Diagn\_TotalGet

PUBLIC :: Diagn\_AutoFillLevelDefined

PUBLIC :: Diagn\_Print

PUBLIC :: Diagn\_DefineFromConfig

PUBLIC :: DiagnCont\_Find

PUBLIC :: DiagnCollection\_Create
PUBLIC :: DiagnCollection\_Cleanup
PUBLIC :: DiagnCollection\_Get

PUBLIC :: DiagnCollection\_Set

PUBLIC :: DiagnCollection\_GetDefaultDelta
PUBLIC :: DiagnCollection\_IsTimeToWrite
PUBLIC :: DiagnCollection\_LastTimesSet

PUBLIC :: DiagnFileOpen
PUBLIC :: DiagnFileGetNext
PUBLIC :: DiagnFileClose
PUBLIC :: DiagnBundle\_Cleanup
PUBLIC :: DiagnBundle\_Init

### PRIVATE MEMBER FUNCTIONS:

PRIVATE :: DiagnList\_Cleanup
PRIVATE :: DiagnCont\_Init

PRIVATE :: DiagnCont\_PrepareOutput

PRIVATE :: DiagnCont\_Link\_2D
PRIVATE :: DiagnCont\_Link\_3D
PRIVATE :: DiagnCont\_Cleanup

PRIVATE :: DiagnCollection\_DefineID
PRIVATE :: DiagnCollection\_Find
PRIVATE :: Diagn\_UpdateDriver
PRIVATE :: Diagn\_UpdateSp0d
PRIVATE :: Diagn\_UpdateSp2d
PRIVATE :: Diagn\_UpdateSp3d
PRIVATE :: Diagn\_UpdateDp0d

PRIVATE :: Diagn\_UpdateDp2d PRIVATE :: Diagn\_UpdateDp3d

INTERFACE Diagn\_Update

MODULE PROCEDURE Diagn\_UpdateSp0d

```
MODULE PROCEDURE Diagn_UpdateSp2d
MODULE PROCEDURE Diagn_UpdateSp3d
MODULE PROCEDURE Diagn_UpdateDp0d
MODULE PROCEDURE Diagn_UpdateDp2d
MODULE PROCEDURE Diagn_UpdateDp3d
END INTERFACE
```

## **REVISION HISTORY:**

```
19 Dec 2013 - C. Keller
                         - Initialization
08 Jul 2014 - R. Yantosca - Now use F90 free-format indentation
08 Jul 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
01 Aug 2014 - C. Keller - Added manual output frequency
                         - Added cumulative sum option
12 Aug 2014 - C. Keller
09 Jan 2015 - C. Keller
                         - Added diagnostics collections
03 Apr 2015 - C. Keller - Now tie output frequency to collection instead
                           of individual diagnostic containers.
06 Nov 2015 - C. Keller
                         - Added argument OutTimeStamp to collection to
                            control the file output time stamp (beginning,
                           middle, end of diagnostics interval).
25 Jan 2016 - R. Yantosca - Added bug fixes for pgfortran compiler
19 Sep 2016 - R. Yantosca - Add extra overloaded functions to the
                           Diagn_Update interface to avoid Gfortran errors
```

# 1.6.1 HcoDiagn\_autoupdate

Subroutine HCODIAGN\_AUTOUPDATE updates the AutoFill diagnostics at species level. This routine should be called after running HEMCO core and all extensions.

### **INTERFACE:**

```
SUBROUTINE HcoDiagn_AutoUpdate( am_I_Root, HcoState, RC )  {\bf USES:} \\
```

```
USE HCO_STATE_MOD, ONLY : HCO_GetHcoID USE HCO_STATE_MOD, ONLY : HCO_State
```

## **INPUT PARAMETERS:**

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

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object INTEGER, INTENT(INOUT) :: RC ! Failure or success
```

```
19 Dec 2013 - C. Keller - Initial version
11 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
11 Jun 2014 - R. Yantosca - Now use F90 freeform indentation
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

## 1.6.2 HcoDiagn\_Init

Subroutine HCODIAGN\_INIT initializes the three built-in HEMCO diagnostic collections: default, restart, and manual. The identification ID of each collection is written into public variable HcoDiagnIDDefault, HcoDiagnIDRestart, and HcoDiagnIDManual, respectively. Those are used to easily refer to one of the diagnostics when adding fields ('containers') to a collection or fetching it's content.

### **INTERFACE:**

```
SUBROUTINE HcoDiagn_Init( am_I_Root, HcoState, RC )
```

### **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_GetHcoID
USE HCO_STATE_MOD, ONLY : HCO_State
USE HCO_ExtList_Mod, ONLY : GetExtOpt
USE HCO_ExtList_Mod, ONLY : CoreNr
USE CHARPAK_MOD, ONLY : TRANLC
```

#### INPUT PARAMETERS:

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

## INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object INTEGER, INTENT(INOUT) :: RC ! Failure or success
```

### REVISION HISTORY:

```
03 Apr 2015 - C. Keller - Initial version
10 Apr 2015 - C. Keller - Now create diagnostics based on entries in the HEMCO diagnostics definition file.
06 Nov 2015 - C. Keller - Added OutTimeStamp.
```

# 1.6.3 Diagn\_DefineFromConfig

Subroutine Diagn\_DefineFromConfig defines HEMCO diagnostic containers as specified in the diagnostics input file.

This routine reads information from a HEMCO diagnostics definition file (specified in the main HEMCO configuration file) and creates HEMCO diagnostic containers for each entry of the diagnostics definition file. Each line of the diagnostics definition file represents a diagnostics container and is expected to consist of 7 entries: container name (character), HEMCO species (character), extension number (integer), emission category (integer), emission hierarchy (integer), space dimension (2 or 3), output unit (character).

The HEMCO setting 'DiagnFile' can be used to specify a diagnostic file. This setting should be placed in the settings section of the HEMCO configuration file.

If argument 'Add2MaplExp' is set to true, the diagnostics field defined in the diagnostics definition file are not added to the HEMCO diagnostics collection (yet), but rather added to the MAPL export state. This is useful in an ESMF environment to automate the coupling of HEMCO diagnostics, e.g. subroutine Diagn\_DefineFromConfig can be called during Set-Services to make sure that all diagnostic fields defined in DiagnFile have a corresponding Export state object (and can thus be written out via the MAPL History component).

### **INTERFACE:**

```
SUBROUTINE Diagn_DefineFromConfig( am_I_Root, HcoState, RC )
```

### **USES:**

```
USE HCO_CharTools_Mod

USE CHARPAK_Mod, ONLY : STRREPL, STRSPLIT

USE inquireMod, ONLY : findFreeLUN

USE HCO_STATE_MOD, ONLY : HCO_GetHcoID

USE HCO_STATE_MOD, ONLY : HCO_State

USE HCO_EXTLIST_MOD, ONLY : GetExtOpt
```

#### INPUT PARAMETERS:

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

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object INTEGER, INTENT(INOUT) :: RC ! Failure or success
```

# **REVISION HISTORY:**

```
10 Apr 2015 - C. Keller - Initial version
21 Feb 2016 - C. Keller - Added default diagnostics (optional)
```

# 1.6.4 Diagn\_Create

Subroutine Diagn\_Create creates a new diagnostics. This routine takes the following input arguments:

- am\_I\_Root: is this the root CPU?
- cName: distinct diagnostics (container) name.
- long\_name: long\_name attribute used for netCDF output.
- ExtNr: emissions extension number.
- Cat: emissions category.
- Hier: emissions hierarchy.
- HcoID: HEMCO species ID of diagnostics species.

- SpaceDim: spatial dimension: 1 (scalar), 2 (lon-lat), or 3 (lon-lat-lev).
- OutUnit: output unit. Emissions will be converted to this unit. Conversion factors will be determined using the HEMCO unit module (see HCO\_UNITS\_Mod.F90). No unit conversions will be performed if the argument OutOper is set (see below).
- HcoState: HEMCO state object. Used to determine the species properties if any of arguments MW\_g, EmMW\_g or MolecRatio is missing.
- OutOper: output operation for non-standard units. If this argument is used, the specified operation is performed and all unit specifications are ignored. Can be one of 'Mean', 'Sum', 'CumulSum', or 'Instantaneous'.
- AutoFill: containers with an AutoFill flag of 1 will be auto- matically updated by the HEMCO standard diagnostics calls (e.g. in hco\_calc\_mod.F90). If set to 0, the diagnostics updates have to be set manually.
- Trgt2D: 2D target array. If specified, the diagnostics array will point to this data. This disables all time averaging, unit conversions, etc., and the data will be written to disk as is.
- Trgt3D: as Trgt2D, but for 3D data.
- MW\_g: species molecular weight. Used to determine unit conversion factors. Not needed for target containers or if argument OutOper is specified. Can be omitted if HcoState is given.
- EmMW\_g: Molecular weight of emitted species. Used to determine unit conversion factors. Not needed for target containers or if argument OutOper is specified. Can be omitted if HcoState is given.
- MolecRatio: Molecules of species per emitted molecule. Used to determine unit conversion factors. Not needed for target containers or if argument OutOper is specified. Can be omitted if HcoState is given.
- ScaleFact: constant scale factor. If provided, the diagnostics are scaled uniformly by this value before outputting. Will be applied on top of any other unit conversions. Does not work on data pointers.
- cID: assigned container ID. Useful for later reference to this diagnostics container.
- RC: HEMCO return code.

```
SUBROUTINE Diagn_Create( am_I_Root, HcoState,
                                                    cName,
                                                                 &
                           ExtNr,
                                       Cat,
                                                    Hier,
                                                                 &
                                       SpaceDim,
                                                    OutUnit,
                           HcoID,
                                                                 &
                           OutOper,
                                       LevIdx,
                                                    AutoFill,
                                                                 &
                           Trgt2D,
                                       Trgt3D,
                                                    MW_g,
                           EmMW_g,
                                       MolecRatio, ScaleFact,
                                                                 &
                           cID,
                                       RC,
                                              COL, OkIfExist,
                                                                 &
                           long_name
```

#### **USES:**

```
USE HCO_State_Mod, ONLY : HCO_State

USE HCO_Unit_Mod, ONLY : HCO_Unit_GetMassScal

USE HCO_Unit_Mod, ONLY : HCO_Unit_GetAreaScal

USE HCO_Unit_Mod, ONLY : HCO_Unit_GetTimeScal
```

#### INPUT PARAMETERS:

```
:: am_I_Root
                                                            ! Root CPU?
LOGICAL.
                  INTENT(IN
                              )
TYPE(HCO_State), POINTER
                                           :: HcoState
                                                            ! HEMCO state obj.
                                           :: cName
CHARACTER(LEN=*), INTENT(IN
                                                            ! Diagnostics name
                              )
                                           :: OutUnit
CHARACTER(LEN=*), INTENT(IN
                                                            ! Output units
                                                            ! Spatial dimension
                              ), OPTIONAL :: SpaceDim
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: ExtNr
                                                            ! Extension #
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: Cat
INTEGER,
                  INTENT(IN
                                                            ! Category
                              ), OPTIONAL :: Hier
                                                            ! Hierarchy
INTEGER,
                  INTENT(IN
INTEGER,
                              ), OPTIONAL :: HcoID
                                                            ! HEMCO species ID
                  INTENT(IN
CHARACTER(LEN=*), INTENT(IN
                              ), OPTIONAL :: OutOper
                                                            ! Output operation
                              ), OPTIONAL :: LevIdx
                                                            ! Level index to use
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: AutoFill
INTEGER,
                  INTENT(IN
                                                            ! 1=fill auto.;0=don't
                              ), OPTIONAL :: Trgt2D(:,:)
                                                            ! 2D target data
REAL(sp),
                  INTENT(IN
REAL(sp),
                              ), OPTIONAL :: Trgt3D(:,:,:) ! 3D target data
                  INTENT(IN
REAL(hp),
                              ), OPTIONAL :: MW_g
                                                            ! species MW (g/mol)
                  INTENT(IN
REAL(hp),
                              ), OPTIONAL :: EmMW_g
                                                            ! emission MW (g/mol)
                  INTENT(IN
REAL(hp),
                  INTENT(IN
                              ), OPTIONAL :: MolecRatio
                                                            ! molec. emission ratio
REAL(hp),
                              ), OPTIONAL :: ScaleFact
                                                            ! uniform scale factor
                  INTENT(IN
                              ), OPTIONAL :: COL
                                                            ! Collection number
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: cID
                                                            ! Container ID
INTEGER,
                  INTENT(IN
                  INTENT(IN
                              ), OPTIONAL :: OkIfExist
                                                            ! Is it ok if already exists?
LOGICAL,
                              ), OPTIONAL :: long_name
CHARACTER(LEN=*), INTENT(IN
                                                            ! long name attribute
```

# INPUT/OUTPUT PARAMETERS:

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

#### REVISION HISTORY:

```
19 Dec 2013 - C. Keller - Initialization
05 Mar 2015 - C. Keller - container ID can now be set by the user
31 Mar 2015 - C. Keller - added argument OkIfExist
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 1.6.5 Diagn\_UpdateSp0d

Subroutine Diagn\_UpdateSp0d is the wrapper routine to update the diagnostics for single precision scalar values. It invokes the main diagnostics update routine with the appropriate arguments.

```
SUBROUTINE Diagn_UpdateSpOd( am_I_Root, HcoState, cID, cName, ExtNr, & Cat, Hier, HcoID, AutoFill, & Scalar, Total, PosOnly, COL, & MinDiagnLev, RC )
```

## **INPUT PARAMETERS:**

```
LOGICAL,
                                           :: am_I_Root
                                                             ! Root CPU?
                  INTENT(IN
                              )
TYPE(HCO_State),
                                                              ! HEMCO state obj
                  POINTER
                                           :: HcoState
                                                             ! Assigned
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: cID
                                                             ! container ID
CHARACTER(LEN=*), INTENT(IN
                                                             ! Diagnostics
                              ), OPTIONAL :: cName
                                                                name
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: ExtNr
                                                              ! Extension #
                              ), OPTIONAL :: Cat
INTEGER,
                                                              ! Category
                  INTENT(IN
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: Hier
                                                             ! Hierarchy
                              ), OPTIONAL :: HcoID
INTEGER,
                  INTENT(IN
                                                             ! HEMCO species
                                                              ! ID number
                              ), OPTIONAL :: AutoFill
                                                              ! 1=yes; 0=no;
INTEGER,
                  INTENT(IN
                                                              ! -1=either
REAL(sp),
                                           :: Scalar
                                                             ! OD scalar
                  INTENT(IN
REAL(sp),
                  INTENT(IN
                              ), OPTIONAL :: Total
                                                             ! Total
                              ), OPTIONAL :: PosOnly
LOGICAL,
                  INTENT(IN
                                                             ! Use only vals
                                                             ! >= 0?
                              ), OPTIONAL :: COL
                                                             ! Collection Nr.
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: MinDiagnLev
                                                             ! minimum diagn level
INTEGER,
                  INTENT(IN
```

# INPUT/OUTPUT PARAMETERS:

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

### **REVISION HISTORY:**

```
20 Apr 2015 - C. Keller - Initialization
19 Sep 2016 - R. Yantosca - Rewritten for Gfortran: remove Scalar and
Array3d (put those in other overloaded methods)
```

# 1.6.6 Diagn\_UpdateSp2d

Subroutine Diagn\_UpdateSp2d is the wrapper routine to update the diagnostics for single precision 2-D arrays. It invokes the main diagnostics update routine with the appropriate arguments.

```
SUBROUTINE Diagn_UpdateSp2d( am_I_Root, HcoState, cID, cName, ExtNr, & Cat, Hier, HcoID, AutoFill, & Array2D, Total, PosOnly, COL, & MinDiagnLev, RC )
```

### INPUT PARAMETERS:

```
INTENT(IN
                                           :: am_I_Root
                                                              ! Root CPU?
LOGICAL,
TYPE(HCO_State),
                                           :: HcoState
                                                              ! HEMCO state obj
                  POINTER
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: cID
                                                              ! Assigned
                                                                container ID
CHARACTER(LEN=*), INTENT(IN
                              ), OPTIONAL :: cName
                                                             ! Diagnostics
                                                                name
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: ExtNr
                                                             ! Extension #
                                                              ! Category
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: Cat
                              ), OPTIONAL :: Hier
                                                             ! Hierarchy
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: HcoID
                                                             ! HEMCO species
INTEGER,
                  INTENT(IN
                                                              ! ID number
                              ), OPTIONAL :: AutoFill
                                                              ! 1=yes; 0=no;
INTEGER,
                  INTENT(IN
                                                              ! -1=either
REAL(sp),
                                           :: Array2D(:,:)
                                                              ! 2D array
                  INTENT(IN
                              ), OPTIONAL :: Total
REAL(sp),
                  INTENT(IN
                                                              ! Total
LOGICAL,
                  INTENT(IN
                              ), OPTIONAL :: PosOnly
                                                              ! Use only vals
                                                                >= 0?
                  INTENT(IN
                              ), OPTIONAL :: COL
                                                              ! Collection Nr.
INTEGER,
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: MinDiagnLev
                                                              ! minimum diagn level
```

### INPUT/OUTPUT PARAMETERS:

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

### **REVISION HISTORY:**

```
20 Apr 2015 - C. Keller - Initialization
19 Sep 2016 - R. Yantosca - Rewritten for Gfortran: remove Scalar and
Array3d (put those in other overloaded methods)
```

## 1.6.7 Diagn\_UpdateSp3d

Subroutine Diagn\_UpdateSp is the wrapper routine to update the diagnostics for single precision 3-D arrays. It invokes the main diagnostics update routine with the appropriate arguments.

## **INTERFACE:**

```
SUBROUTINE Diagn_UpdateSp3d( am_I_Root, HcoState, cID, cName, ExtNr, & Cat, Hier, HcoID, AutoFill, & Array3D, Total, PosOnly, COL, & MinDiagnLev, RC )
```

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

TYPE(HCO_State), POINTER :: HcoState ! HEMCO state obj

INTEGER, INTENT(IN ), OPTIONAL :: cID ! Assigned
```

```
! container ID
CHARACTER(LEN=*), INTENT(IN
                               ), OPTIONAL :: cName
                                                              ! Diagnostics
                                                                 name
                               ), OPTIONAL :: ExtNr
                                                              ! Extension #
INTEGER,
                  INTENT(IN
INTEGER,
                  INTENT(IN
                               ), OPTIONAL :: Cat
                                                              ! Category
INTEGER,
                               ), OPTIONAL :: Hier
                                                              ! Hierarchy
                  INTENT(IN
                               ), OPTIONAL :: HcoID
                                                              ! HEMCO species
INTEGER,
                  INTENT(IN
                                                              ! ID number
INTEGER,
                  INTENT(IN
                               ), OPTIONAL :: AutoFill
                                                              ! 1=ves; 0=no;
                                                              ! -1=either
REAL(sp),
                                           :: Array3D(:,:,:) ! 3D array
                  INTENT(IN
REAL(sp),
                               ), OPTIONAL :: Total
                                                              ! Total
                  INTENT(IN
LOGICAL,
                               ), OPTIONAL :: PosOnly
                                                              ! Use only vals
                  INTENT(IN
                                                              ! >= 0?
                  INTENT(IN
                               ), OPTIONAL :: COL
                                                              ! Collection Nr.
INTEGER,
                               ), OPTIONAL :: MinDiagnLev
                                                              ! minimum diagn level
INTEGER,
                  INTENT(IN
```

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

### **REVISION HISTORY:**

```
20 Apr 2015 - C. Keller - Initialization
19 Sep 2016 - R. Yantosca - Rewritten for Gfortran: remove Scalar and
Array2d (put those in other overloaded methods)
```

## 1.6.8 Diagn\_UpdateDp0d

Subroutine Diagn\_UpdateSp0d is the wrapper routine to update the diagnostics for double-precision scalar values. It invokes the main diagnostics update routine with the appropriate arguments.

#### **INTERFACE:**

```
SUBROUTINE Diagn_UpdateDpOd( am_I_Root, HcoState, cID, cName, ExtNr, & Cat, Hier, HcoID, AutoFill, & Scalar, Total, PosOnly, COL, & MinDiagnLev, RC )
```

```
INTENT(IN
                                           :: am_I_Root
                                                              ! Root CPU?
LOGICAL,
                                                              ! HEMCO state obj
TYPE(HCO_State),
                  POINTER
                                           :: HcoState
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: cID
                                                              ! Assigned
                                                              ! container ID
CHARACTER(LEN=*), INTENT(IN
                              ), OPTIONAL :: cName
                                                              ! Diagnostics
                                                                name
                              ), OPTIONAL :: ExtNr
                                                              ! Extension #
INTEGER,
                  INTENT(IN
```

```
INTEGER,
                  INTENT(IN
                               ), OPTIONAL :: Cat
                                                              ! Category
INTEGER,
                  INTENT(IN
                               ), OPTIONAL :: Hier
                                                              ! Hierarchy
                              ), OPTIONAL :: HcoID
                                                              ! HEMCO species
INTEGER,
                  INTENT(IN
                                                              ! ID number
INTEGER,
                  INTENT(IN
                               ), OPTIONAL :: AutoFill
                                                              ! 1=yes; 0=no;
                                                              ! -1=either
REAL(dp),
                                                              ! 1D scalar
                  INTENT(IN
                                           :: Scalar
REAL(dp),
                  INTENT(IN
                               ), OPTIONAL :: Total
                                                              ! Total
                               ), OPTIONAL :: PosOnly
LOGICAL,
                  INTENT(IN
                                                              ! Use only vals
                                                                 >= 0?
                               ), OPTIONAL :: COL
INTEGER,
                  INTENT(IN
                                                              ! Collection Nr.
INTEGER,
                  INTENT(IN
                               ), OPTIONAL :: MinDiagnLev
                                                              ! minimum diagn level
```

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

### **REVISION HISTORY:**

```
20 Apr 2015 - C. Keller - Initialization

19 Sep 2016 - R. Yantosca - Rewritten for Gfortran: remove Array2d and
Array3d (put those in other overloaded methods)
```

# 1.6.9 Diagn\_UpdateDp2d

Subroutine Diagn\_UpdateSp2d is the wrapper routine to update the diagnostics for single precision 2D arrays. It invokes the main diagnostics update routine with the appropriate arguments.

### **INTERFACE:**

```
SUBROUTINE Diagn_UpdateDp2d( am_I_Root, HcoState, cID, cName, ExtNr, & Cat, Hier, HcoID, AutoFill, & Array2D, Total, PosOnly, COL, & MinDiagnLev, RC
```

```
:: am_I_Root
LOGICAL,
                  INTENT(IN
                              )
                                                              ! Root CPU?
TYPE(HCO_State),
                                           :: HcoState
                                                              ! HEMCO state obj
                  POINTER
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: cID
                                                              ! Assigned
                                                                 container ID
CHARACTER(LEN=*), INTENT(IN
                              ), OPTIONAL :: cName
                                                              ! Diagnostics
                                                              ! name
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: ExtNr
                                                              ! Extension #
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: Cat
                                                              ! Category
INTEGER,
                              ), OPTIONAL :: Hier
                  INTENT(IN
                                                              ! Hierarchy
                              ), OPTIONAL :: HcoID
                                                              ! HEMCO species
INTEGER,
                  INTENT(IN
                                                              ! ID number
```

```
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: AutoFill
                                                              ! 1=yes; 0=no;
                                                              ! -1=either
REAL(dp),
                                           :: Array2D(:,:)
                                                             ! 2D array
                  INTENT(IN
REAL(dp),
                  INTENT(IN
                              ), OPTIONAL :: Total
                                                              ! Total
LOGICAL,
                  INTENT(IN
                              ), OPTIONAL :: PosOnly
                                                             ! Use only vals
                                                              ! >= 0?
                              ), OPTIONAL :: COL
                                                             ! Collection Nr.
INTEGER,
                  INTENT(IN
                                                              ! minimum diagn level
                              ), OPTIONAL :: MinDiagnLev
INTEGER,
                  INTENT(IN
```

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

### REVISION HISTORY:

```
20 Apr 2015 - C. Keller - Initialization
19 Sep 2016 - R. Yantosca - Rewritten for Gfortran: remove Scalar and
Array3d (put those in other overloaded methods)
```

# 1.6.10 Diagn\_UpdateDp3d

Subroutine Diagn\_UpdateSp3d is the wrapper routine to update the diagnostics for single precision arrays. It invokes the main diagnostics update routine with the appropriate arguments.

#### **INTERFACE:**

```
SUBROUTINE Diagn_UpdateDp3d( am_I_Root, HcoState, cID, cName, ExtNr, & Cat, Hier, HcoID, AutoFill, & Array3D, Total, PosOnly, COL, & MinDiagnLev, RC
```

## **USES:**

```
USE HCO_State_Mod, ONLY : HCO_State
```

```
)
                                           :: am_I_Root
                                                             ! Root CPU?
LOGICAL,
                  INTENT(IN
TYPE(HCO_State),
                  POINTER
                                           :: HcoState
                                                             ! HEMCO state obj
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: cID
                                                             ! Assigned
                                                             ! container ID
CHARACTER(LEN=*), INTENT(IN
                              ), OPTIONAL :: cName
                                                             ! Diagnostics
                                                             ! name
                                                             ! Extension #
INTEGER,
                              ), OPTIONAL :: ExtNr
                  INTENT(IN
                              ), OPTIONAL :: Cat
                                                             ! Category
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: Hier
                                                             ! Hierarchy
INTEGER,
                  INTENT(IN
                              ), OPTIONAL :: HcoID
                                                             ! HEMCO species
INTEGER,
                  INTENT(IN
                                                             ! ID number
                  INTENT(IN
                              ), OPTIONAL :: AutoFill
                                                             ! 1=yes; 0=no;
INTEGER,
```

```
! -1=either
REAL(dp),
                               )
                                            :: Array3D(:,:,:) ! 3D array
                   INTENT(IN
REAL(dp),
                   INTENT(IN
                               ), OPTIONAL :: Total
                                                               ! Total
                   INTENT(IN
LOGICAL,
                               ), OPTIONAL :: PosOnly
                                                               ! Use only vals
                                                                  >= 0?
                               ), OPTIONAL :: COL
INTEGER,
                   INTENT(IN
                                                               ! Collection Nr.
                               ), OPTIONAL :: MinDiagnLev
INTEGER,
                  INTENT(IN
                                                               ! minimum diagn level
```

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

#### REVISION HISTORY:

```
20 Apr 2015 - C. Keller - Initialization

19 Sep 2016 - R. Yantosca - Rewritten for Gfortran: remove Scalar and

Array2d (put those in other overloaded methods)
```

## 1.6.11 Diagn\_UpdateDriver

Subroutine Diagn\_UpdateDriver updates the content of a diagnostics container. The container to be updated is determined from the passed variables. If a valid (i.e. positive) container ID is provided, this container is used. Otherwise, if a valid HEMCO species ID (HcoID) is provided, all containers with the same combination of HcoID, extension number (ExtNr), emission category (Cat) and hierarchy (Hier) are updated. If no valid HcoID and no valid cID is given, the container name has to be provided. The passed data array (Scalar, Array2D, or Array3D) needs to match the spatial dimension of the given container. For 2D diagnostics, a 3D array can be passed, in which case the level index specified during initialization ('LevIdx') is used. If LevIdx is set to -1, the column sum is used (default).

If no matching container is found, the subroutine leaves with no error. This allows automatic diagnostics generation, e.g. of intermediate emission fields created in HCO\_CALC\_Mod.F90.

The optional input argument 'MinDiagnLev' determines how 'deep' this routine will search for diagnostics with matching HcoID, ExtNr, etc. For example, if a HcoID, an ExtNr, and a category is provided, HEMCO by default will only update diagnostics containers with exactly the same HcoID, ExtNr, and category - but not diagnostics of 'lower level', e.g. with the same HcoID and ExtNr but no assigned category. This behavior can be changed by explicitly setting MinDiagnLev to the minimum diagnostics level. In the given example, setting MinDiagnLev to 1 would also update level 1 and level 2 diagnostics of the same HcoID (e.g. diagnostics with the same HcoID and no assigned ExtNr and category; as well as diagnostics with the same HcoID and ExtNr and no assigned category).

### Notes:

• For a given time step, the same diagnostics container can be updated multiple times. The field average is always defined as temporal average, e.g. multiple updates on the same time step will not increase the averaging weight of that time step.

- If the passed array is empty (i.e. not associated), it is treated as empty values (i.e. zeros).
- The collection number can be set to -1 to scan trough all existing diagnostic collections.

### INTERFACE:

```
SUBROUTINE Diagn_UpdateDriver(am_I_Root, HcoState,
                                                       cID,
                                                                    cName,
                                                                                 &
                                ExtNr,
                                           Cat,
                                                       Hier,
                                                                   HcoID,
                                                                                 &
                                AutoFill,
                                           Scalar,
                                                       Array2D,
                                                                    Array3D,
                               Total,
                                           Scalar_SP,
                                                       Array2D_SP, Array3D_SP,
                               Total_SP, Scalar_HP,
                                                       Array2D_HP, Array3D_HP, &
                               Total_HP, PosOnly,
                                                       COL,
                                                                   MinDiagnLev, &
                               RC
                                                                                  )
```

### **USES:**

USE HCO\_Arr\_Mod, ONLY : HCO\_ArrAssert

#### **INPUT PARAMETERS:**

```
LOGICAL,
                  INTENT(IN
                               )
                                                    :: am_I_Root
                                                                          ! Root CPU?
TYPE(HCO_State),
                                                    :: HcoState
                                                                          ! HEMCO state obj
                  POINTER
                               ), OPTIONAL
INTEGER,
                  INTENT(IN
                                                    :: cID
                                                                          ! container ID
CHARACTER(LEN=*), INTENT(IN
                               ), OPTIONAL
                                                    :: cName
                                                                          ! Dgn name
                               ), OPTIONAL
                                                    :: ExtNr
                                                                          ! Extension #
INTEGER,
                  INTENT(IN
INTEGER,
                  INTENT(IN
                               ), OPTIONAL
                                                    :: Cat
                                                                          ! Category
                               ), OPTIONAL
                                                    :: Hier
                                                                          ! Hierarchy
INTEGER,
                  INTENT(IN
                               ), OPTIONAL
INTEGER,
                  INTENT(IN
                                                    :: HcoID
                                                                          ! HEMCO species ID
                               ), OPTIONAL
                                                                          ! 1=yes; 0=no;
INTEGER,
                  INTENT(IN
                                                    :: AutoFill
                                                                          ! -1=either
REAL(dp),
                  INTENT(IN
                               ), OPTIONAL
                                                    :: Scalar
                                                                          ! 1D scalar
REAL(dp),
                  INTENT(IN
                               ), OPTIONAL, TARGET :: Array2D
                                                                  (:,:)
                                                                          ! 2D array
REAL(dp),
                               ), OPTIONAL, TARGET :: Array3D
                                                                  (:,:,:) ! 3D array
                  INTENT(IN
REAL(dp),
                  INTENT(IN
                               ), OPTIONAL
                                                    :: Total
                                                                          ! Total
REAL(sp),
                               ), OPTIONAL
                                                    :: Scalar_SP
                  INTENT(IN
                                                                          ! 1D scalar
REAL(sp),
                               ), OPTIONAL, TARGET :: Array2D_SP(:,:)
                  INTENT(IN
                                                                          ! 2D array
                               ), OPTIONAL, TARGET :: Array3D_SP(:,:,:) ! 3D array
REAL(sp),
                  INTENT(IN
REAL(sp),
                               ), OPTIONAL
                                                    :: Total_SP
                                                                          ! Total
                  INTENT(IN
REAL(hp),
                  INTENT(IN
                               ), OPTIONAL
                                                    :: Scalar_HP
                                                                          ! 1D scalar
REAL(hp),
                               ), OPTIONAL, TARGET :: Array2D_HP(:,:)
                                                                          ! 2D array
                  INTENT(IN
REAL(hp),
                               ), OPTIONAL, TARGET :: Array3D_HP(:,:,:) ! 3D array
                  INTENT(IN
REAL(hp),
                               ), OPTIONAL
                                                    :: Total_HP
                                                                          ! Total
                  INTENT(IN
                               ), OPTIONAL
                                                    :: PosOnly
LOGICAL,
                  INTENT(IN
                                                                          ! Use only vals
                                                                          ! >= 0?
                               ), OPTIONAL
                                                    :: COL
                                                                          ! Collection Nr.
INTEGER,
                  INTENT(IN
                               ), OPTIONAL
                                                    :: MinDiagnLev
INTEGER,
                  INTENT(IN
                                                                          ! Collection Nr.
```

## INPUT/OUTPUT PARAMETERS:

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

## **REVISION HISTORY:**

```
19 Dec 2013 - C. Keller - Initialization
25 Sep 2014 - C. Keller - Now allow updating multiple diagnostics
11 Mar 2015 - C. Keller - Now allow scanning of all diagnostic collections
13 Mar 2015 - C. Keller - Bug fix: only prompt warning if it's a new timestep
17 Jun 2015 - C. Keller - Added argument MinDiagnLev
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 1.6.12 Diagn\_Get

Subroutine Diagn\_Get returns a diagnostics container from the diagnostics list, with the data converted to the output unit specified during initialization. Only diagnostics that contain data, i.e. with an update counter higher than zero, are returned. If EndOfIntvOnly is set to TRUE, only containers at the end of their time averaging interval are returned. The current HEMCO time will be used to determine which containers are at the end of their interval. The IsOutFormat flag of the container is set to true, making sure that the currently saved data will be erased during the next update (Diagn\_Update).

If DgnCont is already associated, the search continues from the container next to DgnCont. If DgnCont is empty (null), the search starts from the first container of the diagnostics list ListDiagn. If the optional attribute cName or cID is provided, this particular container is searched (through the entire diagnostics list), but is only returned if it is at the end of it's interval or if EndOfIntvOnly is disabled.

The optional argument InclManual denotes whether or not containers with a manual update frequency shall be considered. This argument is only valid if EndOfIntvOnly is set to FALSE.

The return flag FLAG is set to HCO\_SUCCESS if a container is found, and to HCO\_FAIL otherwise.

### INTERFACE:

```
SUBROUTINE Diagn_Get( am_I_Root, HcoState, & EndOfIntvOnly, DgnCont, & FLAG, RC, cName, & cID, AutoFill, COL, & SkipZeroCount
```

#### **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_State
```

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

TYPE(HCO_State), POINTER :: HcoState ! HEMCO state obj

LOGICAL, INTENT(IN ) :: EndOfIntvOnly ! End of
```

```
! interval
                                                            ! only?
    CHARACTER(LEN=*), INTENT(IN ), OPTIONAL :: cName
                                                            ! container name
    INTEGER,
                    INTENT(IN ), OPTIONAL :: cID
                                                           ! container ID
                                                          ! 0=no; 1=yes;
    INTEGER,
                    INTENT(IN ), OPTIONAL :: AutoFill
                                                            ! -1=either
                    INTENT(IN ), OPTIONAL :: COL
                                                            ! Collection Nr.
    INTEGER,
                     INTENT(IN ), OPTIONAL :: SkipZeroCount ! Skip if counter
    LOGICAL,
                                                            ! is zero
OUTPUT PARAMETERS:
    TYPE(DiagnCont), POINTER
                                           :: DgnCont
                                                            ! Return
                                                            ! container
INPUT/OUTPUT PARAMETERS:
    INTEGER,
                     INTENT(INOUT)
                                                            ! Return flag
                                          :: FLAG
    INTEGER,
                     INTENT(INOUT)
                                          :: RC
                                                            ! Return code
REVISION HISTORY:
   19 Dec 2013 - C. Keller: Initialization
   26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
1.6.13 Diagn_TotalGet
Subroutine Diagn_TotalGet returns the total of a given diagnostics container.
INTERFACE:
  SUBROUTINE Diagn_TotalGet( am_I_Root, Diagn, cName, cID,
                                                         COL, &
                           FOUND,
                                  Total, Reset, RC
INPUT PARAMETERS:
                                          :: am_I_Root
                                                           ! Root CPU?
    LOGICAL.
                     INTENT(IN
    TYPE(DiagnBundle), POINTER
                                           :: Diagn
                                                          ! Diagn bundle obj
                                ), OPTIONAL :: cName
    CHARACTER(LEN=*), INTENT(IN
                                                          ! container name
                    INTENT(IN ), OPTIONAL :: cID
                                                          ! container ID
    INTEGER,
    INTEGER,
                    INTENT(IN ), OPTIONAL :: COL
                                                          ! Collection Nr.
                    INTENT(IN ), OPTIONAL :: Reset
                                                           ! Reset total?
    LOGICAL,
OUTPUT PARAMETERS:
    LOGICAL,
                    INTENT( OUT), OPTIONAL :: FOUND
                                                         ! Container found
    REAL(sp),
                     INTENT( OUT)
                                      :: Total
                                                           ! Container total
INPUT/OUTPUT PARAMETERS:
                     INTENT(INOUT)
                                  :: RC ! Return code
    INTEGER,
REVISION HISTORY:
   15 Mar 2015 - C. Keller: Initialization
   26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

## 1.6.14 DiagnList\_Cleanup

Subroutine DiagnList\_Cleanup cleans up all the diagnostics containers of the given diagnostics list.

## **INTERFACE:**

```
SUBROUTINE DiagnList_Cleanup ( DiagnList )
```

#### INPUT PARAMETERS:

```
TYPE(DiagnCont), POINTER :: DiagnList ! List to be removed
```

#### REVISION HISTORY:

```
19 Dec 2013 - C. Keller - Initialization
25 Jan 2016 - R. Yantosca - Bug fix for pgfortran compiler: Test if the
TMPCONT object is associated before deallocating
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

### 1.6.15 Diagn\_AutoFillLevelDefined

Function Diagn\_AutoFillLevelDefined returns .TRUE. if there is at least one AutoFill diagnostics container defined for the given level (1=Species level, 2=ExtNr level, 3=Category level, 4=Hierarchy level).

### **INTERFACE:**

```
FUNCTION Diagn_AutoFillLevelDefined( Diagn, Level, COL ) RESULT ( IsDefined )
```

## **INPUT PARAMETERS:**

```
TYPE(DiagnBundle),POINTER :: Diagn ! Diagn bundle obj
INTEGER, INTENT(IN) :: Level ! Level of interest
INTEGER, INTENT(IN), OPTIONAL :: COL ! Collection Nr.
```

#### RETURN VALUE:

```
LOGICAL :: IsDefined ! Return argument
```

#### REVISION HISTORY:

```
19 Dec 2013 - C. Keller: Initialization
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

## 1.6.16 DiagnCollection\_Get

Subroutine DiagnCollection\_Get returns variables assigned to a given diagnostic collection.

```
SUBROUTINE DiagnCollection_Get( Diagn,
                                                  COL,
                                   InUse,
                                                  Prefix,
                                   nnDiagn,
                                                  DeltaYMD,
                                                  DeltaHMS, LastHMS, &
                                   LastYMD,
                                   OutTimeStamp, RC
   !INPUT ARGUMENTS:
                       INTENT(IN), OPTIONAL :: COL    ! Collection Nr.
     INTEGER,
OUTPUT PARAMETERS:
     TYPE(DiagnBundle), POINTER
                                             :: Diagn
                       INTENT(OUT), OPTIONAL :: InUse
     LOGICAL,
     CHARACTER(LEN=*), INTENT(OUT), OPTIONAL :: Prefix
     INTEGER,
                      INTENT(OUT), OPTIONAL :: nnDiagn
                    INTENT(OUT), OPTIONAL :: DeltaYMD
INTENT(OUT), OPTIONAL :: LastYMD
INTENT(OUT), OPTIONAL :: DeltaHMS
INTENT(OUT), OPTIONAL :: LastHMS
     INTEGER,
     INTEGER,
     INTEGER,
                       INTENT(OUT), OPTIONAL :: LastHMS
     INTEGER,
     INTEGER,
                       INTENT(OUT), OPTIONAL :: OutTimeStamp
INPUT/OUTPUT PARAMETERS:
                       INTENT(INOUT)
                                      :: RC
     INTEGER,
REVISION HISTORY:
    19 Dec 2013 - C. Keller: Initialization
    26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
1.6.17 DiagnCollection_Set
Subroutine DiagnCollection_Set sets variables assigned to a given diagnostic collection.
INTERFACE:
  SUBROUTINE DiagnCollection_Set( Diagn, COL, InUse, LastYMD, LastHMS, RC )
   !INPUT ARGUMENTS:
     TYPE(DiagnBundle), POINTER
                                             :: Diagn ! Diagn bundle
                       INTENT(IN), OPTIONAL :: COL    ! Collection Nr.
     INTEGER,
OUTPUT PARAMETERS:
     LOGICAL,
                       INTENT(OUT), OPTIONAL :: InUse
                       INTENT(IN ), OPTIONAL :: LastYMD
     INTEGER,
                       INTENT(IN ), OPTIONAL :: LastHMS
     INTEGER,
INPUT/OUTPUT PARAMETERS:
                       INTENT(INOUT)
                                      :: RC
     INTEGER.
REVISION HISTORY:
```

REVISION HISTORY:

19 Dec 2013 - C. Keller: Initialization

26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts

## 1.6.18 DiagnCont\_Init

Subroutine DiagnCont\_Init initializes a new (blank) diagnostics container DgnCont.

### **INTERFACE:**

```
SUBROUTINE DiagnCont_Init( OutCont )
```

#### **OUTPUT PARAMETERS:**

```
TYPE(DiagnCont), POINTER :: OutCont ! Created container
```

### **REVISION HISTORY:**

```
19 Dec 2013 - C. Keller: Initialization
```

## 1.6.19 DiagnCont\_Cleanup

Subroutine DiagnCont\_Cleanup cleans up diagnostics container DgnCont.

#### **INTERFACE:**

```
SUBROUTINE DiagnCont_Cleanup( DgnCont )
```

### **USES:**

```
USE HCO_ARR_Mod, ONLY : HCO_ArrCleanup
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(DiagnCont), POINTER :: DgnCont ! Container to be cleaned
```

### **REVISION HISTORY:**

```
19 Dec 2013 - C. Keller: Initialization
```

## 1.6.20 DiagnCont\_PrepareOutput

Subroutine DiagnCont\_PrepareOutput converts the data of the given diagnostics container to proper output units.

## **INTERFACE:**

```
SUBROUTINE DiagnCont_PrepareOutput (am_I_Root, HcoState, DgnCont, RC)
```

### **USES:**

```
USE HCO_State_Mod, ONLY : HCO_State
USE HCO_Arr_Mod, ONLY : HCO_ArrAssert
```

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

TYPE(HCO_State), POINTER :: HcoState ! HEMCO state obj
```

```
TYPE(DiagnCont), POINTER :: DgnCont ! diagnostics container INTEGER, INTENT(INOUT) :: RC ! Return code
```

### **REVISION HISTORY:**

```
19 Dec 2013 - C. Keller: Initialization
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

## 1.6.21 DiagnCont\_Find

Subroutine DiagnCont\_Find searches for a diagnostics container in ListDiagn. If a valid container ID (¿0) is given, the container with this ID is searched. Otherwise, if a valid HEMCO specied ID (¿0) is given, the container with the same combination of HcoID, extension number (ExtNr), and emission category (Cat) and hierarchy (Hier), is searched. If no valid HcoID and no valid cID is provided, the container with the given container name is searched.

If the optional resume flag is set to TRUE, search will resume after OutCnt. If OutCnt is not associated or resume flag is FALSE, search starts at the beginning of the diagnostics list.

This subroutine does return the diagnostics as is, i.e. in the internal units. It should NOT be used to access the content of a diagnostics but is rather intended to be used in the background, e.g. to check if a diagnostics exists at all. To get the values of a diagnostics, use routine Diagn\_Get. INTERFACE:

```
SUBROUTINE DiagnCont_Find ( Diagn, cID, ExtNr, Cat, Hier, HcoID, & cName, AutoFill, FOUND, OutCnt, Resume, COL )
```

### INPUT PARAMETERS:

```
TYPE(DiagnBundle), POINTEr
                                 :: Diagn
                                              ! diagn bundle
INTEGER,
                   INTENT(IN)
                                 :: cID
                                              ! wanted cont. ID
INTEGER,
                   INTENT(IN)
                                 :: ExtNr
                                              ! wanted ExtNr
INTEGER,
                                              ! wanted category
                   INTENT(IN)
                                 :: Cat
                                 :: Hier
                                              ! wanted hierarchy
INTEGER,
                   INTENT(IN)
                                 :: HcoID
                                              ! wanted spec. ID
INTEGER,
                   INTENT(IN)
CHARACTER(LEN=*),
                                              ! wanted name
                   INTENT(IN)
                                 :: cName
INTEGER,
                                 :: AutoFill ! O=no; 1=yes; -1=either
                    INTENT(IN)
LOGICAL, OPTIONAL, INTENT(IN)
                                              ! Resume at OutCnt?
                                 :: Resume
INTEGER, OPTIONAL, INTENT(IN)
                                 :: COL
                                              ! Collection number
```

## **OUTPUT PARAMETERS:**

```
LOGICAL, INTENT(OUT) :: FOUND ! container found?
```

### INPUT/OUTPUT PARAMETERS:

```
TYPE(DiagnCont), POINTER :: OutCnt ! data container
```

### **REVISION HISTORY:**

```
19 Dec 2013 - C. Keller: Initialization
25 Sep 2014 - C. Keller: Added Resume flag
09 Apr 2015 - C. Keller: Can now search all collections
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

## 1.6.22 DiagnCont\_Link\_2D

Subroutine DiagnCont\_Link\_2D links the data of container DgnCont to the 2D array Tgt2D. This will disable all time averaging, unit conversion, etc., i.e. the data will be returned as is.

#### **INTERFACE:**

```
SUBROUTINE DiagnCont_Link_2D( am_I_Root, DgnCont, ThisColl, Trgt2D, RC, HcoState ) USES:
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(DiagnCont), POINTER :: DgnCont ! diagnostics container INTEGER, INTENT(INOUT) :: RC ! Return code
```

### REVISION HISTORY:

```
19 Dec 2013 - C. Keller: Initialization
```

## 1.6.23 DiagnCont\_Link\_3D

Subroutine DiagnCont\_Link\_3D links the data of container DgnCont to the 3D array Tgt3D. This will disable all time averaging, unit conversion, etc., i.e. the data will be returned as is.

```
SUBROUTINE DiagnCont_Link_3D( am_I_Root, DgnCont, ThisColl, Trgt3D, RC, HcoState )
USES:
```

```
USE HCO_State_Mod, ONLY : HCO_State
!INPUT PARAEMTERS:
                                             :: am_I_Root
                                                              ! Root CPU?
 LOGICAL,
                        INTENT(IN
                                   )
 TYPE (HCO_STATE),
                        POINTER, OPTIONAL
                                            :: HcoState
                                                            ! HEMCO state obj
 REAL(sp),
                        INTENT(IN
                                   ), TARGET :: Trgt3D(:,:,:) ! 3D target data
 TYPE(DiagnCollection), POINTER
                                             :: ThisColl ! Collection
```

```
TYPE(DiagnCont), POINTER :: DgnCont ! diagnostics ! container INTEGER, INTENT(INOUT) :: RC ! Return code
```

#### REVISION HISTORY:

```
19 Dec 2013 - C. Keller: Initialization
```

## 1.6.24 Diagn\_Print

Subroutine Diagn\_Print displays the content of the passed diagnostics container.

#### **INTERFACE:**

```
SUBROUTINE Diagn_Print ( HcoState, Dgn, VerbNr )
```

### **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_STATE
!INPUT ARGUMENTS:
TYPE(HCO_STATE), POINTER :: HcoState
TYPE(DiagnCont), POINTER :: Dgn
INTEGER, INTENT(IN) :: VerbNr
```

## **REVISION HISTORY:**

```
01 Aug 2014 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

## 1.6.25 DiagnCollection\_Create

Subroutine DiagnCollection\_Create creates a new diagnostics collection at position COL. The class arguments are set as specified by the input arguments.

If the given position is already occupied, the routine returns an error if the input argument do not match with the corresponding arguments of the diagnostics class at that position.

### **INTERFACE:**

```
SUBROUTINE DiagnCollection_Create ( am_I_Root, Diagn, NX, NY, NZ, & TS, AM2, PREFIX, & deltaYMD, deltaHMS, OutTimeStamp, & RC, COL, HcoState)
```

### **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_STATE
!INPUT ARGUMENTS:
                                                         ! Root CPU?
 LOGICAL,
                     INTENT(IN)
                                          :: am_I_Root
 TYPE(DiagnBundle), POINTER
                                                         ! Diagn bundle
                                          :: Diagn
 INTEGER,
                     INTENT(IN)
                                          :: NX
                                                         ! # of lons
 INTEGER,
                     INTENT(IN)
                                                         ! # of lats
                                          :: NY
                                                         ! # of levels
 INTEGER,
                     INTENT(IN)
                                         :: NZ
                                                         ! timestep [s]
 REAL(sp),
                     INTENT(IN)
                                          :: TS
 REAL(hp),
                                                         ! grid box areas [m2]
                     POINTER
                                         :: AM2(:,:)
 CHARACTER(LEN=*),
                     INTENT(IN)
                                         :: PREFIX
                                                         ! Output prefix
                                                         ! Output frequency
 INTEGER,
                     INTENT(IN), OPTIONAL :: deltaYMD
                     INTENT(IN), OPTIONAL :: deltaHMS
                                                         ! Output frequency
 INTEGER,
                     INTENT(IN), OPTIONAL :: OutTimeStamp ! Output time stamp
 INTEGER,
                                OPTIONAL :: HcoState
                                                         ! HEMCO state obj
 TYPE(HCO_State),
                     POINTER,
!OUTPUT ARGUMENTS:
                     INTENT( OUT)
                                                      ! Collection Nr.
 INTEGER,
                                       :: COL
!INPUT/OUTPUT ARGUMENTS:
                     INTENT(INOUT) :: RC ! Return code
 INTEGER,
```

#### REVISION HISTORY:

```
08 Jan 2015 - C. Keller - Initial version
06 Nov 2015 - C. Keller - Added OutTimeStamp.
```

# 1.6.26 DiagnCollection\_Cleanup

Subroutine DiagnCollection\_Cleanup cleans up the diagnostics collection for collection COL.

### **INTERFACE:**

```
SUBROUTINE DiagnCollection_Cleanup ( Diagn )
!INPUT ARGUMENTS:
   TYPE(DiagnBundle), POINTER :: Diagn
```

#### REVISION HISTORY:

```
08 Jan 2015 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 1.6.27 DiagnCollection\_DefineID

Subroutine DiagnCollection\_DefineID is a helper routine to return the collection ID.

```
SUBROUTINE DiagnCollection_DefineID ( Diagn, PS, RC, COL, DEF, OkIfAll, & InUse, ThisColl, HcoState )
```

### **USES:**

```
USE HCO_STATE_MOD,
                       ONLY : HCO_STATE
!INPUT ARGUMENTS:
 INTEGER,
                        INTENT(IN
                                   ), OPTIONAL :: COL
                                                      ! desired collection number
                                   ), OPTIONAL :: DEF
                                                            ! default collection number
 INTEGER,
                        INTENT(IN
 LOGICAL,
                        INTENT(IN
                                   ), OPTIONAL :: OkIfAll ! Ok if all (PS=-1)
!INPUT/OUTPUT ARGUMENTS:
 TYPE(DiagnBundle),
                                                            ! Diagn bundle obj
                       POINTER
                                               :: Diagn
                       POINTER,
 TYPE(HCO_STATE),
                                      OPTIONAL :: HcoState
                                                            ! HEMCO state obj
                       INTENT(INOUT)
                                                            ! Assigned collection number
 INTEGER,
                                               :: PS
 INTEGER,
                        INTENT(INOUT)
                                               :: RC
                                                            ! Return code
                        INTENT( OUT), OPTIONAL :: InUse
                                                            ! Is this in use?
 LOGICAL,
!OUTPUT ARGUMENTS:
 TYPE(DiagnCollection), POINTER,
                                     OPTIONAL :: ThisColl
                                                            ! Pointer to collection
```

## **REVISION HISTORY:**

01 Apr 2015 - C. Keller - Initial version

# 1.6.28 DiagnCollection\_Find

Subroutine DiagnCollection\_Find searches the collection linked list for the collection with the given collection ID.

### **INTERFACE:**

```
SUBROUTINE DiagnCollection_Find ( Diagn, PS, FOUND, RC, ThisColl )
```

## **INPUT PARAMETERS:**

```
INTENT(IN
                             )
                                       :: PS
                                                ! desired collection number
INTEGER,
```

OPTIONAL :: ThisColl ! Pointer to collection

# INPUT/OUTPUT PARAMETERS:

```
! Diagn bundle obj
TYPE(DiagnBundle),
                       POINTER
                                              :: Diagn
LOGICAL,
                       INTENT( OUT)
                                              :: FOUND
                                                          ! Collection exists?
                                                          ! Return code
INTEGER,
                       INTENT(INOUT)
                                              :: RC
TYPE(DiagnCollection), POINTER,
```

```
01 Apr 2015 - C. Keller - Initial version
10 Jul 2015 - R. Yantosca - Fixed minor issues in ProTeX header
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 1.6.29 DiagnCollection\_GetDefaultDelta returns the default diagnostics

output intervals based on the 'DiagnFreq' entry of the HEMCO configuration file. This can be one of the following character values: 'Hourly', 'Daily', 'Monthly', 'Annually', 'Always', or 'End'; or two integer explicitly denoting the year-month-day and hour-minute-second interval, respectively (format 00000000 000000). For example, setting DiagnFreq to '00000000 010000' would be the same as setting it to 'Hourly'.

# **INTERFACE:**

#### USES:

```
USE HCO_STATE_MOD, ONLY : HCO_State
USE HCO_ExtList_Mod, ONLY : GetExtOpt
USE HCO_ExtList_Mod, ONLY : CoreNr
```

### INPUT PARAMETERS:

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

TYPE(HCO_STATE), POINTER :: HcoState ! HEMCO state obj
```

# **OUTPUT PARAMETERS:**

```
INTEGER, INTENT( OUT) :: deltaYMD ! delta YYYYMMDD INTEGER, INTENT( OUT) :: deltaHMS ! delta HHMMSS
```

# INPUT/OUTPUT PARAMETERS:

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

### **REVISION HISTORY:**

```
06 Aug 2015 - C. Keller - Initial version
```

# 1.6.30 Function DiagnCollection\_IsTimeToWrite returns true if it is time

to write the provided diagnostics collection (identified by the collection number) to output. Whether it is time to write the diagnostics is based upon the current simulation time, the diagnostics output frequency, and the time span since the last output datetime.

### **INTERFACE:**

```
FUNCTION DiagnCollection_IsTimeToWrite( am_I_Root, HcoState, PS ) &
    RESULT ( TimeToWrite )
```

### **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_State
```

### INPUT PARAMETERS:

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

INTEGER, INTENT(IN ) :: PS ! Diagnostics collection

TYPE(HCO\_State), POINTER :: HcoState ! HEMCO state obj

### **OUTPUT PARAMETERS:**

LOGICAL :: TimeToWrite ! Is it time to write?

### **REVISION HISTORY:**

```
06 Aug 2015 - C. Keller - Initial version
```

30 Sep 2015 - C. Keller - Bug fix: now set current hour from 0 to 24 to

make sure that it will be greater than previous

hour.

# 1.6.31 Function DiagnCollection\_LastTimesSet returns true if there

exists a valid entry for the last datetime that collection PS has been written to disk. This is primarily important to check if the last output date needs be initialized (to non-default values).

## **INTERFACE:**

```
FUNCTION DiagnCollection_LastTimesSet( Diagn, PS ) Result ( LastTimesSet )
```

### **USES:**

### **INPUT PARAMETERS:**

```
TYPE(DiagnBundle), POINTER :: Diagn
```

INTEGER, INTENT(IN ) :: PS ! Diagnostics collection

### **OUTPUT PARAMETERS:**

LOGICAL :: LastTimesSet ! Are last times defined or not?

### **REVISION HISTORY:**

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

Opens a diagnostic configuration file. This is where you tell HEMCO which diagnostics you would like to send directly to netCDF output.

# **INTERFACE:**

```
SUBROUTINE DiagnFileOpen( am_I_Root, HcoConfig, LUN, RC )
```

# **USES:**

```
USE inquireMod, ONLY : findFreeLUN
```

USE HCO\_ExtList\_Mod, ONLY : CoreNr, GetExtOpt

### **INPUT PARAMETERS:**

LOGICAL, INTENT(IN ) :: am\_I\_Root ! root CPU?

# INPUT/OUTPUT PARAMETERS:

TYPE(ConfigObj), POINTER :: HcoConfig ! HEMCO config obj INTEGER, INTENT(INOUT) :: RC ! Failure or success

### **OUTPUT PARAMETERS:**

INTEGER, INTENT( OUT) :: LUN ! File LUN

### **REVISION HISTORY:**

10 Apr 2015 - C. Keller - Initial version

# 1.6.32 DiagnFileGetNext returns the diagnostics entries of the next

line of the diagnostics list file. Gets information from the next line of the diagnostic configuration file.

## **INTERFACE:**

```
SUBROUTINE DiagnFileGetNext( am_I_Root, HcoConfig, LUN, cName, & SpcName, ExtNr, Cat, & Hier, SpaceDim, OutUnit, & EOF, RC, lName, & UnitName
```

## **USES:**

USE HCO\_CharTools\_Mod

USE CHARPAK\_Mod, ONLY : STRREPL, STRSPLIT

# INPUT PARAMETERS:

LOGICAL, INTENT(IN ) :: am\_I\_Root ! root CPU? INTEGER, INTENT(IN ) :: LUN ! file LUN

# INPUT/OUTPUT PARAMETERS:

TYPE(ConfigObj), POINTER :: HcoConfig

LOGICAL, INTENT(INOUT) :: EOF

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

### **OUTPUT PARAMETERS:**

```
CHARACTER(LEN=*), INTENT( OUT)
                                          :: cName
CHARACTER(LEN=*), INTENT( OUT)
                                          :: SpcName
                 INTENT( OUT)
                                          :: ExtNr
INTEGER,
                 INTENT( OUT)
                                          :: Cat
INTEGER,
                 INTENT( OUT)
                                          :: Hier
INTEGER,
                 INTENT( OUT)
                                          :: SpaceDim
INTEGER,
                                          :: OutUnit
CHARACTER(LEN=*), INTENT( OUT)
CHARACTER(LEN=*), INTENT( OUT), OPTIONAL :: 1Name
CHARACTER(LEN=*), INTENT( OUT), OPTIONAL :: UnitName
```

# **REVISION HISTORY:**

```
10 Apr 2015 - C. Keller - Initial version
23 Feb 2016 - C. Keller - Added 1Name and UnitName arguments
```

# 1.6.33 DiagnFileClose

Closes the diagnostic configuration file.

# **INTERFACE:**

SUBROUTINE DiagnFileClose ( LUN )

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: LUN ! File LUN

### **REVISION HISTORY:**

10 Apr 2015 - C. Keller - Initial version

# 1.6.34 DiagnBundle\_Init

Creates an empty diagnostics bundle

### **INTERFACE:**

SUBROUTINE DiagnBundle\_Init ( Diagn )

# INPUT/OUTPUT PARAMETERS:

TYPE(DiagnBundle), POINTER :: Diagn

# **REVISION HISTORY:**

17 Feb 2016 - C. Keller - Initial version

# 1.6.35 DiagnBundle\_Cleanup

Cleans up a diagnostics bundle

### **INTERFACE:**

SUBROUTINE DiagnBundle\_Cleanup ( Diagn )

# INPUT/OUTPUT PARAMETERS:

TYPE(DiagnBundle), POINTER :: Diagn

# **REVISION HISTORY:**

17 Feb 2016 - C. Keller - Initial version

# 1.7 Fortran: Module Interface hco\_driver\_mod.F90

Module HCO\_Driver\_Mod contains the driver routines (INIT, RUN, FINAL) for the HEMCO core module. It calls all the subroutines to initialize, execute and finalize the HEMCO core emissions calculations, i.e. all emissions not calculated in a HEMCO extension (See module hcox\_driver\_mod.F90 for the extensions).

Call this module at the HEMCO - model interface level to execute the HEMCO core operations.

# **INTERFACE:**

```
MODULE HCO_Driver_Mod
```

### **USES:**

```
USE HCO_Error_Mod
USE HCO_State_Mod, ONLY : HCO_State
IMPLICIT NONE
PRIVATE
```

### PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: HCO_Run
PUBLIC :: HCO_Final
```

# **REVISION HISTORY:**

```
27 May 2012 - C. Keller - Initialization
11 Jun 2014 - R. Yantosca - Now indended with F90 free-format
11 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
```

### 1.7.1 HCO\_Run

Subroutine HCO\_Run is the HEMCO core run routine. It calculates the HEMCO emissions as specified in the HEMCO configuration file. All calculation settings, such as the extension number, the lowest and highest species ID, and the lowest and highest emission category, are passed through the HEMCO options object (HcoStateThe time stamp is taken from the HEMCO clock object. Subroutine HcoClock\_Set should be used to update the HEMCO clock (see module hco\_clock\_mod.F90). This should be done at the HEMCO - model interface level.

#### **INTERFACE:**

```
SUBROUTINE HCO_Run( am_I_Root, HcoState, Phase, RC )
```

### **USES:**

```
USE HCO_Calc_Mod, ONLY : HCO_CalcEmis

USE HCO_ReadList_Mod, ONLY : ReadList_Read

USE HCO_Clock_Mod, ONLY : HcoClock_Get

USE HCO_Clock_Mod, ONLY : HcoClock_First

USE HCO_Clock_Mod, ONLY : HcoClock_InitTzPtr

USE HCOIO_DIAGN_MOD, ONLY : HcoDiagn_Write
```

### INPUT PARAMETERS:

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

INTEGER, INTENT(IN ) :: Phase ! Run phase (1 or 2)
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object INTEGER, INTENT(INOUT) :: RC ! Success or failure?
```

# **REVISION HISTORY:**

```
27 May 2012 - C. Keller - Initialization
16 Jul 2014 - R. Yantosca - Cosmetic changes
23 Dec 2014 - C. Keller - ReadList_to_EmisList is now obsolete.

Containers are added to EmisList within routine ReadList_Read.
23 Feb 2015 - R. Yantosca - Now call HcoClock_InitTzPtr on the first emissions timestep to initialize the pointer to the timezones data (i.e. hours from UTC)
01 Apr 2015 - C. Keller - Added run phases
```

### 1.7.2 HCO\_Init

Subroutine HCO\_INIT initializes the HEMCO core modules. This routine assumes that the HEMCO configuration file has already been read to buffer (subroutine Config\_ReadFile in HCO\_CONFIG\_MOD.F90) and that the HEMCO state object has already been initialized. This has to be done at the HEMCO - model interface level.

### **INTERFACE:**

```
SUBROUTINE HCO_Init( am_I_Root, HcoState, RC )
```

# USES:

```
USE HCO_Diagn_Mod, ONLY : HcoDiagn_Init
USE HCO_tIdx_Mod, ONLY : tIDx_Init
USE HCO_Clock_Mod, ONLY : HcoClock_Init
USE HCO_Config_Mod, ONLY : SetReadList
```

# INPUT PARAMETERS:

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

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HcoState object INTEGER, INTENT(INOUT) :: RC ! Failure or success
```

# **REVISION HISTORY:**

```
27 May 2012 - C. Keller - Initialization
11 Jun 2014 - R. Yantosca - Now indended with F90 free-format
11 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
16 Jul 2014 - R. Yantosca - Remove reference to gigc_errcode_mdo.F90
```

# 1.7.3 HCO\_Final

Subroutine HCO\_Final finalizes HEMCO core.

#### INTERFACE:

```
SUBROUTINE HCO_Final( am_I_Root, HcoState, ERROR, RC )
```

### **USES:**

```
USE HCO_Clock_Mod, ONLY : HcoClock_Cleanup
USE HCO_tIdx_Mod, ONLY : tIDx_Cleanup
USE HCO_DataCont_Mod, ONLY : cIDList_Cleanup
USE HCO_ReadList_Mod, ONLY : ReadList_Cleanup
USE HCO_DataCont_Mod, ONLY : ListCont_Cleanup
USE HCO_ExtList_Mod, ONLY : ExtFinal
USE HCOIO_DIAGN_MOD, ONLY : HcoDiagn_Write
```

### INPUT PARAMETERS:

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

LOGICAL, INTENT(IN ) :: ERROR ! Cleanup because of crash?
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HcoState object INTEGER, INTENT(INOUT) :: RC ! Failure or success
```

## **REMARKS:**

- (1) ConfigFile\_Cleanup also cleans up the data containers, while routine EmisList\_Cleanup and ReadList\_Cleanup only removes the pointers to them. Hence, we have to call these routines before ConfigFile\_Cleanup!
- (2) HcoState is cleaned up in the HEMCO-module interface.

```
27 May 2012 - C. Keller - Initialization
11 Jun 2014 - R. Yantosca - Now indended with F90 free-format
11 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
16 Jul 2014 - R. Yantosca - Cosmetic changes
```

# 1.8 Fortran: Module Interface hco\_emislist\_mod.F90

Module HCO\_EmisList\_Mod contains routines and variables for the HEMCO emissions list EmisList. EmisList is a sorted collection of all data containers needed for emission calculation. The containers are sorted by data type, species, emission category, and emission hierarchy (in this order).

### **INTERFACE:**

```
MODULE HCO_EMISLIST_MOD
```

### **USES:**

```
USE HCO_ERROR_MOD
USE HCO_TYPES_MOD
USE HCO_STATE_MOD, ONLY: HCO_State

IMPLICIT NONE
PRIVATE
```

### PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCO\_GetPtr

PUBLIC :: EmisList\_Pass

PUBLIC :: EmisList\_Update

### PRIVATE MEMBER FUNCTIONS:

PRIVATE :: EmisList\_Add
PRIVATE :: Add2EmisList

### REVISION HISTORY:

```
04 Dec 2012 - C. Keller - Initialization
08 Jul 2014 - R. Yantosca - Now use F90 free-format indentation
08 Jul 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
```

### 1.8.1 EmisList\_Add

Subroutine EmisList\_Add adds the passed data container Dct to EmisList. Within EmisList, Dct becomes placed with increasing data type, species ID, category and hierarchy (in this order).

### **INTERFACE:**

```
SUBROUTINE EmisList_Add( am_I_Root, Dct, HcoState, RC )
```

# **USES:**

```
USE HCO_DATACONT_MOD, ONLY : ListCont_Find
USE HCO_LOGFILE_MOD, ONLY : HCO_PrintDataCont
```

# INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Root CPU?
TYPE(DataCont), POINTER :: Dct ! Data cont.
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state
```

# INPUT/OUTPUT PARAMETERS:

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

### REVISION HISTORY:

```
04 Dec 2012 - C. Keller - Initialization
02 Feb 2015 - C. Keller - Moved tIDx_Assign call to hco_readlist_mod
so that this module can also be used by
hco_clock_mod.
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 1.8.2 Add2EmisList

Subroutine Add2EmisList adds list container Lct to EmisList. Base emission fields (Data type = 1) are sorted based on species ID, category and hierarchy (for fields of same category). Scale fields and masks are added to the end of EmisList.

#### **INTERFACE:**

```
SUBROUTINE Add2EmisList( am_I_Root, HcoState, Lct, RC )
```

### INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state
TYPE(ListCont), POINTER :: Lct
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

### **REVISION HISTORY:**

```
06 Dec 2012 - C. Keller - Initial version
```

### 1.8.3 EmisList\_Pass

Subroutine EmisList\_Pass passes (the ReadList) container Lct to EmisList. This routine mostly checks for additive arrays, i.e. if arrays from multiple containers have to be added together prior to emission calculation (e.g. sectoral data).

### **INTERFACE:**

```
SUBROUTINE EmisList_Pass( am_I_Root, HcoState, Lct, RC )
```

### **USES:**

```
USE HCO_DATACONT_MOD, ONLY : ListCont_Find USE HCO_FILEDATA_MOD, ONLY : FileData_ArrCheck
```

### INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am\_I\_Root TYPE(HCO\_State), POINTER :: HcoState

TYPE(ListCont), POINTER :: Lct ! list container

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC ! Success

### REVISION HISTORY:

### 1.8.4 HCO\_GetPtr\_3D

Subroutine HCO\_GetPtr\_3D returns the 3D data pointer Ptr3D of EmisList that is associated with data container DctName. By default, the routine returns an error if the given container name is not found. This can be avoided by calling the routine with the optional argument FOUND, in which case only this argument will be set to FALSE. Similarly, the FILLED flag can be used to control the behaviour if the data container is found but empty, e.g. no data is associated with it.

This routine returns the unevaluated data field, e.g. no scale factors or masking is applied to the data. Use routine HCO\_EvalFld in hco\_calc\_mod.F90 to get evaluated fields.

## **INTERFACE:**

```
SUBROUTINE HCO_GetPtr_3D( am_I_Root, HcoState, DctName, Ptr3D, & RC, TIDX, FOUND, FILLED )
```

### **USES:**

```
USE HCO_DATACONT_MOD, ONLY : ListCont_Find
```

### INPUT PARAMETERS:

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

TYPE(HCO_State), POINTER :: HcoState ! HEMCO state obj

CHARACTER(LEN=*), INTENT(IN ) :: DctName ! container name

INTEGER, INTENT(IN), OPTIONAL :: TIDX ! time index

! (default=1)
```

### **OUTPUT PARAMETERS:**

```
REAL(sp), POINTER :: Ptr3D(:,:,:) ! output array LOGICAL, INTENT(OUT), OPTIONAL :: FOUND ! cont. found? LOGICAL, INTENT(OUT), OPTIONAL :: FILLED ! array filled?
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC ! Success/fail
```

### REVISION HISTORY:

```
04 Sep 2013 - C. Keller - Initialization
19 May 2015 - C. Keller - Added argument FILLED
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 1.8.5 HCO\_GetPtr\_2D

Subroutine HCO\_GetPtr\_2D returns the 2D data pointer Ptr2D of EmisList that is associated with data container DctName. See HCO\_GetPtr\_3D for more details.

# **INTERFACE:**

```
SUBROUTINE HCO_GetPtr_2D( am_I_Root, HcoState, DctName, Ptr2D, & RC, TIDX, FOUND, FILLED )
```

# **USES:**

```
USE HCO_DATACONT_MOD, ONLY : ListCont_Find
```

# INPUT PARAMETERS:

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

TYPE(HCO_State), POINTER :: HcoState ! HEMCO state obj

CHARACTER(LEN=*), INTENT(IN ) :: DctName ! container name

INTEGER, INTENT(IN), OPTIONAL :: TIDX ! time index

! (default=1)
```

# **OUTPUT PARAMETERS:**

```
REAL(sp), POINTER :: Ptr2D(:,:) ! output array LOGICAL, INTENT(OUT), OPTIONAL :: FOUND ! cont. found? LOGICAL, INTENT(OUT), OPTIONAL :: FILLED ! array filled?
```

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC ! Success/fail

### **REVISION HISTORY:**

```
04 Sep 2013 - C. Keller - Initialization
19 May 2015 - C. Keller - Added argument FILLED
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

### 1.9 Fortran: Module Interface hoo error mod.F90

Module HCO\_Error\_Mod contains routines and variables for error handling and logfile messages in HEMCO. It also contains definitions of some globally used parameter, such as the single/double precision as well as the HEMCO precision definitions. The HEMCO precision is used for almost all HEMCO internal data arrays and can be changed below if required.

The error settings are specified in the HEMCO configuration file and error handling is performed according to these settings. They include:

- 1. HEMCO logfile: all HEMCO information is written into the specified logfile. The logfile can be set to the wildcard character, in which case the standard output will be used (this may be another opened logfile).
- 2. Verbose: Number indicating the verbose level to be used. 0 = no verbose, 3 = very verbose. The verbose level can be set in the HEMCO configuration file. The default value is 0.
- 3. Warnings: Number indicating the warning level to be shown. 0 = no warnings, 3 = all warnings.

The error settings are set via subroutine HCO\_ERROR\_SET, called when reading section 'settings' of the HEMCO configuration file (subroutine Config\_ReadFile in hco\_config\_mod.F90). The currently active verbose settings can be checked using subroutines HCO\_IsVerb and HCO\_VERBOSE\_INQ. Messages can be written into the logfile using subroutine HCO\_MSG. Note that the logfile actively need to be opened (HCO\_LOGFILE\_OPEN) before writing to it.

The verbose and warning settings are all set to false if it's not the root CPU.

As of HEMCO v2.0, all HEMCO error variables are organized in derived type object Hco-Err. HcoErr is a component of the HEMCO configuration object (type ConfigObj, see hco\_types\_mod.F90). It must be passed explicitly to all error routines. This design allows the invocation of multiple independent HEMCO instances at the same time (which may have different HEMCO error settings). **INTERFACE:** 

```
MODULE HCO_Error_Mod
```

### **USES:**

IMPLICIT NONE PRIVATE

### PUBLIC MEMBER FUNCTIONS:

```
PUBLIC
                 :: HCO_ERROR
 PUBLIC
                 :: HCO_WARNING
                 :: HCO_MSG
 PUBLIC
                 :: HCO_ENTER
 PUBLIC
 PUBLIC
                 :: HCO_LEAVE
 PUBLIC
                 :: HCO_ERROR_SET
                 :: HCO_ERROR_FINAL
 PUBLIC
 PUBLIC
                 :: HCO_IsVerb
                 :: HCO_VERBOSE_INQ
 PUBLIC
 PUBLIC
                 :: HCO_LOGFILE_OPEN
 PUBLIC
                  :: HCO_LOGFILE_CLOSE
 !MODULE VARIABLES:
  ! Double and single precision definitions
 INTEGER, PARAMETER, PUBLIC :: dp = KIND( REAL( 0.0, 8 ) ) ! Double (r8)
 INTEGER, PARAMETER, PUBLIC :: sp = KIND( REAL( 0.0, 4 ) ) ! Single (r4)
#if defined( USE_REAL8 )
 INTEGER, PARAMETER, PUBLIC :: hp = KIND( REAL( 0.0, 8 ) ) ! HEMCO prec r8
#else
 INTEGER, PARAMETER, PUBLIC :: hp = KIND( REAL( 0.0, 4 ) ) ! HEMCO prec r4
#endif
 INTEGER, PARAMETER, PUBLIC :: i4 = 4
                                                           ! FourByteInt
                                                           ! EightByteInt
 INTEGER, PARAMETER, PUBLIC :: i8 = 8
  ! Error success/failure definitions
  INTEGER, PARAMETER, PUBLIC :: HCO_SUCCESS = 0
 INTEGER, PARAMETER, PUBLIC :: HCO_FAIL = -999
  ! Tiny value for math operations:
  ! --> deprecated. Use TINY(1.0_hp) instead!
 REAL(hp), PARAMETER, PUBLIC :: HCO_TINY = 1.0e-32_hp
  ! Missing value
  ! Note: define missing value as single precision because all data arrays
  ! are read/stored in single precision.
 REAL(sp), PARAMETER, PUBLIC :: HCO_MISSVAL = -1.e31_sp
  ! HEMCO version number.
 CHARACTER(LEN=12), PARAMETER, PUBLIC :: HCO_VERSION = 'v2.0.003'
 INTERFACE HCO_Error
    MODULE PROCEDURE HCO_ErrorNoErr
    MODULE PROCEDURE HCO_ErrorErr
 END INTERFACE HCO_Error
 INTERFACE HCO_Warning
    MODULE PROCEDURE HCO_WarningNoErr
```

```
MODULE PROCEDURE HCO_WarningErr
END INTERFACE HCO_Warning

INTERFACE HCO_MSG

MODULE PROCEDURE HCO_MsgNoErr

MODULE PROCEDURE HCO_MsgErr
```

# **REVISION HISTORY:**

END INTERFACE HCO\_MSG

```
23 Sep 2013 - C. Keller - Initialization

12 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers

12 Jun 2014 - R. Yantosca - Now use F90 freeform indentation

03 Mar 2015 - C. Keller - Added HCO_CFLAG_* and HCO_DCTTYPE_*

15 Feb 2016 - C. Keller - Update to v2.0: error variables now organized in derived type HcoErr.

23 Nov 2016 - R. Yantosca - Now rewrite KIND definitions to prevent 4-byte and 8-byte variables from being elevated when using -r8 (or equivalent flags)
```

# 1.9.1 HCO\_Error

Subroutine HCO\_Error promts an error message and sets RC to HCO\_FAIL. Note that this routine does not stop a run, but it will cause a stop at higher level (when RC gets evaluated).

### **INTERFACE:**

```
SUBROUTINE HCO_ErrorErr( Err, ErrMsg, RC, THISLOC )
```

### INPUT PARAMETERS:

```
TYPE(HcoErr), POINTER :: Err
CHARACTER(LEN=*), INTENT(IN ) :: ErrMsg
CHARACTER(LEN=*), INTENT(IN ), OPTIONAL :: THISLOC
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

# **REVISION HISTORY:**

```
23 Sep 2013 - C. Keller - Initialization
```

# 1.9.2 HCO\_Error

Subroutine HCO\_Error promts an error message and sets RC to HCO\_FAIL. Note that this routine does not stop a run, but it will cause a stop at higher level (when RC gets evaluated).

### **INTERFACE:**

```
SUBROUTINE HCO_ErrorNoErr( ErrMsg, RC, THISLOC )
```

### INPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(IN ) :: ErrMsg CHARACTER(LEN=*), INTENT(IN ), OPTIONAL :: THISLOC
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

# **REVISION HISTORY:**

```
23 Sep 2013 - C. Keller - Initialization
```

# 1.9.3 HCO\_Warning

Subroutine HCO\_Warning promts a warning message without forcing HEMCO to stop, i.e. return code is set to HCO SUCCESS.

### **INTERFACE:**

```
SUBROUTINE HCO_WarningErr( Err, ErrMsg, RC, WARNLEV, THISLOC )
!INPUT PARAMETERS"

TYPE(HcoErr), POINTER :: Err
CHARACTER(LEN=*), INTENT(IN ) :: ErrMsg
INTEGER , INTENT(IN ), OPTIONAL :: WARNLEV
CHARACTER(LEN=*), INTENT(IN ), OPTIONAL :: THISLOC
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

### REVISION HISTORY:

```
23 Sep 2013 - C. Keller - Initialization
26 Mar 2015 - C. Keller - Added warning levels
```

# 1.9.4 HCO\_Warning

Subroutine HCO\_Warning promts a warning message without forcing HEMCO to stop, i.e. return code is set to HCO\_SUCCESS.

## INTERFACE:

```
SUBROUTINE HCO_WarningNoErr( ErrMsg, RC, WARNLEV, THISLOC )
!INPUT PARAMETERS"

CHARACTER(LEN=*), INTENT(IN ) :: ErrMsg
INTEGER , INTENT(IN ), OPTIONAL :: WARNLEV
CHARACTER(LEN=*), INTENT(IN ), OPTIONAL :: THISLOC
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

#### **REVISION HISTORY:**

```
23 Sep 2013 - C. Keller - Initialization
26 Mar 2015 - C. Keller - Added warning levels
```

#### 1.9.5 HCO\_MSG

Subroutine HCO\_MSG passes message msg to the HEMCO logfile (or to standard output if the logfile is not open). Sep1 and Sep2 denote line delimiters before and after the message, respectively. The optional argument Verb denotes the minimum verbose level associated with this message. The message will only be prompted if the verbose level on this CPU (e.g. of this Err object) is at least as high as Verb.

### **INTERFACE:**

```
SUBROUTINE HCO_MSGErr( Err, Msg, Sep1, Sep2, Verb )
```

# **INPUT PARAMETERS:**

```
TYPE(HcoErr),
                 POINTER
                                           :: Err
CHARACTER(LEN=*), INTENT(IN
                              ), OPTIONAL
                                          :: Msg
CHARACTER(LEN=1), INTENT(IN
                              ), OPTIONAL
                                          :: Sep1
CHARACTER(LEN=1), INTENT(IN
                              ), OPTIONAL
                                          :: Sep2
INTEGER,
                 INTENT(IN
                              ), OPTIONAL
                                          :: Verb
```

## **REVISION HISTORY:**

```
23 Sep 2013 - C. Keller - Initialization
20 May 2015 - R. Yantosca - Minor formatting fix: use '(a)' instead of * to avoid line wrapping around at 80 columns.
```

# 1.9.6 HCO<sub>-</sub>MSG

Subroutine HCO\_MSG passes message msg to the HEMCO logfile (or to standard output if the logfile is not open). Sep1 and Sep2 denote line delimiters before and after the message, respectively. The optional argument Verb denotes the minimum verbose level associated with this message. The message will only be prompted if the verbose level on this CPU (e.g. of this Err object) is at least as high as Verb.

### **INTERFACE:**

```
SUBROUTINE HCO_MSGnoErr( Msg, Sep1, Sep2, Verb )
```

### INPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(IN ), OPTIONAL :: Msg CHARACTER(LEN=1), INTENT(IN ), OPTIONAL :: Sep1 CHARACTER(LEN=1), INTENT(IN ), OPTIONAL :: Sep2 INTEGER, INTENT(IN ), OPTIONAL :: Verb
```

# **REVISION HISTORY:**

```
23 Sep 2013 - C. Keller - Initialization
20 May 2015 - R. Yantosca - Minor formatting fix: use '(a)' instead of * to avoid line wrapping around at 80 columns.
```

## 1.9.7 HCO\_Enter

Subroutine HCO\_Enter is called upon entering a routine. It organizes the traceback handling. It is recommended to call this routine for 'big' routines but NOT for routines/functions that are frequently called, e.g. inside of loops!

Note that all subroutines calling HCO\_Enter must also call HCO\_Leave!

### **INTERFACE:**

```
SUBROUTINE HCO_Enter( Err, thisLoc, RC )
```

# **INPUT PARAMETERS:**

### INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

## **REVISION HISTORY:**

```
23 Sep 2013 - C. Keller - Initialization
```

### 1.9.8 HCO\_Leave

Subroutine HCO\_Leave is called upon leaving a routine. It organizes the traceback handling. It is recommended to call this routine for 'big' routines but NOT for routines/functions that are frequently called, e.g. inside of loops!

Note that all subroutines calling HCO\_Leave must also call HCO\_Enter!

### **INTERFACE:**

```
SUBROUTINE HCO_Leave( Err, RC )
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HcoErr), POINTER :: Err INTEGER, INTENT(INOUT) :: RC
```

### REVISION HISTORY:

```
23 Sep 2013 - C. Keller - Initialization
```

### 1.9.9 HCO\_Error\_Set

Subroutine HCO\_Error\_Set defines the HEMCO error settings. This routine is called at the beginning of a HEMCO simulation. Its input parameter are directly taken from the HEMCO configuration file. If LogFile is set to '\*' (asterik), all output is directed to the standard output.

# **INTERFACE:**

# **INPUT PARAMETERS:**

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

TYPE(HcoErr), POINTER :: Err ! Error object

CHARACTER(LEN=*), INTENT(IN) :: LogFile ! logfile path+name
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: Verbose ! verbose level INTEGER, INTENT(INOUT) :: WarningLevel ! warning level
```

INTEGER, INTENT(INOUT) :: RC

# **REVISION HISTORY:**

```
23 Sep 2013 - C. Keller - Initialization
```

## 1.9.10 HCO\_Error\_Final

Subroutine HCO\_Error\_Final finalizes the error type.

### **INTERFACE:**

```
SUBROUTINE HCO_Error_Final ( Err )
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HcoErr), POINTER :: Err ! Error object
```

```
23 Sep 2013 - C. Keller - Initialization
```

# 1.9.11 HCO\_Verbose\_Inq

Function HCO\_Verbose\_Inq returns the HEMCO verbose number.

### **INTERFACE:**

```
FUNCTION HCO_VERBOSE_INQ ( ERR ) RESULT ( VerbNr )
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HcoErr), POINTER :: Err ! Error object
```

### **OUTPUT PARAMETERS:**

```
INTEGER :: VerbNr
```

### **REVISION HISTORY:**

```
15 Mar 2015 - C. Keller - Initialization
```

### 1.9.12 HCO\_IsVerb

Function HCO\_IsVerb returns true if the HEMCO verbose number is equal to or larger than the passed number.

### **INTERFACE:**

```
FUNCTION HCO_IsVerb ( Err, VerbNr ) RESULT ( IsVerb )
```

# **INPUT PARAMETERS:**

```
TYPE(HcoErr), POINTER :: Err ! Error object
```

INTEGER, INTENT(IN) :: VerbNr

# **OUTPUT PARAMETERS:**

```
LOGICAL :: IsVerb
```

### **REVISION HISTORY:**

```
15 Mar 2015 - C. Keller - Initialization
```

# 1.9.13 HCO\_LOGFILE\_OPEN

Subroutine HCO\_LOGFILE\_OPEN opens the HEMCO logfile (if not yet open).

# **INTERFACE:**

```
SUBROUTINE HCO_LogFile_Open( Err, RC )
```

### **USES:**

USE inquireMod, ONLY : findFreeLUN

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HcoErr), POINTER :: Err ! Error object INTEGER, INTENT(INOUT) :: RC
```

### **REVISION HISTORY:**

```
23 Sep 2013 - C. Keller - Initialization
14 Aug 2014 - R. Yantosca - Add FORM='FORMATTED' to the OPEN statement
so that the HEMCO log will be a text file
22 Jan 2016 - R. Yantosca - Line-buffer the HEMCO log file for pgfortran
```

# 1.9.14 HCO\_LogFile\_Close

Subroutine HCO\_LOGFILE\_CLOSE closes the HEMCO logfile. If argument ShowSummary is enabled, it will prompt a summary of the HEMCO run up to this point (number of warnings, etc.).

### **INTERFACE:**

```
SUBROUTINE HCO_LogFile_Close( Err, ShowSummary )
```

### INPUT PARAMETERS:

```
TYPE(HcoErr), POINTER :: Err ! Error object LOGICAL, INTENT(IN), OPTIONAL :: ShowSummary
```

#### REVISION HISTORY:

```
23 Sep 2013 - C. Keller - Initialization
```

## 1.10 Fortran: Module Interface hco\_extlist\_mod

Module HCO\_EXTLIST\_MOD contains routines and variables to organize HEMCO extensions and the corresponding settings (options). This is done through the ExtList object, which is a simple list containing all enabled HEMCO extensions (name and ext. ID) and the corresponding options, as defined in the HEMCO configuration file. The general HEMCO settings are stored as options of the HEMCO core extension (Extension number = 0). The CORE extension is activated in every HEMCO run, while all other extensions are only activated if enabled in the configuration file.

Extension number -999 is used as 'wildcard' value, e.g. data containers with extension number -999 will always be read by HEMCO but will be ignored for emission calculation. This is particularly useful for data fields that shall be used outside of HEMCO, e.g. stratospheric chemistry prod/loss rates, etc.

Extension options are 'flexible' in a sense that any option name/value pair can be assigned to

an extension. The value of any of these options can be queried using subroutine GetExtOpt or function HCO\_GetOpt. In fact, the HEMCO filename parser (in hco\_chartools\_mod.F90) will attempt to find an option value for any HEMCO 'token' (a character starting with the HEMCO token sign (which is, the dollar sign '\$'). This allows the user to specify as many individual tokens as HEMCO settings as needed.

## **INTERFACE:**

MODULE HCO\_ExtList\_Mod

### **USES:**

USE HCO\_Error\_Mod
USE HCO\_Types\_Mod

IMPLICIT NONE PRIVATE

# PUBLIC MEMBER FUNCTIONS:

PUBLIC :: AddExt

PUBLIC :: AddExtOpt

PUBLIC :: GetExtOpt

PUBLIC :: GetExtNr

PUBLIC :: GetExtSpcStr

PUBLIC :: GetExtSpcVal

PUBLIC :: SetExtNr

PUBLIC :: ExtNrInUse

PUBLIC :: ExtFinal

PUBLIC :: HCO\_GetOpt
PUBLIC :: HCO\_SetDefaultToken

PUBLIC :: HCO\_ROOT

PRIVATE :: HCO\_AddOpt
PRIVATE :: HCO\_CleanupOpt

! Core extension number

INTEGER, PARAMETER, PUBLIC :: CoreNr = -1

```
02 Oct 2013 - C. Keller - Initial version
01 Jul 2014 - R. Yantosca - Now use F90 free-format indentation
01 Jul 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
30 Sep 2014 - R. Yantosca - ThisExt%Spcs now has 2047 chars for extensions having many individual species
20 Sep 2015 - C. Keller - Reorganize options in linked lists. Tokens are now the same as options and can be flexibly set by the user.
```

### 1.10.1 AddExt

Subroutine AddExt adds a new extension to the extensions list. The extension name, number and species (multiple species separated by the HEMCO separator sign) need to be provided. Extension options are left blank but can be added lateron using AddExtOpt.

### **INTERFACE:**

```
SUBROUTINE AddExt( am_I_Root, HcoConfig, ExtName, ExtNr, InUse, Spcs, RC )
USES:
```

```
USE CHARPAK_MOD, ONLY : TRANLC
```

### **INPUT PARAMETERS:**

```
LOGICAL, INTENT(IN ) :: am_I_Root
TYPE(ConfigObj), POINTER :: HcoConfig
CHARACTER(LEN=*), INTENT(IN ) :: ExtName
INTEGER, INTENT(IN ) :: ExtNr
LOGICAL, INTENT(IN ) :: InUse
CHARACTER(LEN=*), INTENT(IN ) :: Spcs
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

### **REVISION HISTORY:**

```
03 Oct 2013 - C. Keller - Initial version
20 Sep 2015 - C. Keller - Options are now linked list
12 Dec 2015 - C. Keller - Added argument InUse
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 1.10.2 AddExtOpt

Function AddExtOpt appends the given string to the options character of the desired extension (identified by its extension number). The options string is expected to contain an option name and value, separated by a colon (:). Function GetExtOpt can be used to extract the option value at a later point.

## **INTERFACE:**

```
SUBROUTINE AddExtOpt( am_I_Root, HcoConfig, Opt, ExtNr, RC, IgnoreIfExist )
USES:
```

```
USE CHARPAK_MOD, ONLY : STRSPLIT, TRANLC
```

### INPUT PARAMETERS:

```
! Root CPU?
LOGICAL,
                  INTENT(IN
                                           :: am_I_Root
                               )
TYPE(ConfigObj), POINTER
                                           :: HcoConfig
                                                              ! Configuration object
CHARACTER(LEN=*), INTENT(IN
                                                              ! Option name & value
                               )
                                           :: Opt
                                                              ! Add to this extension
INTEGER,
                  INTENT(IN
                               )
                                           :: ExtNr
                               ), OPTIONAL :: IgnoreIfExist ! Ignore this entry if it exist
LOGICAL,
                  INTENT(IN
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

# **REVISION HISTORY:**

```
03 Oct 2013 - C. Keller - Initial version
20 Sep 2015 - C. Keller - Options are now linked list
12 Dec 2015 - C. Keller - Added argument IgnoreIfExist
```

# 1.10.3 GetExtOpt

Function GetExtOpt returns the option value for a given extension and option name. The type of the return value depends on the provided argument (real, boolean, character). The optional output argument FOUND returns TRUE if the given option name was found, and FALSE otherwise. If the FOUND argument is provided, no error is returned if the option name is not found! If the ExtNr is set to -999, the settings of all extensions are searched.

### **INTERFACE:**

```
SUBROUTINE GetExtOpt ( HcoConfig, ExtNr, OptName, OptValHp, & OptValSp, OptValDp, OptValInt, & OptValBool, OptValChar, Found, RC )
```

### **USES:**

```
USE CHARPAK_MOD, ONLY : STRSPLIT, TRANLC
```

## INPUT PARAMETERS:

```
TYPE(ConfigObj), POINTER :: HcoConfig INTEGER, INTENT(IN ) :: ExtNr CHARACTER(LEN=*), INTENT(IN ) :: OptName
```

## **OUTPUT PARAMETERS:**

```
REAL(hp), INTENT( OUT), OPTIONAL :: OptValHp
REAL(sp), INTENT( OUT), OPTIONAL :: OptValSp
REAL(dp), INTENT( OUT), OPTIONAL :: OptValDp
INTEGER, INTENT( OUT), OPTIONAL :: OptValInt
LOGICAL, INTENT( OUT), OPTIONAL :: OptValBool
CHARACTER(LEN=*), INTENT( OUT), OPTIONAL :: OptValChar
LOGICAL, INTENT( OUT), OPTIONAL :: Found
```

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

### **REVISION HISTORY:**

```
03 Oct 2013 - C. Keller - Initial version
13 Jan 2015 - R. Yantosca - Add optional variable of flex precision (hp)
14 Feb 2015 - C. Keller - Add option to search all extensions (ExtNr=-999).
17 Apr 2015 - C. Keller - Passed option OptName must now exactly match the stored option name to avoid ambiguity.
20 Sep 2015 - C. Keller - Options are now linked list.
20 Jan 2016 - C. Keller - Bug fix: boolean options are now case insensitive.
```

### 1.10.4 GetExtNr

Function GetExtNr returns the extension number of extension ExtName. Returns -999 if no extension with the given name is found.

### **INTERFACE:**

```
FUNCTION GetExtNr( ExtList, ExtName ) Result ( ExtNr )
```

# **USES:**

```
USE CHARPAK_MOD, ONLY: TRANLC
```

### INPUT PARAMETERS:

```
TYPE(Ext), POINTER :: ExtList CHARACTER(LEN=*), INTENT(IN ) :: ExtName
```

# RETURN VALUE:

INTEGER :: ExtNr

# **REVISION HISTORY:**

```
03 Oct 2013 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 1.10.5 GetExtSpcStr

Subroutine GetExtSpcStr returns the HEMCO species names string of all species assigned to the given extension (identified by its extension number).

# **INTERFACE:**

```
SUBROUTINE GetExtSpcStr( HcoConfig, ExtNr, SpcStr, RC )
```

## INPUT PARAMETERS:

```
TYPE(ConfigObj), POINTER :: HcoConfig
INTEGER, INTENT(IN ) :: ExtNr ! Extension Nr.
```

### **OUTPUT PARAMETERS:**

```
CHARACTER(LEN=*), INTENT( OUT) :: SpcStr ! Species string
```

# INPUT/OUTPUT PARAMETERS:

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

### REVISION HISTORY:

```
10 Jan 2014 - C. Keller: Initialization (update)
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 1.10.6 GetExtSpcVal\_Sp

Subroutine GetExtSpcVal\_Sp returns single precision values associated with the species for a given extension. Specifically, this routine searches for extension setting '¡Prefix¿\_SpecName' for every species passed through input argument SpcNames and writes those into output argument SpcScal. The default value DefValue is assigned to all elements of SpcScal with no corresponding extension setting.

### **INTERFACE:**

```
SUBROUTINE GetExtSpcVal_Sp( HcoConfig, ExtNr, NSPC, SpcNames, & Prefix, DefValue, SpcScal, RC
```

# INPUT PARAMETERS:

```
TYPE(ConfigObj),
                                      :: HcoConfig
                       POINTER
INTEGER,
                       INTENT(IN
                                    ) :: ExtNr
                                                        ! Extension Nr.
INTEGER,
                                    ) :: NSPC
                                                        ! # of species
                       INTENT(IN
CHARACTER(LEN=*),
                       INTENT(IN
                                    ) :: SpcNames(NSPC) ! Species string
                                                        ! search prefix
CHARACTER(LEN=*),
                                    ) :: Prefix
                       INTENT(IN
                                   ) :: DefValue
                                                        ! default value
REAL(sp),
                       INTENT(IN
```

# INPUT/OUTPUT PARAMETERS:

```
REAL(sp), ALLOCATABLE, INTENT(INOUT) :: SpcScal(:) ! Species scale factors INTEGER, INTENT(INOUT) :: RC ! Success or failure?
```

```
10 Jun 2015 - C. Keller - Initial version
20 Sep 2015 - C. Keller - Now allocate output array in this routine.
```

# 1.10.7 GetExtSpcVal\_Int

Subroutine GetExtSpcVal\_Int returns integer values associated with the species for a given extension. Specifically, this routine searches for extension setting '¡Prefix¿\_SpecName' for every species passed through input argument SpcNames and writes those into output argument SpcScal. The default value DefValue is assigned to all elements of SpcScal with no corresponding extension setting.

### **INTERFACE:**

```
SUBROUTINE GetExtSpcVal_Int( HcoConfig, ExtNr, NSPC, SpcNames, & Prefix, DefValue, SpcScal, RC )
```

## INPUT PARAMETERS:

```
TYPE(ConfigObj),
                       POINTER
                                      :: HcoConfig
INTEGER,
                       INTENT(IN
                                    ) :: ExtNr
                                                         ! Extension Nr.
INTEGER,
                                    ) :: NSPC
                                                         ! # of species
                       INTENT(IN
                                    ) :: SpcNames(NSPC) ! Species string
CHARACTER(LEN=*),
                       INTENT(IN
CHARACTER(LEN=*),
                                    ) :: Prefix
                                                         ! search prefix
                       INTENT(IN
INTEGER,
                                    ) :: DefValue
                                                         ! default value
                       INTENT(IN
```

# INPUT/OUTPUT PARAMETERS:

### **REVISION HISTORY:**

```
10 Jun 2015 - C. Keller - Initial version
20 Sep 2015 - C. Keller - Now allocate output array in this routine.
```

# 1.10.8 GetExtSpcVal\_Char

Subroutine GetExtSpcVal\_Char returns character values associated with the species for a given extension. Specifically, this routine searches for extension setting '¡Prefix;\_SpecName' for every species passed through input argument SpcNames and writes those into output argument SpcScal. The default value DefValue is assigned to all elements of SpcScal with no corresponding extension setting.

### **INTERFACE:**

```
SUBROUTINE GetExtSpcVal_Char( HcoConfig, ExtNr, NSPC, SpcNames, & Prefix, DefValue, SpcScal, RC)
```

#### INPUT PARAMETERS:

```
TYPE(ConfigObj),
                               POINTER
                                              :: HcoConfig
INTEGER,
                                            ) :: ExtNr
                               INTENT(IN
                                                                 ! Extension Nr.
                                            ) :: NSPC
                                                                 ! # of species
INTEGER,
                               INTENT(IN
                                            ) :: SpcNames(NSPC) ! Species string
CHARACTER(LEN=*),
                               INTENT(IN
CHARACTER(LEN=*),
                                            ) :: Prefix
                                                                 ! search prefix
                               INTENT(IN
CHARACTER(LEN=*),
                                            ) :: DefValue
                                                               ! default value
                               INTENT(IN
```

# INPUT/OUTPUT PARAMETERS:

```
CHARACTER(LEN=*), ALLOCATABLE, INTENT(INOUT) :: SpcScal(:) ! Species scale factors INTEGER, INTENT(INOUT) :: RC ! Success or failure?
```

# **REVISION HISTORY:**

```
10 Jun 2015 - C. Keller - Initial version
20 Sep 2015 - C. Keller - Now allocate output array in this routine.
```

# 1.10.9 GetExtSpcVal\_Dr

Subroutine GetExtSpcVal\_Dr is the GetExtSpcVal driver routine.

### **INTERFACE:**

```
SUBROUTINE GetExtSpcVal_Dr( HcoConfig, ExtNr, NSPC, & SpcNames, Prefix, RC, & DefVal_SP, SpcScal_SP, & DefVal_Char, SpcScal_Char, & DefVal_IN, SpcScal_IN
```

## INPUT PARAMETERS:

```
TYPE(ConfigObj),
                                   POINTER
                                                              :: HcoConfig
                                                              :: ExtNr
INTEGER,
                                   INTENT(IN )
                                                                                  ! Extension Nr.
                                   INTENT(IN
                                                              :: NSPC
INTEGER,
                                                 )
                                                                                  ! # of species
                                                              :: SpcNames(NSPC) ! Species string
CHARACTER(LEN=*),
                                   INTENT(IN )
                                   INTENT(IN ) :: Prefix ! search prefix
INTENT(IN ), OPTIONAL :: DefVal_SP ! default value
INTENT(IN ), OPTIONAL :: DefVal_IN ! default value
CHARACTER(LEN=*),
REAL(sp),
INTEGER,
                                   INTENT(IN ), OPTIONAL :: DefVal_Char ! default value
CHARACTER(LEN=*),
```

# **OUTPUT PARAMETERS:**

```
REAL(sp), INTENT( OUT), OPTIONAL :: SpcScal_SP(NSPC) ! Species valuated in the species of the sp
```

## INPUT/OUTPUT PARAMETERS:

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

```
10 Jun 2015 - C. Keller - Initial version
20 Sep 2015 - C. Keller - Options are now linked list.
```

### 1.10.10 SetExtNr

Subroutine SetExtNr overwrites the extension number of a given extension. The extension of interest is provided in argument ExtName. If this argument is omitted, the extension numbers of all extensions currently listed in ExtList will be set to the provided number. This is useful to disable all extensions by setting the ExtNr to a negative value.

### **INTERFACE:**

```
SUBROUTINE SetExtNr( am_I_Root, HcoConfig, ExtNr, ExtName, RC )
```

### **USES:**

```
USE CHARPAK_MOD, ONLY: TRANLC
```

### **INPUT PARAMETERS:**

```
LOGICAL, INTENT(IN ) :: am_I_Root
TYPE(ConfigObj), POINTER :: HcoConfig
INTEGER, INTENT(IN ) :: ExtNr
CHARACTER(LEN=*), INTENT(IN ), OPTIONAL :: ExtName
!INPUT/OUTPUT PARAMETER:
INTEGER, INTENT(INOUT) :: RC
```

### REVISION HISTORY:

```
12 Jan 2015 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

### 1.10.11 ExtNrInUse

Function ExtNrInUse checks if extension number ExtNr is in the list of used extensions or not.

### **INTERFACE:**

```
FUNCTION ExtNrInUse( ExtList, ExtNr ) Result ( InUse )
```

### INPUT PARAMETERS:

```
TYPE(Ext), POINTER :: ExtList INTEGER, INTENT(IN ) :: ExtNr
```

## RETURN VALUE:

```
LOGICAL :: InUse
```

```
03 Oct 2013 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

### 1.10.12 ExtFinal

Function ExtFinal finalizes the extensions list.

### **INTERFACE:**

```
SUBROUTINE ExtFinal( ExtList )
!INPUT/OUTPUT ARGUMENT:
    TYPE(Ext), POINTER :: ExtList
```

### REVISION HISTORY:

```
03 Oct 2013 - C. Keller - Initial version
20 Sep 2015 - C. Keller - Options are now linked list.
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 1.10.13 HCO\_AddOpt

Subroutine HCO\_AddOpt adds a option name/value pair to the list of options.

# **INTERFACE:**

```
SUBROUTINE HCO_AddOpt ( am_I_Root, HcoConfig, OptName, OptValue, ExtNr, RC, & VERB, IgnoreIfExist )
```

# INPUT PARAMETERS:

```
INTENT(IN
                                    :: am_I_Root ! Root CPU?
LOGICAL,
                           )
                                     :: HcoConfig
                                                      ! HEMCO config obj
TYPE(ConfigObj), POINTER
                                    :: OptName ! OptName :: OptValue ! OptValue
CHARACTER(LEN=*), INTENT(IN )
CHARACTER(LEN=*), INTENT(IN )
INTEGER,
                                      :: ExtNr
                                                      ! Extension Nr.
               INTENT(IN )
               INTENT(IN ), OPTIONAL :: VERB
LOGICAL,
                                                      ! Verbose on
LOGICAL,
           INTENT(IN ), OPTIONAL :: IgnoreIfExist ! Ignore if already exists
```

## **OUTPUT PARAMETERS:**

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

```
18 Sep 2015 - C. Keller - Initial version
12 Dec 2015 - C. Keller - Added argument IgnoreIfExist
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 1.10.14 HCO\_GetOpt

Subroutine HCO\_GetOpt returns a option value for the given option name.

### **INTERFACE:**

```
FUNCTION HCO_GetOpt ( ExtList, OptName, ExtNr ) RESULT ( OptValue )
```

### INPUT PARAMETERS:

```
TYPE(Ext), POINTER :: ExtList ! Extension list CHARACTER(LEN=*), INTENT(IN ) :: OptName ! OptName
```

INTEGER, INTENT(IN ), OPTIONAL :: ExtNr ! Extension Nr.

## **OUTPUT PARAMETERS:**

```
CHARACTER(LEN=OPTLEN) :: OptValue ! OptValue
```

# **REVISION HISTORY:**

```
18 Sep 2015 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 1.10.15 HCO\_ROOT

Function HCO\_ROOT returns the root character string. This is a wrapper routine equivalent to HCO\_GetOpt('ROOT'). Since the ROOT character is called very frequently, it is recommended to use this routine instead.

### **INTERFACE:**

```
FUNCTION HCO_ROOT ( HcoConfig ) RESULT ( OutRoot )
```

## INPUT PARAMETERS:

### **OUTPUT PARAMETERS:**

```
TYPE(ConfigObj), POINTER :: HcoConfig CHARACTER(LEN=OPTLEN) :: OutRoot ! Root output
```

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

# 1.10.16 HCO\_CleanupOpt

Subroutine HCO\_CleanupOpt cleans up the given options linked list.

### **INTERFACE:**

```
SUBROUTINE HCO_CleanupOpt ( OptList )
```

### INPUT PARAMETERS:

### **OUTPUT PARAMETERS:**

```
TYPE(Opt), POINTER :: OptList
```

## **REVISION HISTORY:**

```
18 Sep 2015 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 1.10.17 HCO\_SetDefaultToken

Subroutine HCO\_SetDefaultToken is a wrapper routine to initialize the default set of HEMCO tokens. These can be obtained at any place in the HEMCO code via subroutine HCO\_GetOpt, e.g. HCO\_GetOpt('RES') will return the 'RES' token.

# **INTERFACE:**

```
{\tt SUBROUTINE\ HCO\_SetDefaultToken\ (\ am\_I\_Root,\ CF,\ RC\ )}
```

## **USES:**

# INPUT PARAMETERS:

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

TYPE(ConfigObj), POINTER :: CF
```

# **OUTPUT PARAMETERS:**

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

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

### 1.11 Fortran: Module Interface hco\_filedata\_mod.F90

Module HCO\_Filedata\_Mod contains routines and variables to handle the HEMCO file data object FileData. FileData holds all information of source file data, such as file name, update frequency, temporal resolution, the data array itself, etc. These values are specified in the HEMCO configuration file. Many of these attributes are primarily used for reading/updating the data from file using the HEMCO generic file reading routines. Within an ESMF environment, these attributes may be obsolete.

FileData consists of the following elements:

- ncFile: path and filename to the source file, as specified in the configuration file.
- ncPara: file parameter (variable) of interest, as specified in the configuration file.
- ncYrs: range of years in the source file, as specified in the configuration file through the timestamp attribute.
- ncMts: range of months in the source file, as specified in the configuration file through the timestamp attribute.
- ncDys: range of days in the source file, as specified in the configuration file through the timestamp attribute.
- ncHrs: range of hours in the source file, as specified in the configuration file through the timestamp attribute.
- CycleFlag: determines how to deal with time stamps that do not correspond to one of the source file time slices. If set to 1, the closest available time slice (in the past) is used (or the first available time slice if model time is before first available time slice). If set to 2, the file data is ignored if model time is outside of the source file range. If CycleFlag is set to 3, an error is returned if none of the file time slices matches the model time.
- MustFind: if yes, the code returns with an error if no field can be found for the given simulation time (and according to the cycle flag and time attribute settings). Only of relevance for cycle flags range and exact.
- UpdtFlag: determines the update frequency of the data. This is currently only used to distinguish containers that are updated on every time step (always) or according to the frequency provided in the HEMCO configuration file via attribute 'srcTime'.
- ncRead: logical denoting whether or not we need to read this data container. ncRead is set to false for containers whose data is directly specified in the configuration file. For internal use only.
- OrigUnit: original unit of data.
- ArbDimName: name of additional (arbitrary) file dimension.
- ArbDimVal: desired value of arbitrary dimension.
- IsConc: Set to true if data is concentration. Concentration data will be added to the concentration array instead of the emission array.

- IsLocTime: Set to true if data is in local time. Defaults to false and becomes only true if data is scalar (e.g. uniform diurnal scale factors), country-specific data (read from ASCII), or weekdaily data.
- V3: vector of 3D fields. For 3D-data, this vector will hold the 3D arrays of all time slices kept in memory (e.g. 24 elements for hourly data).
- V2: vector of 2D fields. For 2D-data, this vector will hold the 2D arrays of all time slices kept in memory (e.g. 24 elements for hourly data).
- tIDx: derived type used for proper indexing of the time slices in memory. Internal use only.
- Cover: data coverage on this CPU: 0=no overlap; 1=full overlap; -1=partial overlap. As determined from the mask regions specified in the configuration file.
- SpaceDim: spatial dimension of data array: 1 = spatially uniform (x=y=z=1); 2 = 2D data (x,y); 3 = 3D data (x,y,z).
- Levels: handling of vertical levels (3D data only). For internal use only.
- nt: time dimension. length of vector V3 or V2. For internal use only.
- DeltaT: time interval between time slices. For internal use only. ID i (e.g. cIDList(3) points to data-container w/ cID = 3).
- DoShare: will be set to True if this file data object is shared by multiple data containers. For internal use only.
- IsInList: will be set to True if this file data object is part of the emissions list EmisList. For internal use only.
- IsTouched: will be set to True as soon as the container becomes touched for the first time. For internal use only.

# **INTERFACE:**

MODULE HCO\_FileData\_Mod

### **USES:**

USE HCO\_TYPES\_MOD USE HCO\_ERROR\_MOD USE HCO\_ARR\_MOD

IMPLICIT NONE PRIVATE

# PUBLIC MEMBER FUNCTIONS:

PUBLIC :: FileData\_Init

PUBLIC :: FileData\_Cleanup

PUBLIC :: FileData\_ArrCheck

PUBLIC :: FileData\_ArrIsDefined

PUBLIC :: FileData\_ArrIsTouched

PUBLIC :: FileData\_ArrInit

# PRIVATE MEMBER FUNCTIONS:

PRIVATE :: FileData\_ArrCheck2D
PRIVATE :: FileData\_ArrCheck3D

## REVISION HISTORY:

```
19 Dec 2013 - C. Keller - Initialization
01 Jul 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
01 Jul 2014 - R. Yantosca - Now use F90 free-format indentation
21 Aug 2014 - C. Keller - Added concentration
23 Dec 2014 - C. Keller - Added argument IsInList
06 Oct 2015 - C. Keller - Added argument MustFind
```

### 1.11.1 FileData Init

Subroutine FileData\_Init initializes a new (blank) file data object.

# **INTERFACE:**

```
SUBROUTINE FileData_Init( FileDta )
```

### **INPUT PARAMETERS:**

```
TYPE(FileData), POINTER :: FileDta
```

## **REVISION HISTORY:**

```
19 Dec 2013 - C. Keller - Initialization
21 Aug 2014 - C. Keller - Added concentration
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 1.11.2 FileData\_Cleanup

Subroutine FileData\_Cleanup cleans up the file data object FileDta. If DeepClean is set to False, only the data arrays will be removed.

# **INTERFACE:**

```
SUBROUTINE FileData_Cleanup( FileDta, DeepClean )
```

## INPUT PARAMETERS:

```
TYPE(FileData), POINTER :: FileDta
LOGICAL, INTENT(IN) :: DeepClean
```

```
19 Dec 2013 - C. Keller: Initialization
```

### 1.11.3 FileData\_ArrCheck2D

Subroutine FileData\_ArrCheck2D allocates the 2D data array vector of the given file data object if it is not yet allocated. If already allocated, it compares the array dimensions against the passed dimensions.

### **INTERFACE:**

```
SUBROUTINE FileData_ArrCheck2D( HcoConfig, FileDta, nx, ny, nt, RC )
```

# **INPUT PARAMETERS:**

```
TYPE(ConfigObj), POINTER
                              :: HcoConfig ! HEMCO config object
TYPE(FileData), POINTER
                              :: FileDta
                                          ! file data object
INTEGER,
                INTENT(IN)
                                           ! x-dim
                              :: nx
INTEGER,
                INTENT(IN)
                                           ! v-dim
                              :: ny
INTEGER,
                INTENT(IN)
                              :: nt
                                           ! time dim => vector length
```

## INPUT/OUTPUT PARAMETERS:

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

### REVISION HISTORY:

```
20 Apr 2013 - C. Keller - Initial version
```

### 1.11.4 FileData\_ArrCheck3D

Subroutine FileData\_ArrCheck3D allocates the 3D data array vector of the given file data object if it is not yet allocated. If already allocated, it compares the array dimensions against the passed dimensions.

### **INTERFACE:**

```
SUBROUTINE FileData_ArrCheck3D( HcoConfig, FileDta, nx, ny, nz, nt, RC)
USES:
```

### INPUT PARAMETERS:

```
TYPE(ConfigObj), POINTER :: HcoConfig ! HEMCO config object
TYPE(FileData), POINTER
                             :: FileDta ! Container
INTEGER,
               INTENT(IN)
                                          ! x-dim
                             :: nx
                                          ! y-dim
INTEGER,
               INTENT(IN)
                              :: ny
                                          ! z-dim
INTEGER,
               INTENT(IN)
                             :: nz
                                          ! Time dim => vector length
INTEGER,
               INTENT(IN)
                             :: nt
```

## INPUT/OUTPUT PARAMETERS:

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

```
20 Apr 2013 - C. Keller - Initial version
```

## 1.11.5 FileData\_ArrIsDefined

Function FileData\_ArrIsDefined returns true if the data array of the given file data object is defined.

#### INTERFACE:

```
FUNCTION FileData_ArrIsDefined( FileDta ) RESULT( IsDefined )
```

## INPUT PARAMETERS:

```
TYPE(FileData), POINTER :: FileDta ! Container
```

## RETURN VALUE:

LOGICAL :: IsDefined

# **REVISION HISTORY:**

```
20 Apr 2013 - C. Keller - Initial version
```

## 1.11.6 FileData\_ArrIsTouched

Function FileData\_ArrIsTouched returns true if the data array of the given file data object has already been touched, e.g. if the data has already been read (or at least attempted to being read). This information is mostly important for file data objects that are shared by multiple data containers. See ReadList\_Fill in hco\_readlist\_mod.F90 for more details.

## **INTERFACE:**

```
FUNCTION FileData_ArrIsTouched(FileDta) RESULT(IsTouched)
```

## INPUT PARAMETERS:

```
TYPE(FileData), POINTER :: FileDta ! Container
```

#### RETURN VALUE:

LOGICAL :: IsTouched

#### REVISION HISTORY:

```
17 Mar 2015 - C. Keller - Initial version
```

## 1.11.7 FileData\_ArrInit2D

Subroutine FileData\_ArrInit2D is a wrapper routine to initialize 2D data arrays of a file data object. To ensure proper functioning of the file data object and related routines, this routine should always be used to initialize file data arrays (and NOT HCO\_ArrInit directly!).

```
SUBROUTINE FileData_ArrInit2D(FileDta, nt, nx, ny, RC)
```

#### **USES:**

## INPUT PARAMETERS:

## INPUT/OUTPUT PARAMETERS:

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

#### **REVISION HISTORY:**

```
01 Oct 2014 - C. Keller - Initial version
```

## 1.11.8 FileData\_ArrInit3D

Subroutine FileData\_ArrInit3D is a wrapper routine to initialize 3D data arrays of a file data object. To ensure proper functioning of the file data object and related routines, this routine should always be used to initialize file data arrays (and NOT HCO\_ArrInit directly!).

## **INTERFACE:**

**USES:** 

```
SUBROUTINE FileData_ArrInit3D( FileDta, nt, nx, ny, nz, RC )
```

# **INPUT PARAMETERS:**

```
TYPE(FileData), POINTER
                               :: FileDta ! Container
                INTENT(IN)
                                            ! Time dim => vector length
INTEGER,
                               :: nt
                                            ! x-dim
INTEGER,
                INTENT(IN)
                               :: nx
INTEGER,
                INTENT(IN)
                                            ! y-dim
                               :: ny
                                            ! z-dim
INTEGER,
                INTENT(IN)
                               :: nz
```

# INPUT/OUTPUT PARAMETERS:

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

```
20 Apr 2013 - C. Keller - Initial version
```

## 1.12 Fortran: Module Interface hco\_fluxarr\_mod.F90

Module HCO\_FluxArr\_Mod contains routines to handle the HEMCO flux arrays. These are the emissions and deposition arrays listed in the HEMCO state object.

#### **INTERFACE:**

```
MODULE HCO_FluxArr_Mod
USES:
USE HCO_Error_Mod
USE HCO_Arr_Mod
USE HCO_State_Mod, ONLY: HCO_State
IMPLICIT NONE
PRIVATE
```

## PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: HCO_EmisAdd
PUBLIC :: HCO_DepvAdd
PUBLIC :: HCO_FluxarrReset
```

## PRIVATE MEMBER FUNCTIONS:

PRIVATE :: DiagnCheck

## **REMARKS:**

#### **REVISION HISTORY:**

```
05 Jan 2014 - C. Keller - Initial version, adapted from hco_state_mod.F90 21 Oct 2014 - C. Keller - Added error check for negative values to HCO_EmisAdd
```

#### 1.12.1 HCO FluxarrReset

Routine HCO\_FluxarrReset (re)sets all data arrays of the passed HEMCO state object. The (optional) argument Typ indicates whether only emissions (1), deposition (2), or concentration (3) arrays shall be reset. To reset all, set Typ to 0 (default).

## **INTERFACE:**

```
SUBROUTINE HCO_FluxarrReset( HcoState, RC, Typ )
```

## INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState INTEGER, INTENT(INOUT) :: RC
```

## INPUT PARAMETERS:

```
INTEGER, INTENT(IN ), OPTIONAL :: Typ
```

#### **REMARKS:**

## **REVISION HISTORY:**

```
01 May 2013 - C. Keller - Initial version
21 Aug 2014 - C. Keller - Added concentration
```

## 1.12.2 HCO\_EmisAdd\_3D\_Dp

Routine HCO\_EmisAdd\_3D adds the 3D-array Arr3D to the emissions array of species HcoID in HEMCO object HcoState. This routine also updates all autofill diagnostics that are defined for the givne species, extension number, emission category and hierarchy.

#### **INTERFACE:**

```
SUBROUTINE HCO_EmisAdd_3D_Dp( am_I_Root, HcoState, Arr3D, HcoID, & RC, ExtNr, Cat, Hier, & MinDiagnLev )
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState
```

REAL(dp), INTENT(INOUT) :: Arr3D( HcoState%NX, &

HcoState%NY, &
HcoState%NZ )

INTEGER, INTENT(INOUT) :: RC

## **INPUT PARAMETERS:**

```
LOGICAL,
                 INTENT(IN
                             )
                                          :: am_I_Root
INTEGER,
                 INTENT(IN
                             )
                                          :: HcoID
INTEGER,
                 INTENT(IN
                             ), OPTIONAL :: ExtNr
                             ), OPTIONAL :: Cat
INTEGER,
                 INTENT(IN
                             ), OPTIONAL :: Hier
INTEGER,
                 INTENT(IN
                             ), OPTIONAL :: MinDiagnLev
INTEGER,
                 INTENT(IN
```

## **REVISION HISTORY:**

```
01 May 2013 - C. Keller - Initial version
20 Apr 2015 - C. Keller - Added DiagnCheck
```

## 1.12.3 HCO\_EmisAdd\_3D\_Sp

Routine HCO\_EmisAdd\_3D adds the 3D-array Arr3D to the emissions array of species HcoID in HEMCO object HcoState. This routine also updates all autofill diagnostics that are defined for the givne species, extension number, emission category and hierarchy.

```
SUBROUTINE HCO_EmisAdd_3D_Sp ( am_I_Root, HcoState, Arr3D, HcoID, & RC, ExtNr, Cat, Hier, & MinDiagnLev )
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState
```

REAL(sp), INTENT(INOUT) :: Arr3D( HcoState%NX, &

HcoState%NY, &
HcoState%NZ )

INTEGER, INTENT(INOUT) :: RC

## INPUT PARAMETERS:

```
LOGICAL,
                INTENT(IN
                                        :: am_I_Root
INTEGER,
                                         :: HcoID
                INTENT(IN
INTEGER,
                            ), OPTIONAL :: ExtNr
                INTENT(IN
INTEGER,
                INTENT(IN
                            ), OPTIONAL :: Cat
                           ), OPTIONAL :: Hier
INTEGER,
                INTENT(IN
                            ), OPTIONAL :: MinDiagnLev
INTEGER,
                 INTENT(IN
```

## **REVISION HISTORY:**

```
01 May 2013 - C. Keller - Initial version
20 Apr 2015 - C. Keller - Added DiagnCheck
```

## 1.12.4 HCO\_EmisAdd\_2D\_Dp

Routine HCO\_EmisAdd\_2D\_Dp adds the real\*8 2D-array Arr2D to the emission array of species HcoID in HEMCO object HcoState. This routine also updates all autofill diagnostics that are defined for the givne species, extension number, emission category and hierarchy.

## **INTERFACE:**

```
SUBROUTINE HCO_EmisAdd_2D_Dp( am_I_Root, HcoState, Arr2D, HcoID, & RC, ExtNr, Cat, Hier, & MinDiagnLev )
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState
```

REAL(dp), INTENT(INOUT) :: Arr2D(HcoState%NX,HcoState%NY)

INTEGER, INTENT(INOUT) :: RC

#### INPUT PARAMETERS:

```
LOGICAL,
                INTENT(IN
                                        :: am_I_Root
                                        :: HcoID
INTEGER,
                INTENT(IN
                           ), OPTIONAL :: ExtNr
INTEGER,
                INTENT(IN
INTEGER,
                INTENT(IN
                           ), OPTIONAL :: Cat
INTEGER,
                INTENT(IN
                            ), OPTIONAL :: Hier
                           ), OPTIONAL :: MinDiagnLev
INTEGER,
                INTENT(IN
```

## **REVISION HISTORY:**

```
01 May 2013 - C. Keller - Initial version
20 Apr 2015 - C. Keller - Added DiagnCheck
```

## 1.12.5 HCO\_EmisAdd\_2D\_Sp

Routine HCO\_EmisAdd\_2D\_Sp adds the real\*4 2D-array Arr2D to the emission array of species HcoID in HEMCO object HcoState. This routine also updates all autofill diagnostics that are defined for the givne species, extension number, emission category and hierarchy.

#### **INTERFACE:**

```
SUBROUTINE HCO_EmisAdd_2D_Sp( am_I_Root, HcoState, Arr2D, HcoID, & RC, ExtNr, Cat, Hier, & MinDiagnLev)
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState

REAL(sp), INTENT(INOUT) :: Arr2D(HcoState%NX, HcoState%NY)

INTEGER, INTENT(INOUT) :: RC
```

#### INPUT PARAMETERS:

```
LOGICAL,
                 INTENT(IN
                                         :: am_I_Root
                                         :: HcoID
INTEGER,
                 INTENT(IN
INTEGER,
                 INTENT(IN
                             ), OPTIONAL :: ExtNr
                            ), OPTIONAL :: Cat
INTEGER,
                 INTENT(IN
                             ), OPTIONAL :: Hier
INTEGER,
                 INTENT(IN
                            ), OPTIONAL :: MinDiagnLev
INTEGER,
                 INTENT(IN
```

## **REVISION HISTORY:**

```
01 May 2013 - C. Keller - Initial version
20 Apr 2015 - C. Keller - Added DiagnCheck
```

## 1.12.6 HCO\_EmisAdd\_Dp

Routine HCO\_EmisAdd\_Dp adds value iVal to the emission array of species HcoID in HEMCO object HcoState. The value is placed at location I, J, L of the array.

## **INTERFACE:**

```
SUBROUTINE HCO_EmisAdd_Dp( HcoState, iVal, HcoID, I, J, L, RC )
```

## INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState
REAL(dp), INTENT(INOUT) :: iVal
INTEGER, INTENT(INOUT) :: RC
```

#### INPUT PARAMETERS:

```
INTEGER, INTENT(IN ) :: HcoID
INTEGER, INTENT(IN ) :: I
INTEGER, INTENT(IN ) :: J
INTEGER, INTENT(IN ) :: L
```

#### **REVISION HISTORY:**

```
01 May 2013 - C. Keller - Initial version
```

## 1.12.7 HCO\_EmisAdd\_Sp

Routine HCO\_EmisAdd\_Sp adds value iVal to the emission array of species HcoID in HEMCO object HcoState. The value is placed at location I, J, L of the array.

## **INTERFACE:**

```
SUBROUTINE HCO_EmisAdd_Sp( HcoState, iVal, HcoID, I, J, L, RC )
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState
REAL(sp), INTENT(INOUT) :: iVal
INTEGER, INTENT(INOUT) :: RC
```

# **INPUT PARAMETERS:**

```
INTEGER, INTENT(IN ) :: HcoID
INTEGER, INTENT(IN ) :: I
INTEGER, INTENT(IN ) :: J
INTEGER, INTENT(IN ) :: L
```

#### REVISION HISTORY:

```
01 May 2013 - C. Keller - Initial version
```

## 1.12.8 HCO\_DepvAdd\_2D\_Dp

Routine HCO\_DepvAdd\_2D\_Dp adds the real\*8 2D-array Arr2D to the depostion array of species HcoID in HEMCO object HcoState.

```
SUBROUTINE HCO_DepvAdd_2D_Dp( HcoState, Arr2D, HcoID, RC )
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState INTEGER, INTENT(INOUT) :: RC
```

## INPUT PARAMETERS:

```
REAL(dp), INTENT(IN ) :: Arr2D(HcoState%NX,HcoState%NY)
INTEGER, INTENT(IN ) :: HcoID
```

#### REVISION HISTORY:

```
01 May 2013 - C. Keller - Initial version
```

# 1.12.9 HCO\_DepvAdd\_2D\_Sp

Routine HCO\_DepvAdd\_2D\_Sp adds the real\*4 2D-array Arr2D to the depostion array of species HcoID in HEMCO object HcoState.

## **INTERFACE:**

```
SUBROUTINE HCO_DepvAdd_2D_Sp( HcoState, Arr2D, HcoID, RC )
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState INTEGER, INTENT(INOUT) :: RC
```

## **INPUT PARAMETERS:**

```
REAL(sp), INTENT(IN ) :: Arr2D(HcoState%NX,HcoState%NY)
INTEGER, INTENT(IN ) :: HcoID
```

## **REVISION HISTORY:**

```
01 May 2013 - C. Keller - Initial version
```

# 1.12.10 HCO\_DepvAdd\_Dp

Routine HCO\_DepvAdd\_Dp adds value iVal to the deposition array of species HcoID in HEMCO object HcoState. The value is placed at location I, J of the array.

# INTERFACE:

```
SUBROUTINE HCO_DepvAdd_Dp( HcoState, iVal, HcoID, I, J, RC )
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState INTEGER, INTENT(INOUT) :: RC
```

## **INPUT PARAMETERS:**

```
REAL(dp), INTENT(IN ) :: iVal
INTEGER, INTENT(IN ) :: HcoID
INTEGER, INTENT(IN ) :: I
INTEGER, INTENT(IN ) :: J
```

## REVISION HISTORY:

```
01 May 2013 - C. Keller - Initial version
```

# 1.12.11 HCO\_DepvAdd\_Sp

Routine HCO\_DepvAdd\_Sp adds value iVal to the deposition array of species HcoID in HEMCO object HcoState. The value is placed at location I, J of the array.

#### **INTERFACE:**

```
SUBROUTINE HCO_DepvAdd_Sp( HcoState, iVal, HcoID, I, J, RC )
```

## INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState
INTEGER, INTENT(INOUT) :: RC
```

## INPUT PARAMETERS:

```
REAL(sp), INTENT(IN ) :: iVal
INTEGER, INTENT(IN ) :: HcoID
INTEGER, INTENT(IN ) :: I
INTEGER, INTENT(IN ) :: J
```

## **REVISION HISTORY:**

```
01 May 2013 - C. Keller - Initial version
```

## 1.12.12 DiagnCheck

Subroutine DiagnCheck checks if the given emission array needs to be added to any auto-fill diagnostics. The diagnostics to be filled (if any) depend on the passed extension number, emission category and hierarchy, and the HEMCO species ID.

# **INTERFACE:**

```
SUBROUTINE DiagnCheck( am_I_Root, HcoState, ExtNr, Cat, & Hier, HcoID, Arr3D, Arr3Dsp, & Arr2D, Arr2Dsp, MinDiagnLev, RC )
```

## **USES:**

USE HCO\_DIAGN\_MOD

## INPUT PARAMETERS:

```
LOGICAL,
                 INTENT(IN
                                         :: am_I_Root
INTEGER,
                 INTENT(IN
                                         :: HcoID
                             )
INTEGER,
                 INTENT(IN
                             ), OPTIONAL :: ExtNr
INTEGER,
                 INTENT(IN
                             ), OPTIONAL :: Cat
INTEGER,
                 INTENT(IN
                             ), OPTIONAL :: Hier
                            ), OPTIONAL :: MinDiagnLev
INTEGER,
                 INTENT(IN
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER
                                          :: HcoState
REAL(dp),
                 INTENT(INOUT), OPTIONAL :: Arr3D(
                                                     HcoState%NX, &
                                                      HcoState%NY, &
                                                      HcoState%NZ )
REAL(sp),
                 INTENT(INOUT), OPTIONAL :: Arr3Dsp( HcoState%NX, &
                                                      HcoState%NY, &
                                                      HcoState%NZ )
                 INTENT(INOUT), OPTIONAL :: Arr2D(
REAL(dp),
                                                     HcoState%NX, &
                                                      HcoState%NY )
REAL(sp),
                 INTENT(INOUT), OPTIONAL :: Arr2Dsp( HcoState%NX, &
                                                      HcoState%NY )
INTEGER,
                 INTENT(INOUT)
                                         :: RC
```

## REVISION HISTORY:

```
20 Apr 2015 - C. Keller - Initial version
```

# 1.13 Fortran: Module Interface hco\_geotools\_mod.F90

Module HCO\_GeoTools\_Mod contains a collection of helper routines for extracting geographical information. These routines are based upon GEOS-5 data and may need to be revised for other met. fields!

# **INTERFACE:**

```
MODULE HCO_GeoTools_Mod
```

## **USES:**

```
USE HCO_Error_Mod
```

IMPLICIT NONE PRIVATE

## PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: HCO_LandType
PUBLIC :: HCO_ValidateLon
PUBLIC :: HCO_GetSUNCOS
PUBLIC :: HCO_GetHorzIJIndex
PUBLIC :: HCO_CalcVertGrid
PUBLIC :: HCO_SetPBLm
PUBLIC :: HCO_CalcPBLlev
INTERFACE HCO_LandType
   MODULE PROCEDURE HCO_LandType_Dp
   MODULE PROCEDURE HCO_LandType_Sp
END INTERFACE HCO_LandType
INTERFACE HCO_ValidateLon
   MODULE PROCEDURE HCO_ValidateLon_Dp
   MODULE PROCEDURE HCO_ValidateLon_Sp
END INTERFACE HCO_ValidateLon
 INTERFACE HCO_CalcPBLlev
   MODULE PROCEDURE HCO_CalcPBLlev2D
   MODULE PROCEDURE HCO_CalcPBLlev3D
 END INTERFACE HCO_CalcPBLlev
```

#### PRIVATE MEMBER FUNCTIONS:

PRIVATE:: HCO\_LandType\_Dp
PRIVATE:: HCO\_LandType\_Sp
PRIVATE:: HCO\_ValidateLon\_Dp
PRIVATE:: HCO\_ValidateLon\_Sp

## **REVISION HISTORY:**

```
18 Dec 2013 - C. Keller - Initialization
01 Jul 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
01 Jul 2014 - R. Yantosca - Now use F90 free-format indentation
16 Jul 2014 - C. Keller - Added HCO_ValidateLon
```

## 1.13.1 HCO\_LandType\_Sp

Function HCO\_LANDTYPE returns the land type based upon the land water index (0=water,1=land,2=ice) and the surface albedo. Inputs are in single precision.

## **INTERFACE:**

```
FUNCTION HCO_LandType_Sp( WLI, Albedo ) Result ( LandType )
```

## INPUT PARAMETERS:

```
REAL(sp), INTENT(IN) :: WLI ! Land type: 0=water,1=land,2=ice
```

REAL(sp), INTENT(IN) :: Albedo ! Surface albedo

!RETURN VALUE

INTEGER :: LandType ! Land type: 0=water,1=land,2=ice

#### **REMARKS:**

This function is largely based on the GEOS-Chem functions in dao\_mod.F.

#### REVISION HISTORY:

18 Dec 2013 - C. Keller - Initialization!

# $1.13.2 \quad HCO\_LandType\_Dp$

Function HCO\_LandType\_Dp returns the land type based upon the land water index (0=water,1=land,2=ice) and the surface albedo. Inputs are in double precision.

## INTERFACE:

```
FUNCTION HCO_LandType_Dp( WLI, Albedo ) Result ( LandType )
```

## INPUT PARAMETERS:

```
REAL(dp), INTENT(IN) :: WLI ! Land type: 0=water,1=land,2=ice REAL(dp), INTENT(IN) :: Albedo ! Surface albedo
```

## RETURN VALUE:

```
INTEGER :: LandType ! Land type: 0=water,1=land,2=ice
```

# **REMARKS:**

This function is largely based on the GEOS-Chem functions in dao\_mod.F.

## **REVISION HISTORY:**

```
18 Dec 2013 - C. Keller - Initialization
```

# 1.13.3 HCO\_ValidateLon\_Sp

Subroutine HCO\_ValidateLon\_Sp ensures that the passed single precision longitude axis LON is steadily increasing.

# INTERFACE:

```
SUBROUTINE HCO_ValidateLon_Sp ( HcoState, NLON, LON, RC )
```

## **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_STATE
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object
INTEGER, INTENT(IN ) :: NLON ! # of lons
```

# INPUT/OUTPUT PARAMETERS:

```
REAL(sp), INTENT(INOUT) :: LON(NLON) ! longitude axis INTEGER, INTENT(INOUT) :: RC ! Return code
```

## REVISION HISTORY:

```
16 Jul 2014 - C. Keller - Initialization
```

# 1.13.4 HCO\_ValidateLon\_Dp

Subroutine HCO\_ValidateLon\_Sp ensures that the passed double precision longitude axis LON is steadily increasing.

# **INTERFACE:**

```
SUBROUTINE HCO_ValidateLon_Dp ( HcoState, NLON, LON, RC )
```

#### **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_STATE
```

## INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object INTEGER, INTENT(IN ) :: NLON ! # of lons
```

## INPUT/OUTPUT PARAMETERS:

```
REAL(dp), INTENT(INOUT) :: LON(NLON) ! longitude axis INTEGER, INTENT(INOUT) :: RC ! Return code
```

# **REVISION HISTORY:**

```
16 Jul 2014 - C. Keller - Initialization
```

## 1.13.5 HCO\_GetSUNCOS

Subroutine HCO\_GetSUNCOS calculates the solar zenith angle for the given date.

```
SUBROUTINE HCO_GetSUNCOS( am_I_Root, HcoState, SUNCOS, DT, RC )
!USES

USE HCO_STATE_MOD, ONLY: HCO_STATE

USE HCO_CLOCK_MOD, ONLY: HcoClock_Get

USE HCO_CLOCK_MOD, ONLY: HcoClock_GetLocal
```

# INPUT/OUTPUT PARAMETERS:

```
LOGICAL,
               INTENT(IN
```

TYPE(HCO\_State), POINTER

INTEGER, INTENT(IN

#### **OUTPUT PARAMETERS:**

```
REAL(hp),
                INTENT( OUT) :: SUNCOS(HcoState%NX,HcoState%NY)
```

# INPUT/OUTPUT PARAMETERS:

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

## **REVISION HISTORY:**

```
22 May 2015 - C. Keller - Initial version, based on GEOS-Chem's dao_mod.F.
```

10 Jul 2015 - R. Yantosca - Corrected issues in ProTeX header

## 1.13.6 HCO\_GetHorzIJIndex

Function HCO\_GetHorzIJIndex returns the grid box index for the given longitude (deg E, -180...180), and latitude (deg N, -90...90).

# **INTERFACE:**

```
SUBROUTINE HCO_GetHorzIJIndex(am_I_Root, HcoState, N, Lon, Lat, idx, jdx, RC)
!USES
```

#include "MAPL\_Generic.h"

USE ESMF

USE MAPL\_Mod

USE HCO\_STATE\_MOD, ONLY : HCO\_STATE

## INPUT PARAMETERS:

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

:: HcoState TYPE(HCO\_State), POINTER ! HEMCO state object

INTENT(IN INTEGER, ) :: N INTENT(IN ) :: Lon(N) REAL(hp), REAL(hp), INTENT(IN ) :: Lat(N)

## INPUT/OUTPUT PARAMETERS:

INTENT(INOUT) :: RC INTEGER,

## **OUTPUT PARAMETERS:**

INTENT( OUT) :: IDX(N), JDX(N) INTEGER,

#### **REVISION HISTORY:**

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

10 Jul 2015 - R. Yantosca - Corrected issues in ProTeX header

## 1.13.7 HCO\_GetHorzIJIndex

Function HCO\_GetHorzIJIndex returns the grid box index for the given longitude (deg E, -180...180), and latitude (deg N, -90...90).

#### **INTERFACE:**

```
SUBROUTINE HCO_GetHorzIJIndex( am_I_Root, HcoState, N, Lon, Lat, idx, jdx, RC )
```

## **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_STATE
```

## INPUT PARAMETERS:

```
LOGICAL,
                  INTENT(IN
                                  :: am_I_Root
                                                     ! Root CPU?
                                                     ! HEMCO state object
TYPE(HCO_State), POINTER
                                  :: HcoState
INTEGER,
                  INTENT(IN
                                  :: N
REAL(hp),
                                  :: Lon(N)
                  INTENT(IN
REAL(hp),
                  INTENT(IN
                                  :: Lat(N)
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

#### **OUTPUT PARAMETERS:**

```
INTEGER, INTENT( OUT) :: IDX(N), JDX(N)
```

#### REVISION HISTORY:

```
04 Jun 2015 - C. Keller - Initial version
10 Jul 2015 - R. Yantosca - Corrected issues in ProTeX header
```

#### 1.13.8 HCO\_CalcVertGrid

Function HCO\_CalcVertGrid calculates the vertical grid quantities surface pressure PSFC [Pa], surface geopotential height ZSFC [m], grid box height BXHEIGHT [m], and pressure edges PEDGE [Pa]. Any of these fields can be passed explicitly to the routine, in which case these fields are being used. If not passed through the routine (i.e. if the corresponding input argument pointer is nullified), the field is searched in the HEMCO configuration file. If not found in the configuration file, the field is approximated from other quantities (if possible). For example, if surface pressures are provided (either passed as argument or in the HEMCO configuration file as field PSFC), pressure edges are calculated from PSFC and the vertical grid coordinates (Ap and Bp for a hybrid sigma coordinate system). The temperature field TK [K] is needed to approximate box heights and/or geopotential height (via the hydrostatic equation).

```
SUBROUTINE HCO_CalcVertGrid ( am_I_Root, HcoState, PSFC, & ZSFC, TK, BXHEIGHT, PEDGE, RC )
!USES

USE HCO_Arr_Mod, ONLY: HCO_ArrAssert

USE HCO_STATE_MOD, ONLY: HCO_STATE

USE HCO_CALC_MOD, ONLY: HCO_EvalFld
```

#### INPUT PARAMETERS:

```
) :: am_I_Root
                                                    ! Root CPU?
LOGICAL,
                 INTENT(IN
TYPE(HCO_State), POINTER
                                 :: HcoState
                                                    ! HEMCO state object
                                                    ! surface pressure (Pa)
REAL(hp),
                                :: PSFC(:,:)
                 POINTER
                                :: ZSFC(:,:)
:: TK (:,:,:)
                                                    ! surface geopotential height (m)
REAL(hp),
                 POINTER
REAL(hp),
                 POINTER
                                                    ! air temperature (K)
                                 :: BXHEIGHT(:,:,:) ! grid box height (m)
REAL(hp),
                 POINTER
REAL(hp),
                 POINTER
                                :: PEDGE(:,:,:) ! pressure edges (Pa)
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

## **REVISION HISTORY:**

```
28 Sep 2015 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

#### 1.13.9 HCO SetPBLm

Subroutine HCO\_SetPBLm sets the HEMCO PBL mixing height in meters. It first tries to read it from field 'FldName' (from the HEMCO data list), then to fill it from field 'PBLM', and then assigns the default value 'DefVal' to it.

## **INTERFACE:**

```
SUBROUTINE HCO_SetPBLm ( am_I_Root, HcoState, FldName, PBLM, DefVal, RC )
!USES

USE HCO_Arr_Mod, ONLY: HCO_ArrAssert

USE HCO_STATE_MOD, ONLY: HCO_STATE

USE HCO_CALC_MOD, ONLY: HCO_EvalFld
```

#### INPUT PARAMETERS:

```
LOGICAL,
                                         :: am_I_Root
                                                       ! Root CPU?
                 INTENT(IN
                            )
TYPE(HCO_State), POINTER
                                         :: HcoState
                                                       ! HEMCO state object
CHARACTER(LEN=*), OPTIONAL, INTENT(IN
                                      ) :: FldName
                                                       ! field name
REAL(hp),
                 OPTIONAL, POINTER
                                         :: PBLM(:,:) ! pbl mixing height
REAL(hp),
                 OPTIONAL, INTENT(IN
                                      ) :: DefVal
                                                       ! default value
```

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

## **REVISION HISTORY:**

28 Sep 2015 - C. Keller - Initial version

## 1.14 Fortran: Module Interface hco\_interp\_mod.F90

Module HCO\_INTERP\_MOD contains routines to interpolate input data onto the HEMCO grid. This module contains routine for horizontal regridding between regular grids (MAP\_A2A), as well as vertical interpolation amongst GEOS model levels (full ¡–¡, reduced).

Regridding is supported for concentration quantities (default) and index-based values. For the latter, the values in the regridded grid boxes correspond to the value of the original grid that contributes most to the given box.

## **INTERFACE:**

MODULE HCO\_Interp\_Mod

## **USES:**

USE HCO\_Types\_Mod USE HCO\_Error\_Mod USE HCO\_State\_Mod,

ONLY : Hco\_State

IMPLICIT NONE PRIVATE

## PUBLIC MEMBER FUNCTIONS:

PUBLIC :: ModelLev\_Check

PUBLIC :: ModelLev\_Interpolate

PUBLIC :: REGRID\_MAPA2A

# PUBLIC MEMBER FUNCTIONS:

PRIVATE :: GEOS5\_TO\_GEOS4\_LOWLEV

PRIVATE :: COLLAPSE PRIVATE :: INFLATE

```
30 Dec 2014 - C. Keller - Initialization
03 Feb 2015 - C. Keller - Added REGRID_MAPA2A (from hcoio_dataread_mod.F90).
```

## 1.14.1 Regrid\_MAPA2A

Subroutine Regrid\_MAPA2A regrids input array NcArr onto the simulation grid and stores the data in list container Lct. Horizontal regridding is performed using MAP\_A2A algorithm. Vertical interpolation between GEOS levels (full vs. reduced, GEOS-5 vs. GEOS-4), is also supported.

This routine can remap concentrations and index-based quantities.

## **INTERFACE:**

```
SUBROUTINE REGRID_MAPA2A ( am_I_Root, HcoState, NcArr, LonE, LatE, Lct, RC )
```

## **USES:**

```
USE REGRID_A2A_Mod, ONLY : MAP_A2A
```

USE HCO\_FileData\_Mod, ONLY : FileData\_ArrCheck
USE HCO\_UNIT\_MOD, ONLY : HCO\_IsIndexData

#### INPUT PARAMETERS:

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

TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object

REAL(sp), POINTER :: NcArr(:,:,:) ! 4D input data
```

REAL(hp), POINTER :: LonE(:) ! Input grid longitude edges REAL(hp), POINTER :: LatE(:) ! Input grid latitude edges

# INPUT/OUTPUT PARAMETERS:

```
TYPE(ListCont), POINTER :: Lct ! HEMCO list container INTEGER, INTENT(INOUT) :: RC ! Success or failure?
```

# **REVISION HISTORY:**

```
03 Feb 2015 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

#### 1.14.2 ModelLev\_Check

Subroutine ModelLev\_Check checks if the passed number of vertical levels indicates that these are model levels or not.

## **INTERFACE:**

```
SUBROUTINE ModelLev_Check (am_I_Root, HcoState, nLev, IsModelLev, RC)
```

## **USES:**

```
USE HCO_FileData_Mod, ONLY : FileData_ArrCheck
```

## INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root ! Are we on the root CPU? TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object INTEGER, INTENT(IN ) :: nlev ! number of levels
```

## INPUT/OUTPUT PARAMETERS:

```
LOGICAL, INTENT(INOUT) :: IsModelLev ! Are these model levels?

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

## **REVISION HISTORY:**

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

## 1.14.3 ModelLev\_Interpolate

Subroutine ModelLev\_Interpolate puts 3D data from an arbitrary number of model levels onto the vertical levels of the simulation grid. Since the input data is already on model levels, this is only to inflate/collapse fields between native/reduced vertical levels, e.g. from 72 native GEOS-5 levels onto the reduced 47 levels. The vertical interpolation scheme depends on compiler switches. If none of the compiler switches listed below is used, no vertical interpolation is performed, e.g. the vertical levels of the input grid are retained.

The input data (REGR<sub>-4</sub>D) is expected to be already regridded horizontally. The 4th dimension of REGR<sub>-4</sub>D denotes time.

The 3rd dimension of REGR\_3D holds the vertical levels. It is assumed that these are model levels, starting at the surface (level 1). If the input data holds 72 input levels, this is interpreted as native data and will be collapsed onto the reduced grid. If the input data holds X i=47 levels, these levels are interpreted as levels 1-X of the reduced grid. In other words, input data with 33 levels will be interpreted as 33 levels on the reduced grid, and the data is accordingly mapped onto the simulation grid. If data becomes inflated or collapsed, the output data will always extent over all vertical levels of the simulation grid. If necessary, the unused upper levels will be filled with zeros. If no data interpolation is needed, the vertical extent of the output data is limited to the number of used levels. For instance, if the input data has 5 vertical levels, the output array will only extent over those 5 (bottom) levels.

Currently, this routine can remap the following combinations:

- Native GEOS-5 onto reduced GEOS-5 (72 –; 47 levels)
- Reduced GEOS-5 onto native GEOS-5 (47 -; 72 levels)
- Native GEOS-4 onto reduced GEOS-4 (55 –; 30 levels)
- Reduced GEOS-4 onto native GEOS-4 (30 -; 55 levels)
- Native GEOS-5 onto native GEOS-4 (72 –; 55 levels)
- $\bullet$  Reduced GEOS-5 onto native GEOS-4 (47 –; 55 levels)

- Native GEOS-5 onto reduced GEOS-4 (72 -; 30 levels)
- Reduced GEOS-5 onto reduced GEOS-4 (47 -; 30 levels)

Interpolation from GEOS-5 onto GEOS-4 levels is currently not supported.

## **INTERFACE:**

```
SUBROUTINE ModelLev_Interpolate ( am_I_Root, HcoState, REGR_4D, Lct, RC ) USES:
```

```
USE HCO_FileData_Mod, ONLY : FileData_ArrCheck
```

## INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root ! Are we on the root CPU?
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object
REAL(sp), POINTER :: REGR_4D(:,:,:,:) ! 4D input data
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(ListCont), POINTER :: Lct ! HEMCO list container INTEGER, INTENT(INOUT) :: RC ! Success or failure?
```

## **REVISION HISTORY:**

```
30 Dec 2014 - C. Keller - Initial version
24 Feb 2015 - R. Yantosca - Now exit if vertical interpolation isn't needed
12 Aug 2015 - R. Yantosca - Vertically remap MERRA2 as we do for GEOS-FP
24 Sep 2015 - C. Keller - Added interpolation on edges.
06 Dec 2015 - C. Keller - Pass # of GEOS-5 levels to be mapped onto GEOS-4
```

## 1.14.4 GEOS5\_TO\_GEOS4\_LOWLEV

Helper routine to map the lowest 28 GEOS-5 levels onto the lowest 11 GEOS-4 levels. The individual level weights were calculated offline and are hard-coded here. These are the edge pressure values on the lowest 28 GEOS-5 levels: 1013.25, 998.05, 982.76, 967.47, 952.19, 936.91 921.62, 906.34, 891.05, 875.77, 860.49, 845.21, 829.92, 809.55, 784.08, 758.62, 733.15, 707.69, 682.23, 644.05, 605.87, 567.70, 529.54, 491.40, 453.26, 415.15, 377.07, 339.00, 288.92 And these are the edge pressure values on the lowest 12 GEOS-4 levels: 1013.25, 998.16, 968.49, 914.79, 841.15, 752.89, 655.96, 556.85, 472.64, 401.14, 340.43, 288.92 The value at every given GEOS-4 level is determined from the GEOS-5 values by multiplying the (GEOS-5) input data by the normalized level weights. For instance, the first GEOS-5 level is the only level contributing to the 1st GEOS-4 level. For the 2nd GEOS-4 level, contributions from GEOS-5 levels 1-3 are used. Of GEOS-5 level 1, only 0.7is in GEOS-4 level 1), whereas 100level 3 contribute to GEOS-4 level 2. The corresponding normalized weights become 0.00378,0.515, and 0.481, respectively.

The weights don't always add up to exactly 1.00 due to rounding errors.

SUBROUTINE GEOS5\_TO\_GEOS4\_LOWLEV( HcoState, Lct, REGR\_4D, NZ, T, RC)

#### INPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object
REAL(sp), POINTER :: REGR_4D(:,:,:) ! 4D input data
INTEGER, INTENT(IN) :: T ! Time index
```

INTEGER, INTENT(IN) :: NZ ! # of vertical levels to remap. Mu

# INPUT/OUTPUT PARAMETERS:

```
TYPE(ListCont), POINTER :: Lct ! HEMCO list container INTEGER, INTENT(INOUT) :: RC ! Return code
```

#### **REVISION HISTORY:**

```
07 Jan 2015 - C. Keller - Initial version.
24 Sep 2015 - C. Keller - Added option to interpolate edges.
06 Dec 2015 - C. Keller - Added input argument NZ
```

## 1.14.5 COLLAPSE

Helper routine to collapse input levels onto the output grid. The input data is weighted by the grid box thicknesses defined on top of this module. The input parameter T determines the time slice to be considered, and MET denotes the met field type of the input data (4 = GEOS-4 levels, GEOS-5 otherwise).

## **INTERFACE:**

```
SUBROUTINE COLLAPSE ( Lct, REGR_4D, OutLev, InLev1, NLEV, T, MET )
```

# INPUT PARAMETERS:

```
REAL(sp),
                                  :: REGR_4D(:,:,:,:) ! 4D input data
                  POINTER
INTEGER,
                  INTENT(IN)
                                  :: OutLev
                                  :: InLev1
INTEGER,
                  INTENT(IN)
INTEGER,
                                  :: NLEV
                  INTENT(IN)
INTEGER,
                  INTENT(IN)
                                  :: T
                                  :: MET
                                                       ! 4=GEOS-4, else GEOS-5
INTEGER,
                  INTENT(IN)
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(ListCont), POINTER :: Lct ! HEMCO list container
```

```
30 Dec 2014 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

## 1.14.6 **INFLATE**

Helper routine to inflate input levels onto the output grid. The values on the input data are evenly distributed amongst all output levels.

#### **INTERFACE:**

```
SUBROUTINE INFLATE ( Lct, REGR_4D, InLev, OutLev1, NLEV, T )
```

#### INPUT PARAMETERS:

```
REAL(sp), POINTER :: REGR_4D(:,:,:,:) ! 4D input data INTEGER, INTENT(IN) :: InLev INTEGER, INTENT(IN) :: OutLev1 INTEGER, INTENT(IN) :: NLEV INTEGER, INTENT(IN) :: T
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(ListCont), POINTER :: Lct ! HEMCO list container
```

#### REVISION HISTORY:

```
30 Dec 2014 - C. Keller - Initial version
```

## 1.15 Fortran: Module Interface hcoio\_dataread\_mod.F90

Module HCOIO\_DataRead\_Mod controls data processing for HEMCO. Depending on the model environment (standard, ESMF, etc.), it invokes the corresponding routines to read the data from file, convert units as required, and interpolate the data onto the model grid.

Currently, HEMCO can read data from the following data sources:

- Gridded data from netCDF file. The netCDF file should adhere to the COARDS conventions and can hold data on resolutions different than then simulation grid. Regridding is performed as part of the data reading. Routine HCOIO\_DataRead is the driver routine to read data from netCDF file. In an ESMF environment, this routine simply calls down to the MAPL/ESMF generic I/O routines. In a non-ESMF environment, the HEMCO generic reading and remapping algorithms are used. Those support vertical regridding, unit conversion, and more (see below).
- Scalar data directly specified in the HEMCO configuration file. If multiple values separated by the separator sign (/) are provided, they are interpreted as temporally changing values: 7 values = Sun, Mon, ..., Sat; 12 values = Jan, Feb, ..., Dec; 24 values = 0am, 1am, ..., 23pm (local time!). For masks, exactly four values must be provided, interpreted as lower left and upper right mask box corners (lon1/lat1/lon2/lat2).
- Country-specific data specified in a separate ASCII file. This file must end with the suffix '.txt' and hold the country specific values listed by country ID. The IDs must correspond to the IDs of a corresponding (netCDF) mask file. The container name of this mask file must be given in the first line of the file, and must be listed HEMCO

configuration file. ID 0 is reserved for the default values, applied to all countries with no specific values listed. The .txt file must be structured as follows:

# Country mask file name CountryMask

# Country Name Country ID Country Values DEFAULT 0 1.0/1.0/1.0/1.0/1.0/1.0/1/0 USA 840 0.8/0.9/1.0/1.1/1.2/1.1/0.9

The Country Values are interpreted the same way as scalar values, except that they are applied to all grid boxes with the given country ID.

Outside of an ESMF environment, the GEOS-Chem netCDF reading utilities are used to read netCDF data from disk. The selection of the time slice to be read depends on the current simulation time and the datetime settings assigned to a given data container (set in the configuration file). These settings include:

- datetime range (srcTime), given as YYYY/MM/DD/hh. These can be given as fixed date (e.g. 2010/1/1/0), ranges (e.g. 1990-2010/1/1/0 or 2000-2100/1-12/0/0-23), or using tokens (e.g. YYYY/MM/1/0). Data is automatically updated if a 'dynamic' time attribute is given. For instance, for attribute YYYY/1/1/0the filewill beupdate devery year, attribute YY every day, etc. The date time tokens are replaced with the current simulation date-time. If a range is provided, only time stamps within the given range are being used. If there is no exact match between the preferred datetime (determined from srcTime) and the time slices in the netCDF file, the cycle flag determines what time slice index is selected.
- Cycling behavior. This determines what to do if there is no exact match between preferred datetime and available datetimes of a file. The options are cycling (C, default), range (R), exact (E), and interpolation (I). If cycling is used, data is recycled if the simulation time is outside of the available data time interval. If cycling is set to range, a data container is ignored if the \*simulation\* time is outside the given range. For example, if the range is set to 2010-2015/1-12/1/0, this data container is used for simulation dates between 2010 and 2015. If the actual netCDF file data is outside that range, the closest available time slice is selected using the algorithm described below. If cycling is set to exact, HEMCO returns w/ an error if no time slice can be found in the netCDF file that exactly matches the preferred time slices. Finally, if interpolation is selected, data will be interpolated between two time slices if the current preferred datetime cannot be found in the input data. If the preferred datetime does not match with any of the ncdf datetimes, the following method is used to select the time slice to be used: If the preferred datetime is within the range of the available dates, the closest available time stamp in the past is used in most cases. For example, assume a file contains January data between 2005 and 2010, and a simulation starts on July 2007. In this case, the data from Jan 2007 will be used and replaced with Jan 2008 as soon as the simulation date changes to 2008. If the datetimes of the netCDF file contain discontinuities (e.g. don't have the same time interval between all time stamps), an attempt is made to maintain the highest cycling frequency. For instance, if a file contains monthly data for years 2005 and 2020 and the srcTime attribute is set to YYYY/1 –

 $12/1/0. For July 2008, this will use the data from July 2005, and not December 2005 (which would be the closest data of TEST file YYYY. nc VAL 2005-2010/1/1/0 I \dots$ 

## MODULE HCOIO\_DataRead\_Mod

#### **USES:**

```
USE HCO_Types_Mod

USE HCO_Error_Mod

USE HCO_CharTools_Mod

USE HCO_State_Mod, ONLY : Hco_State

IMPLICIT NONE

PRIVATE
```

## PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCOIO\_DataRead

## **REVISION HISTORY:**

```
22 Aug 2013 - C. Keller - Initial version
01 Jul 2014 - R. Yantosca - Now use F90 free-format indentation
01 Jul 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
22 Feb 2016 - C. Keller - Environment specific routines are now in respective modules.
```

#### 1.15.1 HCOIO\_DataRead

Routine HCOIO\_DataRead invokes the appropriate data reading routines for the given model environment.

#### **INTERFACE:**

```
SUBROUTINE HCOIO_DataRead( am_I_Root, HcoState, Lct, RC )
```

#### **USES:**

```
#if defined(ESMF_)
    USE HCOIO_READ_ESMF_MOD, ONLY : HCOIO_READ_ESMF
#else
    USE HCOIO_READ_STD_MOD, ONLY : HCOIO_READ_STD
#endif
```

## INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
TYPE(HCO_State), POINTER :: HcoState
TYPE(ListCont), POINTER :: Lct
```

## INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

```
28 Aug 2013 - C. Keller - Initial version
27 Aug 2014 - R. Yantosca - Err msg now displays hcoio_dataread_mod.F90
22 Feb 2016 - C. Keller - Now calls down to model-specific routines.
24 Mar 2016 - C. Keller - Removed LUN and CloseFile. Not needed any more.
```

# 1.16 Fortran: Module Interface hcoio\_diagn\_mod.F90

Module HCOIO\_Diagn\_Mod.F90 is the data interface module for the HEMCO diagnostics. It contains routines to write out diagnostics into a netCDF file.

In an ESMF/MAPL environment, the HEMCO diagnostics are not directly written to disk but passed to the gridded component export state, where they can be picked up by the MAPL HISTORY component.

## **INTERFACE:**

```
MODULE HCOIO_DIAGN_MOD
```

#### **USES:**

```
USE HCO_ERROR_MOD
```

IMPLICIT NONE PRIVATE

#### PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HcoDiagn\_Write

PUBLIC :: HCOIO\_Diagn\_WriteOut

## **REMARKS:**

HEMCO diagnostics are still in testing mode. We will fully activate them at a later time. They will be turned on when debugging & unit testing.

```
04 May 2014 - C. Keller - Initial version.

11 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers

11 Jun 2014 - R. Yantosca - Now use F90 freeform indentation

28 Jul 2014 - C. Keller - Removed GC specific initialization calls and moved to HEMCO core.

05 Aug 2014 - C. Keller - Added dummy interface for ESMF.

03 Apr 2015 - C. Keller - Added HcoDiagn_Write
```

## 1.16.1 HcoDiagn\_Write

Subroutine HcoDiagn\_Write is the wrapper routine to write out the content of the built-in HEMCO diagnostics. If input argument Restart is set to TRUE, only the restart collection will be written out. Otherwise, the default collection

## **INTERFACE:**

```
SUBROUTINE HcoDiagn_Write( am_I_Root, HcoState, Restart, RC )
```

## **USES:**

```
USE HCO_State_Mod,
                          ONLY : HCO_State
```

USE HCO\_Clock\_Mod, ONLY : HcoClock\_SetLast

## INPUT/OUTPUT PARAMETERS:

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

TYPE(HCO\_State), POINTER ! HEMCO state object

:: Restart INTENT(IN ! write restart (enforced)? LOGICAL, )

# INPUT/OUTPUT PARAMETERS:

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

## **REVISION HISTORY:**

```
- Initial version
03 Apr 2015 - C. Keller
01 Nov 2016 - C. Keller
                         - Also write out default diagnostics collection if
                           RESTART=.TRUE.
```

# 1.16.2 HCOIO\_Diagn\_WriteOut

Subroutine HCOIO\_Diagn\_WriteOut writes diagnostics to output. Depending on the model environment, different subroutines will be invoked.

## **INTERFACE:**

```
SUBROUTINE HCOIO_Diagn_WriteOut( am_I_Root, HcoState, ForceWrite, &
                                RC,
                                             PREFIX,
                                                       UsePrevTime, &
                                OnlyIfFirst, COL
                                                                     )
```

#### **USES:**

```
USE HCO_State_Mod,
                          ONLY : HCO_State
```

#if defined(ESMF\_)

USE HCOIO\_WRITE\_ESMF\_MOD, ONLY : HCOIO\_WRITE\_ESMF

#else

USE HCOIO\_WRITE\_STD\_MOD, ONLY : HCOIO\_WRITE\_STD

#endif

#### INPUT PARAMETERS:

```
) :: am_I_Root
LOGICAL,
                            INTENT(IN
                                                         ! root CPU?
TYPE(HCO_State), POINTER
                                          :: HcoState
                                                         ! HEMCO state object
                                       ) :: ForceWrite ! Write all diagnostics?
LOGICAL,
                            INTENT(IN
CHARACTER(LEN=*), OPTIONAL, INTENT(IN
                                                         ! File prefix
                                       ) :: PREFIX
LOGICAL,
                 OPTIONAL, INTENT(IN
                                        ) :: UsePrevTime ! Use previous time
LOGICAL,
                 OPTIONAL, INTENT(IN
                                        ) :: OnlyIfFirst ! Only write if nnDiagn is 1
                 OPTIONAL, INTENT(IN
                                        ) :: COL
                                                         ! Collection Nr.
INTEGER,
```

# INPUT/OUTPUT PARAMETERS:

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

# **REVISION HISTORY:**

```
12 Sep 2013 - C. Keller
                          - Initial version
11 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
11 Jun 2014 - R. Yantosca - Now use F90 freeform indentation
19 Feb 2015 - C. Keller
                          - Added optional argument OnlyIfFirst
23 Feb 2015 - R. Yantosca - Now make Arr1D REAL(sp) so that we can write
                            out lon & lat as float instead of double
06 Nov 2015 - C. Keller
                          - Output time stamp is now determined from
                            variable OutTimeStamp.
14 Jan 2016 - E. Lundgren - Create netcdf title out of filename prefix
20 Jan 2016 - C. Keller
                          - Added options DiagnRefTime and DiagnNoLevDim.
22 Feb 2016 - C. Keller
                          - Now calls down to environment specific routines.
```

# 1.17 Fortran: Module Interface hcoio\_messy\_mod.F90

Module HCOIO\_MESSY\_MOD interfaces HEMCO with the regridding tool NCREGRID of the Modular Earth Submodel System (MESSy). This regridding scheme is used for vertical regridding and/or for index data, i.e. data with discrete values (e.g. land type integers). This code currently only works for rectilinear (regular lon-lat) grids but can be extended to support curvilinear grids.

## REFERENCES:

• Joeckel, P. Technical note: Recursive rediscretisation of geo- scientific data in the Modular Earth Submodel System (MESSy), ACP, 6, 3557–3562, 2006.

# **INTERFACE:**

```
MODULE HCOIO_MESSY_MOD
```

## **USES:**

```
USE HCO_ERROR_MOD

USE HCO_TYPES_MOD, ONLY : ListCont

USE HCO_STATE_MOD, ONLY : Hco_State

USE MESSY_NCREGRID_BASE, ONLY : NARRAY, AXIS

IMPLICIT NONE

PRIVATE
```

## PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCO\_MESSY\_REGRID

#### PRIVATE MEMBER FUNCTIONS:

```
! Set this value to TRUE if you want to reduce the output array
! to the minimum required number of vertical levels.
LOGICAL, PARAMETER :: ReduceVert = .FALSE.
!MODULE INTERFACES:
```

## REVISION HISTORY:

```
24 Jun 2014 - C. Keller - Initial version
```

## 1.17.1 Hco\_Messy\_Regrid

This is the wrapper routine to regrid a 4D input array NcArr (x,y,z,t) onto the HEMCO emissions grid (defined in HcoState) using the regridding tool NCREGRID. LonEdge, Lat-Edge and LevEdge are the grid point edges of the input grid. The data is written into list container Lct.

If the input grid is 2D (horizontal only), LevEdge must not be specified (null pointer) and the data is regridded in the horizontal only. If the input grid has only one vertical level, it is assumed that this is the surface level and the output data is 3D but with only one vertical level.

For input data with more than one vertical level, the data is mapped onto the entire 3D grid. The module parameter ReduceVert can be used to cap the output data at the lowest possible level. For example, if the input grid only covers three surface levels with a minimum sigma value of 0.75, vertical regridding is performed within this sigma range (1-0.75) and the output grid is reduced accordingly. This option is not used in the standard HEMCO setup because problems can arise if the data array of a given container suddently changes its size (i.e. when updated data covers more/less vertical levels than the data beforehand).

The input argument IsModelLev denotes whether or not the vertical coordinates of the input data are on model levels. If set to yes and LevEdge is not provided (i.e. a nullified pointer), the MESSy regridding routines are only used for the horizontal remapping and subroutine ModelLev\_Interpolate (module hco\_interp\_mod.F90) is used for the vertical remapping.

## **INTERFACE:**

```
SUBROUTINE HCO_MESSY_REGRID ( am_I_Root, HcoState, NcArr, & LonEdge, LatEdge, LevEdge, & Lct, IsModelLev, RC
```

## **USES:**

```
USE HCO_FILEDATA_MOD, ONLY : FileData_ArrCheck
  USE HCO_UNIT_MOD,
                            ONLY : HCO_IsIndexData
  USE HCO_INTERP_MOD, ONLY : ModelLev_Interpolate
  USE MESSY_NCREGRID_BASE, ONLY : RG_INT, RG_IDX
  USE MESSY_NCREGRID_BASE, ONLY: NREGRID
  USE MESSY_NCREGRID_BASE, ONLY : INIT_NARRAY
INPUT/OUTPUT PARAMETERS:
                       INTENT(IN ) :: am_I_Root ! Root CPU?
POINTER :: HcoState ! HEMCO obj.
     LOGICAL,
     TYPE(HCO_State), POINTER
    REAL(sp), POINTER
REAL(hp), POINTER
REAL(hp), POINTER
REAL(hp), POINTER
                                     :: ncArr(:,:,:,:) ! Input array(x,y,z,t)
                                     :: LonEdge(:) ! lon edges
                                    :: LatEdge(:) ! lat edges
                                     :: LevEdge(:,:,:) ! sigma level edges
                      POINTER :: Lct ! Target list container
INTENT(IN ) :: IsModelLev ! Are these model levels?
     TYPE(ListCont), POINTER
     LOGICAL,
                       INTENT(INOUT) :: RC
                                                           ! Return code
     INTEGER,
REVISION HISTORY:
    27 Jun 2014 - C. Keller - Initial version
```

```
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

## 1.17.2 Axis\_Create

Subroutine AXIS\_CREATE creates a MESSy axis type from the grid defined by mid points Lon, Lat, Lev. Lev must be in (unitless) sigma coordinates: sigma(i,j,l) = p(i,j,l) / p\_surface(i,j)

## **INTERFACE:**

```
SUBROUTINE AXIS_CREATE ( am_I_Root, HcoState, lon, lat, lev, ax, RC )
USES:
```

USE MESSY\_NCREGRID\_BASE, ONLY : INIT\_AXIS

## INPUT PARAMETERS:

```
LOGICAL,
                INTENT(IN
                            )
                                      :: am_I_Root
                                       :: HcoState
TYPE(HCO_State), POINTER
TYPE(ListCont), POINTER
                                       :: Lct
              POINTER
REAL(hp),
                                      :: Lon(:)
REAL(hp),
               POINTER
                                       :: Lat(:)
                                       :: Lev(:,:,:)
REAL(hp),
               POINTER
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(axis),
                                           :: ax(:)
                  POINTER
INTEGER,
                  INTENT(INOUT)
                                          :: RC
```

```
22 Jun 2014 - C. Keller - Initial version (from messy_ncregrid_geohyb.f90)
```

## 1.17.3 Axis\_Delete

Subroutine AXIS\_DELETE deletes the specified MESSy axis.

## **INTERFACE:**

```
SUBROUTINE AXIS_DELETE ( ax1, ax2, RC )
```

#### **USES:**

USE MESSY\_NCREGRID\_BASE, ONLY : INIT\_AXIS

# INPUT/OUTPUT PARAMETERS:

```
TYPE(axis), POINTER :: ax1(:)
TYPE(axis), POINTER :: ax2(:)
INTEGER, INTENT(INOUT) :: RC
```

## **REVISION HISTORY:**

```
28 Aug 2013 - C. Keller - Initial version
```

## 1.17.4 Hco2Messy

Subroutine HCO2MESSY converts a HEMCO data array into a messy array-structure.

## **INTERFACE:**

```
SUBROUTINE HCO2MESSY( am_I_Root, HcoState, InArr, narr, ax, RC)
```

## **USES:**

# INPUT/OUTPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
TYPE(HCO_State), POINTER :: HcoState
REAL(sp), POINTER :: InArr(:,:,:,:)
TYPE(narray), POINTER :: narr(:)
TYPE(axis), POINTER :: ax(:)
INTEGER, INTENT(INOUT) :: RC
```

```
27 Jun 2014 - C. Keller - Initial version
```

## 1.17.5 Messy2Hco

Subroutine MESSY2HCO converts a MESSy array structure into a HEMCO data array. This is basically the reverse function of HCO2MESSY.

## **INTERFACE:**

```
SUBROUTINE MESSY2HCO( am_I_Root, HcoState, narr, Lct, LEV, Ptr4D, RC ) USES:
```

## INPUT/OUTPUT PARAMETERS:

```
LOGICAL,
                 INTENT(IN
                                         :: am_I_Root
TYPE(HCO_State), POINTER
                                         :: HcoState
                                         :: narr(:)
TYPE(narray),
                 POINTER
TYPE(ListCont),
                 POINTER
                                         :: Lct
INTEGER,
                 INTENT(IN )
                                         :: LEV
                                         :: Ptr4D(:,:,:,:)
REAL(sp),
                 POINTER
INTEGER,
                 INTENT(INOUT)
                                         :: RC
```

## **REVISION HISTORY:**

```
27 Jun 2014 - C. Keller - Initial version
```

## 1.18 Fortran: Module Interface hcoio\_read\_esmf\_mod.F90

Module HCOIO\_Read\_ESMF\_mod is the HEMCO interface for data reading within the ESMF framework.

#### **INTERFACE:**

```
MODULE HCOIO_Read_ESMF_mod
```

## **USES:**

```
USE HCO_Types_Mod
USE HCO_Error_Mod
USE HCO_State_Mod, ONLY : Hco_State

IMPLICIT NONE
PRIVATE
```

# PUBLIC MEMBER FUNCTIONS:

```
#if defined(ESMF_)
PUBLIC :: HCOIO_Read_ESMF
```

```
22 Aug 2013 - C. Keller - Initial version
01 Jul 2014 - R. Yantosca - Now use F90 free-format indentation
01 Jul 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
22 Feb 2016 - C. Keller - Split off from hcoio_dataread_mod.F90
```

# 1.18.1 HCOIO\_DataRead (ESMF/MAPL version)

Interface routine between ESMF and HEMCO to obtain the data array for a given HEMCO data container. The data is obtained through the ExtData interface. The HEMCO source file attribute is taken to identify the ExtData pointer name.

## **INTERFACE:**

```
SUBROUTINE HCOIO_Read_ESMF( am_I_Root, HcoState, Lct, RC )
```

## **USES:**

```
USE ESMF
USE MAPL_mod
USE HCO_FILEDATA_MOD, ONLY : FileData_ArrInit
```

## **INPUT PARAMETERS:**

# include "MAPL\_Generic.h"

```
LOGICAL, INTENT(IN ) :: am_I_Root
TYPE(HCO_State), POINTER :: HcoState
TYPE(ListCont), POINTER :: Lct
```

## INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

#### **REVISION HISTORY:**

```
28 Aug 2013 - C. Keller - Initial version
27 Aug 2014 - R. Yantosca - Err msg now displays hcoio_dataread_mod.F90
```

## 1.19 Fortran: Module Interface hcoio\_read\_std\_mod.F90

Module HCOIO\_read\_std\_mod controls data processing (file reading, unit conversion, regridding) for HEMCO in the 'standard' environment (i.e. non-ESMF).

#### **INTERFACE:**

```
MODULE HCOIO_read_std_mod
```

# **USES:**

```
USE HCO_Types_Mod
USE HCO_Error_Mod
USE HCO_CharTools_Mod
USE HCO_State_Mod, ONLY : Hco_State
IMPLICIT NONE
PRIVATE
```

# PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCOIO\_ReadOther
PUBLIC :: HCOIO\_CloseAll

#if !defined(ESMF\_)

PUBLIC :: HCOIO\_read\_std

## PRIVATE MEMBER FUNCTIONS:

PRIVATE :: GET\_TIMEIDX
PRIVATE :: Check\_AvailYMDh
PRIVATE :: prefYMDh\_Adjust

PRIVATE :: Set\_tIdx2
PRIVATE :: IsClosest

PRIVATE :: GetIndex2Interp

PRIVATE :: GetWeights
PRIVATE :: YMDh2hrs

PRIVATE :: Normalize\_Area
PRIVATE :: SrcFile\_Parse
PRIVATE :: SigmaMidToEdges
PRIVATE :: CheckMissVal
PRIVATE :: GetArbDimIndex

#endif

PRIVATE :: HCOIO\_ReadCountryValues
PRIVATE :: HCOIO\_ReadFromConfig

PRIVATE :: GetDataVals
PRIVATE :: GetSliceIdx
PRIVATE :: FillMaskBox

## **REVISION HISTORY:**

```
22 Aug 2013 - C. Keller - Initial version
01 Jul 2014 - R. Yantosca - Now use F90 free-format indentation
01 Jul 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
22 Feb 2016 - C. Keller - Split off from hcoio_dataread_mod.F90
```

#### 1.19.1 HCOIO Read std

Reads a netCDF file and returns the regridded array in proper units. This routine uses the HEMCO generic data reading and regridding routines.

Two different regridding algorithm are used: NCREGRID for 3D data with vertical regridding, and map\_a2a for all other data. map\_a2a also supports index-based remapping, while this feature is currently not possible in combination with NCREGRID.

3D data is vertically regridded onto the simulation grid on the sigma interface levels. In order to calculate these levels correctly, the netCDF vertical coordinate description must adhere to the CF - conventions. See routine NC\_Get\_Sigma\_Levels in Ncdf\_Mod for more

details.

A simpler vertical interpolation scheme is used if (a) the number of vertical levels of the input data corresponds to the number of levels on the simulation grid (direct mapping, no remapping), (b) the vertical level variable name (long\_name) contains the word "GEOS-Chem level". In the latter case, the vertical levels of the input data is interpreted as GEOS vertical levels and mapped onto the simulation grid using routine ModelLev\_Interpolate.

## **INTERFACE:**

```
SUBROUTINE HCOIO_read_std( am_I_Root, HcoState, Lct, RC )
```

## **USES:**

```
USE Ncdf_Mod,
                        ONLY : NC_Open
USE Ncdf_Mod,
                        ONLY : NC_Close
USE Ncdf_Mod,
                        ONLY : NC_Read_Var
USE Ncdf_Mod,
                        ONLY : NC_Read_Arr
USE Ncdf_Mod,
                        ONLY : NC_Get_Grid_Edges
USE Ncdf_Mod,
                        ONLY : NC_Get_Sigma_Levels
USE Ncdf_Mod,
                        ONLY : NC_ISMODELLEVEL
USE CHARPAK_MOD,
                        ONLY: TRANLC
USE HCO_Unit_Mod,
                        ONLY : HCO_Unit_Change
USE HCO_Unit_Mod,
                        ONLY : HCO_Unit_ScalCheck
                        ONLY : HCO_IsUnitless
USE HCO_Unit_Mod,
USE HCO_Unit_Mod,
                        ONLY : HCO_IsIndexData
USE HCO_Unit_Mod,
                        ONLY : HCO_UnitTolerance
USE HCO_GeoTools_Mod,
                        ONLY: HCO_ValidateLon
USE HCO_FileData_Mod,
                        ONLY : FileData_ArrCheck
USE HCO_FileData_Mod,
                        ONLY : FileData_Cleanup
USE HCOIO_MESSY_MOD,
                        ONLY : HCO_MESSY_REGRID
USE HCO_INTERP_MOD,
                        ONLY: REGRID_MAPA2A
USE HCO_INTERP_MOD,
                        ONLY : ModelLev_Check
USE HCO_CLOCK_MOD,
                        ONLY : HcoClock_Get
USE HCO_DIAGN_MOD,
                        ONLY : Diagn_Update
USE HCO_EXTLIST_MOD,
                        ONLY : HCO_GetOpt
USE HCO_TIDX_MOD,
                        ONLY : tIDx_IsInRange
```

#### INPUT PARAMETERS:

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

TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object

TYPE(ListCont), POINTER :: Lct ! HEMCO list container
```

# INPUT/OUTPUT PARAMETERS:

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

```
13 Mar 2013 - C. Keller - Initial version
```

```
27 Aug 2014 - R. Yantosca - Err msg now displays hcoio_dataread_mod.F90
01 Oct 2014 - C. Keller
                          - Added file name parser
03 Oct 2014 - C. Keller
                          - Added vertical regridding capability
                          - Don't do vertical regridding if data is already
12 Dec 2014 - C. Keller
                            on GEOS-Chem levels.
31 Dec 2014 - C. Keller
                          - Now call ModelLev_Interpolate for model remapping
                            of model levels.
15 Jan 2015 - C. Keller
                          - Now allow model level interpolation in
                            combination with MESSy (horizontal) regridding.
03 Feb 2015 - C. Keller
                          - Moved map_a2a regridding to hco_interp_mod.F90.
24 Mar 2015 - C. Keller
                          - Added arguments LUN and CloseFile.
27 Mar 2015 - R. Yantosca - Now use a FORMAT statement when printing the
                            filename to the Unix stdout.
08 Apr 2015 - R. Yantosca - Bug fix: set KeepSpec=.TRUE. if there is no
                            species in the container. This prevents
                            diffs in output in sp vs mp runs.
13 Jul 2015 - C. Keller
                          - Write data into diagnostics right after reading
                            (if a diagnostics with the same name exists).
23 Sep 2015 - C. Keller
                          - Support time averaging (cycle flags A and RA).
06 Oct 2015 - C. Keller
                          - Support additional horizontal coordinates. Added
                            MustFind error checks (cycle flags EF and RF).
                          - Bug fix: now use Lun2 if reading second file.
22 Nov 2015 - C. Keller
24 Mar 2016 - C. Keller
                          - Simplified handling of file in buffer. Remove
                            args LUN and CloseFile.
29 Apr 2016 - R. Yantosca - Don't initialize pointers in declaration stmts
```

## 1.19.2 Get\_TimeIdx

Returns the lower and upper time slice index (tidx1 and tidx2, respectively) to be read. These values are determined based upon the time slice information extracted from the netCDF file, the time stamp settings set in the config. file, and the current simulation date.

Return arguments wgt1 and wgt2 denote the weights to be given to the two time slices. This is only of relevance for data that shall be interpolated between two (not necessarily consecutive) time slices. In all other cases, the returned weights are negative and will be ignored.

Also returns the time slice year and month, as these values may be used for unit conversion.

```
SUBROUTINE GET_TIMEIDX( am_I_Root, HcoState, Lct, & ncLun, tidx1, tidx2, & wgt1, wgt2, oYMDh, & YMDh, YMDh1, RC, & Year)
```

#### **USES:**

```
USE Ncdf_Mod, ONLY : NC_Read_Time_YYYYMMDDhh
USE HCO_tIdx_Mod, ONLY : HCO_GetPrefTimeAttr
```

## INPUT PARAMETERS:

```
INTENT(IN
                                          :: am_I_Root ! Root CPU?
LOGICAL,
                             )
TYPE(HCO_State),
                 POINTER
                                          :: HcoState ! HcoState object
                                                       ! List container
TYPE(ListCont),
                 POINTER
                                          :: Lct
INTEGER,
                 INTENT(IN
                             )
                                          :: ncLun
                                                       ! open ncLun
                                                       ! year to be used
INTEGER,
                 INTENT(IN
                             ), OPTIONAL :: Year
```

## **OUTPUT PARAMETERS:**

```
INTEGER,
                 INTENT( OUT)
                                           :: tidx1
                                                        ! lower time idx
               INTENT( OUT)
INTEGER,
                                           :: tidx2
                                                        ! upper time idx
                                                        ! weight to tidx1
REAL(sp),
                                           :: wgt1
                                           :: wgt2
:: oYMDh
:: YMDh
REAL(sp),
                 INTENT( OUT)
                                                        ! weight to tidx2
                                                        ! preferred time slice
INTEGER(8),
                 INTENT( OUT)
                 INTENT( OUT)
                                                        ! selected time slice
INTEGER(8),
                                                        ! 1st time slice in file
INTEGER(8),
                 INTENT( OUT)
                                           :: YMDh1
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

#### REVISION HISTORY:

```
13 Mar 2013 - C. Keller - Initial version
27 Feb 2015 - C. Keller - Added weigths
```

## 1.19.3 Check\_AvailYMDh

Checks if prefYMDh is within the range of availYMDh and returns the location of the closest vector element that is in the past (-; tidx1). tidx1 is set to -1 otherwise.

# **INTERFACE:**

```
SUBROUTINE Check_AvailYMDh( Lct, N, availYMDh, prefYMDh, tidx1 )
```

## INPUT PARAMETERS:

```
TYPE(ListCont), POINTER :: Lct
INTEGER, INTENT(IN) :: N
```

# **OUTPUT PARAMETERS:**

```
INTEGER, INTENT(OUT) :: tidx1
```

```
13 Mar 2013 - C. Keller - Initial version
```

# 1.19.4 prefYMDh\_Adjust

Adjusts prefYMDh to the closest available time attribute. Can be adjusted for year (level=1), month (level=2), or day (level=3).

# **INTERFACE:**

```
SUBROUTINE prefYMDh_Adjust( N, availYMDh, prefYMDh, level, tidx1 )
```

# INPUT PARAMETERS:

```
INTEGER , INTENT(IN) :: N
INTEGER(8), INTENT(IN) :: availyMDh(N)
INTEGER , INTENT(IN) :: level
INTEGER , INTENT(IN) :: tidx1
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER(8), INTENT(INOUT) :: prefYMDh
```

# **REVISION HISTORY:**

```
13 Mar 2013 - C. Keller - Initial version
17 Jul 2014 - C. Keller - Now allow to adjust year, month, or day.
```

#### 1.19.5 Set\_tIdx2

sets the upper time slice index by selecting the range of all elements in availYMDh with the same date (year,month,day) as availYMDh(tidx1).

#### **INTERFACE:**

```
SUBROUTINE Set_tIdx2( N, availYMDh, tidx1, tidx2 )
```

# INPUT PARAMETERS:

```
INTEGER , INTENT(IN) :: N
INTEGER(8), INTENT(IN) :: availYMDh(N)
INTEGER , INTENT(IN) :: tidx1
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER , INTENT(OUT) :: tidx2
```

```
13 Mar 2013 - C. Keller - Initial version
```

# 1.19.6 IsClosest

function IsClosest returns true if the selected time index is the 'closest' one. It is defined as being closest if: (a) the currently selected index exactly matches the preferred one. (b) the time gap between the preferred time stamp and the currently selected index is at least as small as any other gap of consecutive prior time stamps.

# **INTERFACE:**

```
FUNCTION IsClosest (prefYMDh, availYMDh, nTime, ctidx1 ) RESULT (Closest)
```

# **INPUT PARAMETERS:**

```
INTEGER(8), INTENT(IN) :: prefYMDh
```

INTEGER(8), INTENT(IN) :: availYMDh(nTime)

INTEGER, INTENT(IN) :: nTime
INTEGER, INTENT(IN) :: ctidx1

# **OUTPUT PARAMETERS:**

LOGICAL :: Closest

#### **REVISION HISTORY:**

```
03 Mar 2015 - C. Keller - Initial version
```

# 1.19.7 GetIndex2Interp

GetIndex2Interp

#### **INTERFACE:**

```
SUBROUTINE GetIndex2Interp ( am_I_Root, HcoState, Lct, & nTime, availYMDh, & prefYMDh, origYMDh, tidx1, & tidx2, wgt1, wgt2, RC )
```

# **INPUT PARAMETERS:**

```
LOGICAL, INTENT(IN) :: am_I_Root
TYPE(HCO_State), POINTER :: HcoState
TYPE(ListCont), POINTER :: Lct
INTEGER, INTENT(IN) :: nTime
```

INTEGER(8), INTENT(IN) :: availYMDh(nTime)

INTEGER(8), INTENT(IN) :: prefYMDh
INTEGER(8), INTENT(IN) :: origYMDh
INTEGER, INTENT(IN) :: tidx1

# **OUTPUT PARAMETERS:**

# INPUT/OUTPUT PARAMETERS:

```
REAL(sp), INTENT(INOUT) :: wgt1
REAL(sp), INTENT(INOUT) :: wgt2
INTEGER, INTENT(INOUT) :: RC
```

# **REVISION HISTORY:**

```
02 Mar 2015 - C. Keller - Initial version
```

# 1.19.8 GetWeights

Helper function to get the interpolation weights between two datetime intervals (int1, int2) and for a given time cur.

# **INTERFACE:**

```
SUBROUTINE GetWeights ( int1, int2, cur, wgt1, wgt2 )
```

# INPUT PARAMETERS:

# INPUT/OUTPUT PARAMETERS:

```
REAL(sp), INTENT( OUT) :: wgt1, wgt2
```

# **REVISION HISTORY:**

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

# 1.19.9 YMDh2hrs

returns the hours of element YMDh. For simplicity, 30 days are assigned to every month. At the moment, this routine is only called to determine the time interval between two emission time slices (DeltaT) and this approximation is good enough.

# INTERFACE:

```
FUNCTION YMDh2hrs ( YMDh ) RESULT ( hrs )
```

# INPUT PARAMETERS:

```
INTEGER(8), INTENT(IN) :: YMDh
```

# INPUT/OUTPUT PARAMETERS:

INTEGER :: hrs

```
26 Jan 2015 - C. Keller - Initial version
```

#### 1.19.10 Normalize\_Area

Subroutine Normalize\_Area normalizes the given array by the surface area calculated from the given netCDF file.

#### **INTERFACE:**

```
SUBROUTINE Normalize_Area( HcoState, Array, nlon, LatEdge, FN, RC )
```

#### INPUT PARAMETERS:

```
! HEMCO state object
TYPE(HCO_State),
                  POINTER
                                    :: HcoState
INTEGER,
                  INTENT(IN
                               )
                                    :: nlon
                                                           ! # of lon midpoints
REAL(hp),
                  POINTER
                                    :: LatEdge(:)
                                                           ! lat edges
CHARACTER(LEN=*), INTENT(IN
                                                           ! filename
                                    :: FN
```

# INPUT/OUTPUT PARAMETERS:

```
REAL(sp), POINTER :: Array(:,:,:) ! Data
INTEGER, INTENT(INOUT) :: RC ! Return code
```

#### **REVISION HISTORY:**

```
13 Mar 2013 - C. Keller - Initial version
```

#### 1.19.11 SrcFile\_Parse

Routine SrcFile\_Parse parses the source file name ('ncFile') of the provided list container Lct. In particular, it searches for tokens such as ROOT, YYYYY, etc., within the file name and replaces those values with the intendend characters. The parsed file name is returned in string srcFile, while the original file name is retained in Lct.

It now also checks if the file exists. If the file does not exist and the file name contains date tokens, it tries to adjust the file name to the closest available date in the past. The optional flag FUTURE can be used to denote that the next available file in the future shall be selected, even if there is a file that exactly matches the preferred date time. This is useful for interpolation between fields.

#### **INTERFACE:**

```
SUBROUTINE SrcFile_Parse ( am_I_Root, HcoState, Lct, srcFile, FOUND, RC, & FUTURE, Year )
```

#### **USES:**

```
USE HCO_TIDX_MOD, ONLY : HCO_GetPrefTimeAttr
USE HCO_TIDX_MOD, ONLY : tIDx_IsInRange
USE HCO_CHARTOOLS_MOD, ONLY : HCO_CharParse
USE HCO_CLOCK_MOD, ONLY : HcoClock_Get
USE HCO_CLOCK_MOD, ONLY : Get_LastDayOfMonth
```

#### INPUT PARAMETERS:

```
:: am_I_Root ! Root CPU?
LOGICAL,
                INTENT(IN
                            )
TYPE(HCO_State), POINTER
                                       :: HcoState
                                                    ! HEMCO state object
TYPE(ListCont),
                POINTER
                                                     ! HEMCO list container
                                       :: Lct
                            ), OPTIONAL :: FUTURE
                                                    ! If needed, update
LOGICAL,
                INTENT(IN
                                                     ! date tokens to future
                INTENT(IN ), OPTIONAL :: Year
                                                    ! To use fixed year
INTEGER,
```

# **OUTPUT PARAMETERS:**

```
CHARACTER(LEN=*), INTENT( OUT) :: srcFile ! output string LOGICAL, INTENT( OUT) :: FOUND ! Does file exist?
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC ! return code
```

#### REVISION HISTORY:

```
01 Oct 2014 - C. Keller - Initial version
23 Feb 2015 - C. Keller - Now check for negative return values in
HCO_GetPrefTimeAttr
06 Nov 2015 - C. Keller - Bug fix: restrict day to last day of month.
```

# 1.19.12 SigmaMidToEdges

Helper routine to interpolate sigma mid point values to edges. A simple linear interpolation is performed.

# **INTERFACE:**

```
SUBROUTINE SigmaMidToEdges (am_I_Root, HcoState, SigMid, SigEdge, RC)
```

# INPUT PARAMETERS:

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

TYPE(HCO_State), POINTER :: HcoState ! HEMCO state obj

REAL(hp), POINTER :: SigMid(:,:,:) ! sigma levels
```

# **OUTPUT PARAMETERS:**

```
REAL(hp), POINTER :: SigEdge(:,:,:) ! sigma edges INTEGER, INTENT( OUT) :: RC ! return code
```

```
03 Oct 2013 - C. Keller - Initial version
```

# 1.19.13 CheckMissVal

Checks for missing values in the passed array. Missing values of base emissions and masks are set to 0, missing values of scale factors are set to 1.

# **INTERFACE:**

```
SUBROUTINE CheckMissVal ( Lct, Arr )
```

#### INPUT PARAMETERS:

```
TYPE(ListCont), POINTER :: Lct
REAL(sp), POINTER :: Arr(:,:,:,:)
```

# **REVISION HISTORY:**

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

# 1.19.14 GetArbDimIndex

Subroutine GetArbDimIndex returns the index of the arbitrary file dimension. -1 if no such dimension is defined.

# **INTERFACE:**

```
SUBROUTINE GetArbDimIndex( am_I_Root, HcoState, Lun, Lct, ArbIdx, RC )
```

# **USES:**

```
USE m_netcdf_io_checks
USE m_netcdf_io_get_dimlen
USE HCO_ExtList_Mod, ONLY : GetExtOpt
```

# **INPUT PARAMETERS:**

```
LOGICAL, INTENT(IN ) :: am_I_Root
TYPE(HCO_State), POINTER :: HcoState
INTEGER, INTENT(IN ) :: Lun
TYPE(ListCont), POINTER :: Lct
```

# **OUTPUT PARAMETERS:**

```
INTEGER, INTENT( OUT) :: Arbldx INTEGER, INTENT( OUT) :: RC
```

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

# 1.19.15 HCOIO\_ReadOther

Subroutine HCOIO\_ReadOther is a wrapper routine to read data from sources other than netCDF.

If a file name is given (ending with '.txt'), the data are assumed to hold country-specific values (e.g. diurnal scale factors). In all other cases, the data is directly read from the configuration file (scalars).

# **INTERFACE:**

```
SUBROUTINE HCOIO_ReadOther ( am_I_Root, HcoState, Lct, RC )
```

# **USES:**

#### !INPUT PARAMTERS:

LOGICAL, INTENT(IN ) :: am\_I\_Root

TYPE(HCO\_State), POINTER :: HcoState ! HEMCO state

# INPUT/OUTPUT PARAMETERS:

TYPE(ListCont), POINTER :: Lct INTEGER, INTENT(INOUT) :: RC

# **REVISION HISTORY:**

22 Dec 2014 - C. Keller: Initial version

# 1.19.16 HCOIO\_ReadCountryValues

Subroutine HCOIO\_ReadCountryValues

# **INTERFACE:**

```
SUBROUTINE HCOIO_ReadCountryValues ( am_I_Root, HcoState, Lct, RC )
```

#### **USES:**

```
USE inquireMod, ONLY : findFreeLUN
```

USE HCO\_CHARTOOLS\_MOD, ONLY: HCO\_CMT, HCO\_SPC, NextCharPos

USE HCO\_EmisList\_Mod, ONLY : HCO\_GetPtr

USE HCO\_FileData\_Mod, ONLY : FileData\_ArrCheck

!INPUT PARAMTERS:

LOGICAL, INTENT(IN ) :: am\_I\_Root

TYPE(HCO\_State), POINTER :: HcoState ! HEMCO state

# INPUT/OUTPUT PARAMETERS:

TYPE(ListCont), POINTER :: Lct INTEGER, INTENT(INOUT) :: RC

# **REVISION HISTORY:**

```
22 Dec 2014 - C. Keller: Initial version
```

26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts

# 1.19.17 HCOIO\_ReadFromConfig

Subroutine HCOIO\_ReadFromConfig reads data directly from the configuration file (instead of reading it from a netCDF file). These data is always assumed to be spatially uniform, but it is possible to specify multiple time slices by separating the individual time slice values by the HEMCO separator sign ('/' by default). The time dimension of these data is either determined from the srcTime attribute or estimated from the number of time slices provided. For example, if no srcTime is specified and 24 time slices are provided, data is assumed to represent hourly data. Similarly, data is assumed to represent weekdaily or monthly data for 7 or 12 time slices, respectively.

If the srcTime attribute is defined, the time slices are determined from this attribute. Only one time dimension (year, month, day, or hour) can be defined for scalar fields!

#### **INTERFACE:**

```
SUBROUTINE HCOIO_ReadFromConfig (am_I_Root, HcoState, Lct, RC)
USES:
    USE HCO_FILEDATA_MOD,
                            ONLY : FileData_ArrCheck
   !INPUT PARAMTERS:
    LOGICAL,
                      INTENT(IN
                                       :: am_I_Root
    TYPE(HCO_State), POINTER
                                       :: HcoState
                                                      ! HEMCO state
INPUT/OUTPUT PARAMETERS:
    TYPE(ListCont),
                      POINTER
                                       :: Lct
    INTEGER,
                      INTENT (INOUT)
                                       :: RC
```

# **REVISION HISTORY:**

```
24 Jul 2014 - C. Keller: Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 1.19.18 HCOIO\_CloseAll

Subroutine HCOIO\_CloseAll makes sure that there is no open netCDF file left in the stream.

# **INTERFACE:**

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

#### REVISION HISTORY:

```
24 Mar 2016 - C. Keller: Initial version
```

# 1.19.19 GetSliceIdx

gets the time slice index to be used for data directly read from the HEMCO configuration file. prefDt denotes the preferred time attribute (year, month, or day). DtType is used to identify the time attribute type (1=year, 2=month, 3=day). The time slice index will be selected based upon those two variables. IDX is the selected time slice index. It will be set to -1 if the current simulation date is outside of the specified time range and the time cycle attribute is not enabled for this field.

# **INTERFACE:**

```
SUBROUTINE GetSliceIdx ( HcoState, Lct, DtType, prefDt, IDX, RC )
```

# **INPUT PARAMETERS:**

```
TYPE(HCO_State), POINTER :: HcoState
TYPE(ListCont), POINTER :: Lct
INTEGER, INTENT(IN ) :: DtType
INTEGER, INTENT(IN ) :: prefDt
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: IDX
INTEGER, INTENT(INOUT) :: RC
```

#### REVISION HISTORY:

```
13 Mar 2013 - C. Keller - Initial version
```

# 1.19.20 GetDataVals

Subroutine GetDataVals extracts the data values from ValStr and writes them into vector Vals. ValStr is typically a character string read from an external ASCII file or directly from the HEMCO configuration file. Depending on the time specifications provided in the configuration file, Vals will be filled with only a subset of the values of ValStr.

# **INTERFACE:**

```
SUBROUTINE GetDataVals ( am_I_Root, HcoState, Lct, ValStr, Vals, RC )
```

# **USES:**

```
USE HCO_CHARTOOLS_MOD, ONLY : HCO_CharSplit
USE HCO_EXTLIST_MOD, ONLY : HCO_GetOpt
USE HCO_UNIT_MOD, ONLY : HCO_Unit_Change
USE HCO_tIdx_Mod, ONLY : HCO_GetPrefTimeAttr
```

!INPUT PARAMTERS:

LOGICAL, INTENT(IN ) :: am\_I\_Root

TYPE(HCO\_State), POINTER :: HcoState ! HEMCO state

CHARACTER(LEN=\*), INTENT(IN ) :: ValStr

# INPUT/OUTPUT PARAMETERS:

TYPE(ListCont), POINTER :: Lct INTEGER, INTENT(INOUT) :: RC

# **OUTPUT PARAMETERS:**

REAL(hp), POINTER :: Vals(:)

# **REVISION HISTORY:**

22 Dec 2014 - C. Keller: Initial version

# 1.19.21 FillMaskBox

Subroutine FillMaskBox fills the data array of the passed list container Lct according to the mask region provided in Vals. Vals contains the mask region of interest, denoted by the lower left and upper right grid box corners: lon1, lat1, lon2, lat2. The data array of Lct is filled such that all grid boxes are set to 1 whose mid-point is inside of the given box range.

# **INTERFACE:**

```
SUBROUTINE FillMaskBox (am_I_Root, HcoState, Lct, Vals, RC)
```

# **USES:**

# !INPUT PARAMTERS:

LOGICAL, INTENT(IN ) :: am\_I\_Root

TYPE(HCO\_State), POINTER :: HcoState ! HEMCO state

REAL(hp) , POINTER :: Vals(:)

# INPUT/OUTPUT PARAMETERS:

TYPE(ListCont), POINTER :: Lct INTEGER, INTENT(INOUT) :: RC

# REVISION HISTORY:

```
29 Dec 2014 - C. Keller - Initial version
```

19 Nov 2015 - C. Keller - Now support grid point masks

# 1.20 Fortran: Module Interface hcoio\_write\_esmf\_mod.F90

Module HCOIO\_Write\_ESMF\_Mod.F90 is the HEMCO output interface for the ESMF environment. In an ESMF/MAPL environment, the HEMCO diagnostics are not directly written to disk but passed to the gridded component export state, where they can be picked up by the MAPL HISTORY component.

# **INTERFACE:**

```
MODULE HCOIO_WRITE_ESMF_MOD

USES:

USE HCO_ERROR_MOD

USE HCO_DIAGN_MOD
```

IMPLICIT NONE

#### PUBLIC MEMBER FUNCTIONS:

```
#if defined(ESMF_)
PUBLIC :: HCOIO_WRITE_ESMF
```

#### **REMARKS:**

PRIVATE

HEMCO diagnostics are still in testing mode. We will fully activate them at a later time. They will be turned on when debugging & unit testing.

# **REVISION HISTORY:**

```
04 May 2014 - C. Keller - Initial version.

11 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers

11 Jun 2014 - R. Yantosca - Now use F90 freeform indentation

28 Jul 2014 - C. Keller - Removed GC specific initialization calls and moved to HEMCO core.

05 Aug 2014 - C. Keller - Added dummy interface for ESMF.

03 Apr 2015 - C. Keller - Added HcoDiagn_Write

22 Feb 2016 - C. Keller - Split off from hcoio_diagn_mod.F90
```

# 1.20.1 HCOIO\_Diagn\_WriteOut

Subroutine HCOIO\_Diagn\_WriteOut is the interface routine to link the HEMCO diagnostics arrays to the corresponding data pointers of the MAPL/ESMF history component.

Since the history component internally organizes many diagnostics tasks such as output scheduling, file writing, and data averaging, all HEMCO diagnostics are made available to the history component on every time step, e.g. the entire content of the HEMCO diagnostics list is 'flushed' every time this subroutine is called.

For now, all diagnostics data is copied to the corresponding MAPL data pointer so that this routine works for cases where the HEMCO precision is not equal to the ESMF precision.

Once the HEMCO precision is pegged to the ESMF precision, we can just establish pointers between the export arrays and the diagnostics the first time this routine is called.

# **INTERFACE:**

```
SUBROUTINE HCOIO_WRITE_ESMF ( am_I_Root, HcoState, RC, OnlyIfFirst, COL )
USES:
    USE ESMF
    USE MAPL_MOD
    USE HCO_Types_Mod, ONLY : DiagnCont
    USE HCO_State_Mod, ONLY : HCO_State
 # include "MAPL_Generic.h"
INPUT PARAMETERS:
```

```
! root CPU?
LOGICAL,
                           INTENT(IN
                                      ) :: am_I_Root
                                                       ! HEMCO state object
TYPE(HCO_State), POINTER
                                         :: HcoState
                 OPTIONAL, INTENT(IN
                                      ) :: OnlyIfFirst !
LOGICAL,
INTEGER,
                 OPTIONAL, INTENT(IN
                                      ) :: COL
                                                       ! Collection Nr.
```

# INPUT/OUTPUT PARAMETERS:

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

#### **REVISION HISTORY:**

```
05 Aug 2014 - C. Keller
                          - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

#### 1.21 Fortran: Module Interface hcoio\_write\_std\_mod.F90

Module HCOIO\_write\_std\_mod.F90 is the HEMCO data output interface for the 'standard' model environment. It contains routines to write out diagnostics into a netCDF file.

# **INTERFACE:**

```
MODULE HCOIO_WRITE_STD_MOD
USES:
  USE HCO_ERROR_MOD
  USE HCO_DIAGN_MOD
  IMPLICIT NONE
  PRIVATE
 #if !defined(ESMF_)
```

# PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCOIO\_WRITE\_STD

#### PRIVATE MEMBER FUNCTIONS:

PRIVATE :: ConstructTimeStamp

#### **REMARKS:**

HEMCO diagnostics are still in testing mode. We will fully activate them at a later time. They will be turned on when debugging & unit testing.

#### REVISION HISTORY:

```
04 May 2014 - C. Keller - Initial version.

11 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers

11 Jun 2014 - R. Yantosca - Now use F90 freeform indentation

28 Jul 2014 - C. Keller - Removed GC specific initialization calls and moved to HEMCO core.

05 Aug 2014 - C. Keller - Added dummy interface for ESMF.

03 Apr 2015 - C. Keller - Added HcoDiagn_Write

22 Feb 2016 - C. Keller - Split off from hcoio_diagn_mod.F90
```

#### 1.21.1 HCOIO\_write\_std

Subroutine HCOIO\_write\_std writes diagnostics to netCDF file. If the ForceWrite flag is set to TRUE, all diagnostics are written out except they have already been written out during this time step. This option is usually only used at the end of a simulation run. If ForceWrite is False, only the diagnostics that are at the end of their time averaging interval are written. For example, if the current month is different from the previous (emissions) month, all diagnostics with hourly, daily and monthly time averaging intervals are written out. If the optional argument OnlyIfFirst is set to TRUE, diagnostics will only be written out if its nnGetCalls is 1. This can be used to avoid that diagnostics will be written out twice. The nnGetCalls is reset to zero the first time a diagnostics is updated. For diagnostics that point to data stored somewhere else (i.e. that simply contain a data pointer, nnGetCalls is never reset and keeps counting.

#### **INTERFACE:**

```
SUBROUTINE HCOIO_write_std( am_I_Root, HcoState, ForceWrite, & RC, PREFIX, UsePrevTime, & OnlyIfFirst, COL )
```

# **USES:**

```
USE Ncdf_Mod, ONLY : NC_Var_Write
USE Ncdf_Mod, ONLY : NC_Get_RefDateTime
USE CHARPAK_Mod, ONLY : TRANLC
USE HCO_State_Mod, ONLY : HCO_State
USE JulDay_Mod, ONLY : JulDay
USE HCO_EXTLIST_MOD, ONLY : GetExtOpt, CoreNr
USE HCO_Types_Mod, ONLY : DiagnCont
USE HCO_Clock_Mod
```

#### INPUT PARAMETERS:

```
INTENT(IN ) :: am_I_Root ! root CPU?
LOGICAL,
                                       :: HcoState ! HEMCO state object
TYPE(HCO_State), POINTER
LOGICAL,
                          INTENT(IN
                                     ) :: ForceWrite ! Write all diagnostics?
CHARACTER(LEN=*), OPTIONAL, INTENT(IN ) :: PREFIX ! File prefix
                OPTIONAL, INTENT(IN ) :: UsePrevTime ! Use previous time
LOGICAL,
                OPTIONAL, INTENT(IN ) :: OnlyIfFirst ! Only write if nnDiagn is 1
LOGICAL,
                OPTIONAL, INTENT(IN
                                     ) :: COL
                                                     ! Collection Nr.
INTEGER,
```

# INPUT/OUTPUT PARAMETERS:

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

# **REVISION HISTORY:**

```
12 Sep 2013 - C. Keller - Initial version

11 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers

11 Jun 2014 - R. Yantosca - Now use F90 freeform indentation

19 Feb 2015 - C. Keller - Added optional argument OnlyIfFirst

23 Feb 2015 - R. Yantosca - Now make Arr1D REAL(sp) so that we can write out lon & lat as float instead of double

06 Nov 2015 - C. Keller - Output time stamp is now determined from variable OutTimeStamp.

14 Jan 2016 - E. Lundgren - Create netcdf title out of filename prefix

20 Jan 2016 - C. Keller - Added options DiagnRefTime and DiagnNoLevDim.

03 Mar 2016 - M. Sulprizio- Change netCDF format to netCDF-4

26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 1.21.2 ConstructTimeStamp

Subroutine ConstructTimeStamp is a helper routine to construct the time stamp of a given diagnostics collection.

# **INTERFACE:**

```
SUBROUTINE ConstructTimeStamp (am_I_Root, HcoState, PS, PrevTime, Yr, Mt, Dy, hr, mn, RC)
USES:
```

USE HCO\_State\_Mod, ONLY : HCO\_State USE HCO\_Clock\_Mod

USE JULDAY\_MOD

# INPUT/OUTPUT PARAMETERS:

INTENT(IN LOGICAL,

:: am\_I\_Root ! Root CPU?
:: HcoState ! HEMCO state obj
:: PS ! collection ID
:: PrevTime ! Use previous time? TYPE(HCO\_State), POINTER INTEGER, INTENT(IN )

LOGICAL, INTENT(IN

# INPUT/OUTPUT PARAMETERS:

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

# **OUTPUT PARAMETERS:**

INTEGER, INTENT( OUT) :: Yr INTEGER, INTENT( OUT) :: Mt INTEGER, INTENT( OUT) :: Dy INTEGER, INTENT( OUT) :: hr INTEGER, INTENT( OUT) :: mn

# REVISION HISTORY:

06 Nov 2015 - C. Keller - Initial version

# 1.22 Fortran: Module Interface hco\_logfile\_mod

Module HCO\_LOGFILE\_MOD contains some wrapper routines to write data into the HEMCO logfile.

# **INTERFACE:**

MODULE HCO\_LOGFILE\_MOD

# **USES:**

USE HCO\_ERROR\_MOD

IMPLICIT NONE

PRIVATE

# PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCO\_Spec2Log PUBLIC :: HCO\_PrintList PUBLIC :: HCO\_PrintDataCont

# REVISION HISTORY:

27 May 2014 - C. Keller - Initialization

# 1.22.1 hco\_spec2log

Subroutine HCO\_Spec2Log writes information of a species to the logfile.

# **INTERFACE:**

```
SUBROUTINE HCO_Spec2Log( am_I_Root, HcoState, ID )
```

#### **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_State !INPUT PARAMETER
```

LOGICAL, INTENT(IN) :: am\_I\_Root ! Root CPU

TYPE(HCO\_State), POINTER :: HcoState ! HEMCO state object INTEGER, INTENT(IN) :: ID ! HEMCO species ID

# REVISION HISTORY:

```
27 May 2014 - C. Keller - Initialization
```

# 1.22.2 HCO\_PrintList

Subroutine HCO\_PrintList displays the content of List.

# **INTERFACE:**

```
SUBROUTINE HCO_PrintList ( HcoState, List, Verbose )
```

# **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_State
USE HCO_TYPES_MOD, ONLY : ListCont
```

!INPUT ARGUMENTS:

TYPE(HCO\_STATE),POINTER :: HcoState
TYPE(ListCont), POINTER :: List
INTEGER, INTENT(IN) :: Verbose

# **REVISION HISTORY:**

```
20 Apr 2013 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 1.22.3 HCO\_PrintDataCont

Subroutine HCO\_PrintDataCont displays the content of the data container Dct.

# **INTERFACE:**

```
SUBROUTINE HCO_PrintDataCont ( HcoState, Dct, Verbose )
!USES

USE HCO_STATE_MOD, ONLY : HCO_State
USE HCO_TYPES_MOD, ONLY : DataCont, HCO_DCTTYPE_BASE
!INPUT ARGUMENTS:

TYPE(HCO_STATE),POINTER :: HcoState
TYPE(DataCont), POINTER :: Dct
INTEGER, INTENT(IN) :: Verbose
```

#### REVISION HISTORY:

```
20 Apr 2013 - C. Keller - Initial version
16 Mar 2015 - M. Sulprizio- Now print min and max values for debugging
```

# 1.23 Fortran: Module Interface hco\_readlist\_mod.F90

Module HCO\_ReadList\_Mod contains routines and variables for the HEMCO ReadList. ReadList is a collection of all data containers used by HEMCO. They are categorized according to their reading update frequency, i.e all data containers that need to be updated on an annual basis are stored in ReadList 'Year', etc. The following reading update frequencies are supported:

- Year: update every year (annual data)
- Month: update every month (monthly data)
- Day: update every day (daily data)
- Hour: update every hour (hourly data)
- Once: update only once (time-invariant data)
- Always: update every time step

# **INTERFACE:**

```
MODULE HCO_ReadList_Mod
```

# **USES:**

```
USE HCO_Types_Mod
USE HCO_Error_MOD
USE HCO_State_MOD, ONLY : HCO_State

IMPLICIT NONE
PRIVATE
```

# PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: ReadList_Init
PUBLIC :: ReadList_Read
PUBLIC :: ReadList_Set
PUBLIC :: ReadList_Print
PUBLIC :: ReadList_Cleanup
PUBLIC :: ReadList_Remove
```

# PRIVATE MEMBER FUNCTIONS:

```
PRIVATE :: DtCont_Add
PRIVATE :: ReadList_Fill
```

#### **REVISION HISTORY:**

```
20 Apr 2013 - C. Keller - Initial version
01 Jul 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
01 Jul 2014 - R. Yantosca - Now use F90 free-format indentation
```

# 1.23.1 ReadList\_Set

Subroutine ReadList\_Set places the passed data container Dct in one of the reading lists, according to the data update frequency specified in the HEMCO configuration file. Containers are sorted with increasing container ID.

# **INTERFACE:**

```
SUBROUTINE ReadList_Set( am_I_Root, HcoState, Dct, RC )
```

# **USES:**

```
USE HCO_LOGFILE_MOD, ONLY : HCO_PrintDataCont
```

# **INPUT PARAMETERS:**

```
LOGICAL, INTENT(IN ) :: am_I_Root
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState
TYPE(DataCont), POINTER :: Dct
INTEGER, INTENT(INOUT) :: RC
```

```
20 Apr 2013 - C. Keller - Initial version
```

# 1.23.2 ReadList\_Read

Subroutine ReadList\_Read makes sure that all arrays in the reading lists are up to date, i.e. it invokes the data reading calls for those lists that need to be refreshed.

#### INTERFACE:

```
SUBROUTINE ReadList_Read( am_I_Root, HcoState, RC, ReadAll )
```

# **USES:**

```
USE HCO_CLOCK_MOD, ONLY: HcoClock_NewYear
USE HCO_CLOCK_MOD, ONLY: HcoClock_NewMonth
USE HCO_CLOCK_MOD, ONLY: HcoClock_NewDay
USE HCO_CLOCK_MOD, ONLY: HcoClock_NewHour
USE HCO_CLOCK_MOD, ONLY: HcoClock_First
```

# **INPUT PARAMETERS:**

```
LOGICAL, INTENT(IN ) :: am_I_Root ! root CPU?
LOGICAL, OPTIONAL, INTENT(IN ) :: ReadAll ! read all fields?
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object INTEGER, INTENT(INOUT) :: RC ! Success or failure?
```

#### REVISION HISTORY:

```
20 Apr 2013 - C. Keller - Initial version
```

# 1.23.3 ReadList\_Fill

Subroutine ReadList\_Fill (re-)reads the data from all containers of the passed ReadList. In a non-ESMF environment, this routine calls the HEMCO generic (netCDF) reading and remapping routines. In an ESMF environment, the arrays are obtained through the ESMF/MAPL software framework. ReadLIst\_Fill provides the interface between HEMCO and the data reading interface. See module HCOI\_DATAREAD\_MOD.F90 for more details on data reading.

The ReadList containers are added to EmisList immediately after data filling. This has the advantage that data arrays are immediately available through routine HCO\_GetPtr. This is required for country mappings that depend on the country mask input field.

#### **INTERFACE:**

```
SUBROUTINE ReadList_Fill( am_I_Root, HcoState, ReadList, RC )
```

#### **USES:**

```
USE HCOIO_DataRead_Mod, ONLY : HCOIO_DataRead
USE HCOIO_Read_Std_Mod, ONLY : HCOIO_ReadOther
USE HCOIO_Read_Std_Mod, ONLY : HCOIO_CloseAll
USE HCO_FileData_Mod, ONLY : FileData_ArrIsDefined
USE HCO_FileData_Mod, ONLY : FileData_ArrIsTouched
USE HCO_EmisList_Mod, ONLY : EmisList_Pass
USE HCO_DataCont_Mod, ONLY : DataCont_Cleanup
```

# USE HCO\_TIDX\_MOD, ONLY : tIDx\_Assign

#### INPUT PARAMETERS:

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

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object
TYPE(ListCont), POINTER :: ReadList ! Current reading list
INTEGER, INTENT(INOUT) :: RC ! Success or failure?
```

#### **REMARKS:**

Different HCOI\_DATAREAD routines may be invoked depending on the model environment.

#### REVISION HISTORY:

```
20 Apr 2013 - C. Keller - Initial version

23 Dec 2014 - C. Keller - Now pass container to EmisList immediately after reading the data. Added second loop to remove data arrays that are not used in EmisList.

02 Feb 2015 - C. Keller - Now call tIDx_Assign here instead of in hco_emislist_mod. This way, hco_emislist_mod can also be used by hco_clock_mod.

24 Mar 2015 - C. Keller - Now avoid closing/reopening the same file all the time.

24 Mar 2016 - C. Keller - Remove GetFileLUN and SaveFileLUN. This is now handled in hcoio_read_std_mod.F90.

26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

#### 1.23.4 DtCont\_Add

Subroutine DtCont\_Add adds a new container to the specified reading list.

# **INTERFACE:**

```
SUBROUTINE DtCont_Add( ReadList, Dct )
```

# INPUT PARAMETERS:

```
TYPE(ListCont), POINTER :: ReadList
TYPE(DataCont), POINTER :: Dct
```

# **REVISION HISTORY:**

```
20 Apr 2013 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

#### 1.23.5 ReadList\_Init

Subroutine ReadList\_Init initializes the ReadList.

#### **INTERFACE:**

```
SUBROUTINE ReadList_Init( am_I_Root, ReadLists, RC )
```

# INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(RdList), POINTER :: ReadLists
```

INTEGER, INTENT(INOUT) :: RC

# REVISION HISTORY:

```
20 Apr 2013 - C. Keller - Initial version
```

# 1.23.6 ReadList\_Print

Subroutine ReadList\_Print displays the content of ReadList.

# **INTERFACE:**

```
SUBROUTINE ReadList_Print( HcoState, ReadLists, verb )
```

# **USES:**

```
USE HCO_LOGFILE_MOD, ONLY : HCO_PrintList
```

!INPUT ARGUMENTS

TYPE(HCO\_State), POINTER :: HcoState TYPE(RdList), POINTER :: ReadLists

#### REVISION HISTORY:

```
20 Apr 2013 - C. Keller - Initial version
```

15 Mar 2015 - C. Keller - Added verbose number as input argument

# 1.23.7 ReadList\_Remove

Subroutine ReadList\_Remove removes the container given by name from the ReadList. If no container with the given name exist, nothing is done. This routine returns an error if the container already holds data.

# **INTERFACE:**

```
SUBROUTINE ReadList_Remove( am_I_Root, HcoState, cName, RC )
USES:
```

# INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
TYPE(HCO_State), POINTER :: HcoState
CHARACTER(LEN=*), INTENT(IN ) :: cName
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

# **REVISION HISTORY:**

```
13 Jan 2015 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 1.23.8 ReadList\_Cleanup

Subroutine ReadList\_Cleanup removes all content of ReadList. If RemoveDct is set to True, the content of the data containers will be also removed, otherwise the corresponding pointer is just nullified.

# **INTERFACE:**

```
SUBROUTINE ReadList_Cleanup( ReadLists, RemoveDct )
```

# **USES:**

```
USE HCO_DataCont_Mod, ONLY : ListCont_Cleanup
```

#### INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: RemoveDct
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(RdList), POINTER :: ReadLists
```

```
20 Apr 2013 - C. Keller - Initial version
```

# 1.24 Fortran: Module Interface hco\_restart\_mod.F90

Module HCO\_RESTART\_MOD contains wrapper routines to define, get and write restart fields.

Restart variables are required by some of the HEMCO extensions. The HEMCO restart variables can be organized through the HEMCO restart diagnostics collection. At the end of a simulation, all diagnostic fields ('containers') of the restart collection are written to the HEMCO restart file.

All fields from the HEMCO restart file can be easily read back into HEMCO via the HEMCO I/O infrastructure, i.e. by listing them in the HEMCO configuration file.

In an ESMF/MAPL environment, restart variables should be organized through the ESMF internal state object. This is particularly important for simulation that rely on checkpoint files (e.g. replay simulations). In this cases, the restart variables are obtained from / written to the ESMF internal state object, rather than the HEMCO restart file.

This module contains wrapper routines to define, obtain and write restart fields for the two aforementioned restart types. The routines work both for 'traditional' and ESMF restart variables. In an ESMF application, the first check is always performed within the internal state, e.g. it is first checked if the given field variable exists in the internal state of the gridded component that HEMCO sits in. If so, the field is obtained from / written to the internal state. If no internal state object exist, an attempt is made to obtain the field through the HEMCO data list, i.e. it is checked if the restart variable is specified in the HEMCO configuration file. A HEMCO diagnostics container is created in the diagnostics restart collection in both the traditional and the ESMF environment.

Routine HCO\_RestartDefine should be called during the initialization stage. Routine HCO\_RestartGet should be called on the first run call and after each rewinding of the clock. HEMCO routines HcoClock\_First and HcoClock\_Rewind can be used to determine if it's time to read/update the restart variable. HCO\_RestartWrite should be called \*on every time step\*. This is important in ESMF applications that rely on checkpoint files (e.g. replay simulations) that are written out by ESMF/MAPL throughout the simulation. In a non-ESMF environment, the HCO\_RestartWrite call is basically void but it should be called nevertheless.

# **INTERFACE:**

MODULE HCO\_RESTART\_MOD

# **USES:**

USE HCO\_ERROR\_MOD

IMPLICIT NONE PRIVATE

#### PUBLIC MEMBER FUNCTIONS:

! defined in all environment

```
PUBLIC :: HCO_RestartDefine
PUBLIC :: HCO_RestartGet
PUBLIC :: HCO_RestartWrite
```

#### PRIVATE MEMBER FUNCTIONS:

```
#if defined(ESMF_)
PRIVATE :: HCO_CopyFromIntnal_ESMF
#endif

INTERFACE HCO_RestartDefine
MODULE PROCEDURE HCO_RestartDefine_3D
MODULE PROCEDURE HCO_RestartDefine_2D
END INTERFACE HCO_RestartDefine

INTERFACE HCO_RestartGet
MODULE PROCEDURE HCO_RestartGet_3D
MODULE PROCEDURE HCO_RestartGet_2D
END INTERFACE HCO_RestartGet

INTERFACE HCO_RestartGet

INTERFACE HCO_RestartWrite
MODULE PROCEDURE HCO_RestartWrite_3D
MODULE PROCEDURE HCO_RestartWrite_2D
END INTERFACE HCO_RestartWrite_2D
END INTERFACE HCO_RestartWrite
```

#### **REVISION HISTORY:**

```
10 Mar 2015 - C. Keller - Initial version
```

# 1.24.1 HCO\_RestartDefine\_3D

TYPE(HCO\_State),

Subroutine HCO\_RestartDefine\_3D defines a restart diagnostics. This adds a diagnostics with output frequency 'End' to the HEMCO diagnostics list. Arr3D is the 3D field of interest. The diagnostics will not copy the current content of Arr3D but establish a 'link' (e.g. pointer) to it. This way, any updates to Arr3D will automatically be seen by the diagnostics and there is no need to explicitly update the content of the diagnostics.

# **INTERFACE:**

```
SUBROUTINE HCO_RestartDefine_3D( am_I_Root, HcoState, Name, Arr3D, & Unit, RC )

USES:

USE HCO_DIAGN_MOD, ONLY: Diagn_Create
USE HCO_STATE_MOD, ONLY: HCO_State
!INPUT ARGUMENTS:
LOGICAL, INTENT(IN ) :: am_I_Root! Root CPU?
```

:: HcoState ! HEMCO state obj.

POINTER

! Return code

```
CHARACTER(LEN=*),
                        INTENT(IN
                                    )
                                               :: Name
                                                             ! Name of restart variable
 ! Array with data of interest
 REAL(sp),
                        INTENT(IN
                                    ), TARGET :: Arr3D(HcoState%NX,HcoState%NY,HcoState%NZ)
 CHARACTER(LEN=*),
                                    )
                                                             ! Units of Arr3D
                        INTENT(IN
                                               :: Unit
!INPUT/OUTPUT ARGUMENTS:
 INTEGER,
                        INTENT(INOUT)
                                               :: RC
                                                             ! Return code
```

# **REVISION HISTORY:**

11 Mar 2015 - C. Keller - Initial version

# 1.24.2 HCO\_RestartDefine\_2D

Subroutine HCO\_RestartDefine\_2D defines a restart diagnostics. This adds a diagnostics with output frequency 'End' to the HEMCO diagnostics list. Arr2D is the 2D field of interest. The diagnostics will not copy the current content of Arr2D but establish a 'link' (e.g. pointer) to it. This way, any updates to Arr2D will automatically be seen by the diagnostics and there is no need to explicitly update the content of the diagnostics.

#### **INTERFACE:**

```
SUBROUTINE HCO_RestartDefine_2D( am_I_Root, HcoState, Name, Arr2D, &
                                                 RC
                                     Unit,
USES:
     USE HCO_DIAGN_MOD,
                            ONLY : Diagn_Create
     USE HCO_STATE_MOD,
                            ONLY : HCO_State
   !INPUT ARGUMENTS:
     LOGICAL,
                           INTENT(IN
                                                  :: am_I_Root ! Root CPU?
     TYPE(HCO_State),
                           POINTER
                                                  :: HcoState
                                                               ! HEMCO state obj.
     CHARACTER(LEN=*),
                           INTENT(IN
                                                  :: Name
                                                                ! Name of restart variable
                                       )
     ! Array with data of interest
     REAL(sp),
                           INTENT(IN
                                       ), TARGET :: Arr2D(HcoState%NX,HcoState%NY)
     CHARACTER(LEN=*),
                           INTENT(IN
                                       )
                                                                ! Units of Arr2D
                                                  :: Unit
   !INPUT/OUTPUT ARGUMENTS:
```

:: RC

#### **REVISION HISTORY:**

INTEGER,

11 Mar 2015 - C. Keller - Initial version

INTENT(INOUT)

# 1.24.3 HCO\_RestartGet\_3D

Subroutine HCO\_RestartGet\_3D attempts to read a restart field. In an ESMF environment, it first checks if the given field (name) is included in the internal state object, in which case the data object is filled with these values. If not found or if not in an ESMF environment, the HEMCO data list (specified in the HEMCO configuration file) is searched. A default

! Return code

value can be specified in case that no field could be imported via ESMF and/or the HEMCO interface.

# **INTERFACE:**

```
SUBROUTINE HCO_RestartGet_3D( am_I_Root, HcoState, Name,
                                                               Arr3D, &
                                 RC,
                                             FILLED,
                                                       Def3D,
                                                               DefVal )
USES:
     USE HCO_STATE_MOD,
                           ONLY : HCO_State
     USE HCO_EMISLIST_MOD, ONLY : HCO_GetPtr
   !INPUT ARGUMENTS:
     LOGICAL,
                          INTENT(IN
                                       )
                                                   :: am_I_Root ! Root CPU?
                                                   :: HcoState ! HEMCO state object
     TYPE(HCO_State),
                          POINTER
     CHARACTER(LEN=*),
                          INTENT(IN
                                       )
                                                                ! Name of restart variable
                                                   :: Name
     ! Default value to be used if restart variable could not be found
                                       ), OPTIONAL :: Def3D(HcoState%NX,HcoState%NY,HcoState%NZ
     REAL(sp),
                          INTENT(IN
     ! Default uniform value to be used if restart variable could not be found and
     ! Def2D is not defined.
     REAL(sp),
                          INTENT(IN
                                       ), OPTIONAL :: DefVal
   !OUTPUT ARGUMENTS:
     LOGICAL,
                          INTENT( OUT), OPTIONAL :: FILLED ! Was the restart variable found
   !INPUT/OUTPUT ARGUMENTS:
     ! Data field with restart variable
                          INTENT(INOUT)
                                                   :: Arr3D(HcoState%NX, HcoState%NY, HcoState%NZ
     REAL(sp),
```

:: RC

# **REVISION HISTORY:**

INTEGER,

```
11 Mar 2015 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

INTENT(INOUT)

# 1.24.4 HCO\_RestartGet\_2D

Subroutine HCO\_RestartGet\_2D attempts to read a restart field. In an ESMF environment, it first checks if the given field (name) is included in the internal state object, in which case the data object is filled with these values. If not found or if not in an ESMF environment, the HEMCO data list (specified in the HEMCO configuration file) is searched. A default value can be specified in case that no field could be imported via ESMF and/or the HEMCO interface.

# **INTERFACE:**

```
SUBROUTINE HCO_RestartGet_2D( am_I_Root, HcoState, Name, Arr2D, & RC, FILLED, Def2D, DefVal )
```

# **USES:**

```
USE HCO_STATE_MOD,
                          ONLY : HCO_State
    USE HCO_EMISLIST_MOD, ONLY : HCO_GetPtr
   !INPUT ARGUMENTS:
    LOGICAL,
                                                :: am_I_Root ! Root CPU?
                         INTENT(IN
                                      )
    TYPE(HCO_State),
                         POINTER
                                                  :: HcoState ! HEMCO state object
    CHARACTER(LEN=*),
                                                  :: Name
                                                              ! Name of restart variable
                         INTENT(IN
                                      )
     ! Default value to be used if restart variable could not be found
                                     ), OPTIONAL :: Def2D(HcoState%NX,HcoState%NY)
    REAL(sp),
                          INTENT(IN
     ! Default uniform value to be used if restart variable could not be found and
     ! Def2D is not defined.
    REAL(sp),
                          INTENT(IN
                                     ), OPTIONAL :: DefVal
   !OUTPUT ARGUMENTS:
                         INTENT( OUT), OPTIONAL :: FILLED ! Was the restart variable found
    LOGICAL,
   !INPUT/OUTPUT ARGUMENTS:
     ! Data field with restart variable
                                                 :: Arr2D(HcoState%NX,HcoState%NY)
    REAL(sp),
                         INTENT(INOUT)
    INTEGER,
                         INTENT(INOUT)
                                                 :: RC
                                                              ! Return code
REVISION HISTORY:
    11 Mar 2015 - C. Keller - Initial version
    26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

#### 1.24.5 HCO\_RestartWrite\_3D

Subroutine HCO\_RestartWrite\_3D writes a restart variable to the ESMF internal state. This is only of relevance in an ESMF environment. The 'regular' HEMCO diagnostics created in HCO\_RestartDefine becomes automatically written to disk.

# **INTERFACE:**

```
{\tt SUBROUTINE~HCO\_RestartWrite\_3D(~am\_I\_Root,~HcoState,~Name,~Arr3D,~RC,~FOUND~)}
```

:: RC

# **USES:**

```
USE HCO_STATE_MOD,
                        ONLY : HCO_State
!INPUT ARGUMENTS:
 LOGICAL,
                       INTENT(IN
                                               :: am_I_Root
                                                :: HcoState
 TYPE(HCO_State),
                       POINTER
                                               :: Name
 CHARACTER(LEN=*),
                       INTENT(IN
                                   )
!OUTPUT ARGUMENTS:
                       INTENT( OUT), OPTIONAL :: FOUND
 LOGICAL,
!INPUT/OUTPUT ARGUMENTS:
 REAL(sp),
                       INTENT(INOUT)
                                               :: Arr3D(HcoState%NX, HcoState%NY, HcoState%NZ
```

INTENT(INOUT)

# **REVISION HISTORY:**

INTEGER,

```
11 Mar 2015 - C. Keller - Initial version
```

# 1.24.6 HCO\_RestartWrite\_2D

Subroutine HCO\_RestartWrite\_2D writes a restart variable to the ESMF internal state. This is only of relevance in an ESMF environment. The 'regular' HEMCO diagnostics created in HCO\_RestartDefine becomes automatically written to disk.

# **INTERFACE:**

```
SUBROUTINE HCO_RestartWrite_2D( am_I_Root, HcoState, Name, Arr2D, RC, FOUND )
```

# **USES:**

```
USE HCO_STATE_MOD,
                        ONLY : HCO_State
!INPUT ARGUMENTS:
 LOGICAL,
                                    )
                                                :: am_I_Root
                       INTENT(IN
 TYPE(HCO_State),
                       POINTER
                                                :: HcoState
 CHARACTER(LEN=*),
                       INTENT(IN
                                                :: Name
                                    )
!OUTPUT ARGUMENTS:
 LOGICAL,
                       INTENT( OUT), OPTIONAL :: FOUND
!INPUT/OUTPUT ARGUMENTS:
 REAL(sp),
                       INTENT(INOUT)
                                                :: Arr2D(HcoState%NX,HcoState%NY)
                       INTENT(INOUT)
                                                :: RC
 INTEGER,
```

# **REVISION HISTORY:**

```
11 Mar 2015 - C. Keller - Initial version
```

# 1.24.7 HCO\_CopyFromIntnal\_ESMF

Subroutine HCO\_CopyFromIntnal\_ESMF attempts to transfer data to and from the ESMF/MAPL internal state.

# **INTERFACE:**

```
SUBROUTINE HCO_CopyFromIntnal_ESMF ( am_I_Root, HcoState, Name, & Direction, Found, RC, Arr2D, Arr3D )
```

# **USES:**

```
#include "MAPL_Generic.h"
   USE ESMF
   USE MAPL_Mod
   USE HCO_STATE_MOD, ONLY : Hco_State
```

# **ARGUMENTS:**

```
:: am_I_Root
LOGICAL,
                     INTENT(IN
                                 )
TYPE(HCO_State),
                     POINTER
                                              :: HcoState
CHARACTER(LEN=*),
                     INTENT(IN
                                 )
                                              :: Name
INTEGER,
                     INTENT(IN
                                              :: Direction
                                                              ! 1: internal to Arr2D; -1:
                                 )
                                              :: Found
LOGICAL,
                     INTENT( OUT)
```

# REVISION HISTORY:

```
10 Mar 2015 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 1.25 Fortran: Module Interface hco\_state\_mod.F90

Module HCO\_State\_Mod contains definitions and sub- routines for the HEMCO state derived type. The HEMCO state object (HcoState) contains all information related to the HEMCO run, such as the HEMCO clock, information on the emission grid and the data fields to be read, details on all used species, various physical constants, etc. It also contains the final assembled 3D flux and 2D deposition arrays (to be passed to the overlaying model) and a pointer to the HEMCO configuration object (Config). The latter contains error and traceback information and holds the data fields (in the data list ConfigList).

The HEMCO state object (typically called HcoState) for a given HEMCO run must be defined on the HEMCO-model interface level (subroutine HcoState\_Init).

#### **INTERFACE:**

```
MODULE HCO_State_Mod
USES:
USE HCO_Types_Mod
USE HCO_Error_Mod
USE HCO_Arr_Mod
USE HCO_VertGrid_Mod

#if defined(ESMF_)
USE ESMF
#endif

IMPLICIT NONE
PRIVATE
```

# PUBLIC MEMBER FUNCTIONS:

! HCO\_State: Main HEMCO State derived type

```
PUBLIC :: HcoState_Init

PUBLIC :: HcoState_Final

PUBLIC :: HCO_GetModSpcID

PUBLIC :: HCO_GetHcoID

PUBLIC :: HCO_GetExtHcoID
```

```
TYPE, PUBLIC :: HCO_State
  !%%%% Species information %%%%%
  INTEGER
                            :: nSpc
                                         ! # of species
  TYPE(HcoSpc),
                     POINTER :: Spc(:)
                                        ! list of species
  !%%%% Emission grid information %%%%%
                            :: NX
                                         ! # of x-pts (lons) on this CPU
  INTEGER
                            :: NY
                                         ! # of y-pts (lats) on this CPU
                                         ! # of z-pts (levs) on this CPU
  INTEGER
                            :: NZ
                                         ! HEMCO grid information
  TYPE(HcoGrid),
                    POINTER :: Grid
  TYPE(HcoClock),
                    POINTER :: Clock
                                         ! HEMCO clock
  ! Data array
  TYPE(Arr3D_HP),
                    POINTER :: Buffer3D
                                          ! Placeholder to store temporary
                                          ! 3D array. Emissions will be
                                          ! written into this array if
                                          ! option FillBuffer = .TRUE.
  !%%%% Constants and timesteps %%%%%
  TYPE(HcoPhys),
                     POINTER :: Phys
                                         ! Physical constants
  REAL(sp)
                            :: TS_EMIS
                                         ! Emission timestep [s]
  REAL(sp)
                            :: TS_CHEM
                                          ! Chemical timestep [s]
  REAL(sp)
                            :: TS_DYN
                                          ! Dynamic timestep [s]
  !%%%% Aerosol quantities %%%%%
  INTEGER
                            :: nDust
                                          ! # of dust species
  TYPE(HcoMicroPhys), POINTER :: MicroPhys ! Microphysics settings
  !%%%% Run time options %%%%%
                            :: isESMF
  LOGICAL
                                          ! Are we using ESMF?
                   POINTER :: Options
                                         ! HEMCO run options
  TYPE(HcoOpt),
  !%%%% ReadLists %%%%%
  TYPE(RdList), POINTER :: ReadLists
  LOGICAL
                            :: SetReadListCalled
  !%%%% Emissions linked list %%%%%%
  TYPE(ListCont), POINTER
                           :: EmisList
  INTEGER
                            :: nnEmisCont = 0 ! # of container in EmisList
  !%%%% Data container indeces %%%%%
  ! Element i of cIDList will point to data-container with container
  ! ID i (e.g. cIDList(3) points to data-container with cID = 3).
  TYPE(cIDListPnt), POINTER :: cIDList(:) => NULL()
  ! # of defined data containers. Will be automatically increased
```

```
! by one when creating a new data container (DataCont_Init)
     INTEGER
                                 :: nnDataCont = 0
     ! Define object based on TimeIdxCollection derived type
     TYPE(TimeIdxCollection), POINTER :: AlltIDx => NULL()
     ! HEMCO configuration object
     TYPE(ConfigObj), POINTER
                                :: Config => NULL()
     ! Pointer to beginning of collections linked list
     TYPE(DiagnBundle), POINTER :: Diagn => NULL()
     !%%%% ESMF objects
#if defined(ESMF_)
     TYPE(ESMF_GridComp), POINTER :: GridComp
     TYPE(ESMF_State),
                         POINTER :: IMPORT
     TYPE(ESMF_State),
                         POINTER :: EXPORT
#endif
 END TYPE HCO_State
```

#### **REVISION HISTORY:**

```
20 Aug 2013 - C. Keller - Initial version, adapted from gigc_state_chm_mod.F90

07 Jul 2014 - R. Yantosca - Cosmetic changes

30 Sep 2014 - R. Yantosca - Add HcoMicroPhys derived type to HcoState

08 Apr 2015 - C. Keller - Added MaskFractions to HcoState options.

13 Jul 2015 - C. Keller - Added option 'Field2Diagn'.

15 Feb 2016 - C. Keller - Update to v2.0
```

#### 1.25.1 HcoState\_Init

Routine HcoState\_Init initializes the HEMCO state object. This initializes (nullifies) all pointers and sets all HEMCO settings and options to default values. The here defined pointers are defined/connected at the HEMCO-model interface level. The passed HEMCO configuration object (HcoConfig) must be defined, e.g. this subroutine must be called after having read (at least stage 1 of) the HEMCO configuration file (Config\_ReadFile in hco\_config\_mod.F90).

# **INTERFACE:**

**USES:** 

```
SUBROUTINE HcoState_Init( am_I_Root, HcoState, HcoConfig, nSpecies, RC )
```

# USE HCO\_EXTLIST\_MOD, ONLY : GetExtOpt, CoreNr USE HCO\_UNIT\_MOD, ONLY : HCO\_UnitTolerance

# INPUT PARAMETERS:

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

INTEGER, INTENT(IN) :: nSpecies ! # HEMCO species
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO State object
TYPE(ConfigObj), POINTER :: HcoConfig ! HEMCO Config object
INTEGER, INTENT(INOUT) :: RC ! Return code
```

# **REVISION HISTORY:**

# 1.25.2 HcoState\_Final

Routine HcoState\_CLEANUP cleans up HcoState.

# INTERFACE:

```
SUBROUTINE HcoState_Final( HcoState )
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO State object
```

# REVISION HISTORY:

```
20 Aug 2013 - C. Keller - Adapted from gigc_state_chm_mod.F90
24 Sep 2014 - R. Yantosca - Add an extra safety check when deallocating the pointer field HcoState%Spc
```

# 1.25.3 HCO\_GetModSpcId

Function HCO\_GetModSpcId returns the model species index of a species by name. Returns -1 if given species is not found, 0 if name corresponds to the HEMCO wildcard character.

# **INTERFACE:**

```
FUNCTION HCO_GetModSpcID( name, HcoState ) RESULT( Indx )
USES:
```

```
USE HCO_EXTLIST_MOD, ONLY : HCO_GetOpt
```

# INPUT PARAMETERS:

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

# INPUT/OUTPUT PARAMETERS:

TYPE(HCO\_State), INTENT(INOUT) :: HcoState ! HEMCO State

#### RETURN VALUE:

INTEGER :: Indx ! Index of this species

# REVISION HISTORY:

20 Aug 2013 - C. Keller - Adapted from gigc\_state\_chm\_mod.F90

#### 1.25.4 HCO\_GetHcoId

Function HCO\_GetHcoIdHCO returns the HEMCO species index of a species by name. Returns -1 if given species is not found, 0 if name corresponds to the HEMCO wildcard character.

# **INTERFACE:**

```
FUNCTION HCO_GetHcoID( name, HcoState ) RESULT( Indx )
```

# **USES:**

USE HCO\_EXTLIST\_MOD, ONLY : HCO\_GetOpt

# INPUT PARAMETERS:

CHARACTER(LEN=\*), INTENT(IN) :: name ! Species name TYPE(HCO\_State), INTENT(INOUT) :: HcoState ! HEMCO State

# RETURN VALUE:

INTEGER :: Indx ! Index of this species

# REVISION HISTORY:

20 Aug 2013 - C. Keller - Adapted from gigc\_state\_chm\_mod.F90

# 1.25.5 HCO\_GetExtHcoID

Subroutine HCO\_GetExtHcoID returns the HEMCO species IDs and names for all species assigned to the given extension (identified by its extension number).

# **INTERFACE:**

```
SUBROUTINE HCO_GetExtHcoID( HcoState, ExtNr, HcoIDs, & SpcNames, nSpc, RC )
```

#### **USES:**

```
USE CHARPAK_MOD, ONLY : STRSPLIT
USE HCO_EXTLIST_MOD, ONLY : GetExtSpcStr
USE HCO_EXTLIST_MOD, ONLY : HCO_GetOpt
```

#### INPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState
```

# **OUTPUT PARAMETERS:**

```
INTEGER, ALLOCATABLE, INTENT( OUT) :: HcoIDs(:) ! Species IDs
```

# INPUT/OUTPUT PARAMETERS:

```
CHARACTER(LEN=*), ALLOCATABLE, INTENT(INOUT) :: SpcNames(:) ! Species names
INTEGER, INTENT(INOUT) :: nSpc ! # of species
INTEGER, INTENT(INOUT) :: RC ! Success/fail
```

# REVISION HISTORY:

```
10 Jan 2014 - C. Keller: Initialization (update)
29 Sep 2014 - C. Keller: Now allows species lists up to 2047 instead of 255 characters.
```

# 1.26 Fortran: Module Interface hco\_tidx\_mod.F90

Module HCO\_tIdx\_Mod contains routines and variables to organize and index data array time slices.

The HEMCO data containers can hold multiple 2D or 3D data arrays (aligned in a vector), providing a 4th dimension (time). During emission calculation, only the vector element ('time slice') representative for the given time will be used. Currently, the following time slice intervals are supported:

- Constant: Only one time slice (default)
- Hourly: Between 2-24 time slices. These slices will be split into even day bins, and are cycled through accordingly. the local time is used to obtain the current valid index at each longitude.
- Hourly\_gridded: As hourly, but uses the same time slice index across all longitudes (based upon UTC time).
- Weekdaily: Seven time slices, representing the days of the week: Sun, Mon, ..., Sat. Uses local time.
- Monthly: 12 time slices, representing the months of the year: Jan, ..., Dec. Uses local time.

The time slice cycling frequency is automatically determined during creation of a data container - based upon the time stamp settings in the HEMCO configuration file and the time information read from the data (netCDF) file.

Spatial uniform data (i.e. nx = ny = 1) is always assigned the local time cycle intervals (hourly, weekdaily, or monthly), e.g. the local time is used at every grid box when picking the time slice at a given time. For gridded data, it's assumed that local-time effects are already taken into account and UTC time is used at all locations to select the currently valid time slice. The exception is weekdaily data, which is always assumed to be in local time.

Structure AlltIDx organizes the indexing of the vector arrays. It contains the current valid time slice index for each of the above defined time slice intervals. Each data container points to one of the elements of AlltIDx, according to the temporal dimension of its array. The values of AlltIDx become update on every HEMCO time step.

#### **INTERFACE:**

```
MODULE HCO_tIdx_Mod
```

#### **USES:**

```
USE HCO_Error_Mod
USE HCO_Types_Mod, ONLY: TimeIdx
USE HCO_Types_Mod, ONLY: TimeIdxCollection
IMPLICIT NONE
PRIVATE
```

# PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: tIDx_Assign

PUBLIC :: tIDx_Init

PUBLIC :: tIDx_GetIndx

PUBLIC :: tIDx_Cleanup

PUBLIC :: tIDx_IsInRange

PUBLIC :: HCO_GetPrefTimeAttr

PUBLIC :: HCO_ExtractTime
```

# **REMARKS:**

```
The current local time implementation assumes a regular grid, i.e. local time does not change with latitude!
```

```
29 Dec 2012 - C. Keller - Initialization
22 Aug 2013 - C. Keller - Some time slice updates.
08 Jul 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
08 Jul 2014 - R. Yantosca - Now use F90 free-format indentation
03 Dec 2014 - C. Keller - Major update: now calculate the time slice
```

indeces on the fly instead of storing them in precalculated vectors.

25 Feb 2015 - R. Yantosca - Comment out WEEKDAY\_GRID, it is not used anymore. This avoids seg faults.

# 1.26.1 tIDx\_Init

Subroutine tIDx\_Init initializes the time slice index collection.

# **INTERFACE:**

```
SUBROUTINE tIDx_Init( HcoState, RC )
```

# **USES:**

USE HCO\_State\_Mod, ONLY : HCO\_State

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! Hemco state INTEGER, INTENT(INOUT) :: RC ! Return code
```

# REVISION HISTORY:

29 Dec 2012 - C. Keller - Initialization

# $1.26.2 \quad tIDx\_Set$

Subroutine tIDx\_Set linkes the passed TimeIDx type to the corresponding element in the TimeIdx collection, according to the given TypeID. TypeID can be one of the following:

- 1: Constant
- 24: Hourly
- 241: Hourly\_Grid
- 7: Weekday
- 71: Weekday\_Grid
- 12: Monthly

#### **INTERFACE:**

```
SUBROUTINE tIDx_Set( HcoState, ctIDx, TypeID )
```

# **USES:**

```
USE HCO_State_Mod, ONLY : HCO_State
```

#### INPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state
TYPE(TimeIdx), POINTER :: ctIDx ! container TimeIDx
INTEGER, INTENT(IN) :: TypeID ! type ID
```

## **REVISION HISTORY:**

```
29 Dec 2012 - C. Keller - Initialization
```

# 1.26.3 tIDx\_Cleanup

Subroutine tIDx\_Cleanup deallocates the time slice index collection.

## **INTERFACE:**

```
SUBROUTINE tIDx_Cleanup( AlltIDx )
!Input/output arguments:
```

```
TYPE(TimeIdxCollection), POINTER :: AlltIDx
```

## **REVISION HISTORY:**

```
29 Dec 2012 - C. Keller - Initialization
```

#### $1.26.4 \quad tIDx\_GetIndx$

Subroutine tIDx\_GetIndx calculates the current valid index values for the given file data time slice type and longitude location

#### **INTERFACE:**

```
FUNCTION tIDx_GetIndx ( am_I_Root, HcoState, Dta, I, J ) RESULT ( Indx )
USES:
```

```
USE HCO_State_Mod, ONLY : HCO_State
USE HCO_Types_Mod, ONLY : FileData
```

USE HCO\_CLOCK\_MOD, ONLY : HcoClock\_Get, HcoClock\_GetLocal

# INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root ! Longitude index of interest
```

```
TYPE(HCO_State), POINTER :: HcoState ! Hemco state
TYPE(FileData), POINTER :: Dta ! File data object
```

INTEGER, INTENT(IN) :: I ! Longitude index of interest INTEGER, INTENT(IN) :: J ! Latitude index of interest

# INPUT/OUTPUT PARAMETERS:

```
INTEGER :: Indx ! Index
```

```
02 Dec 2014 - C. Keller - Initial version
```

## 1.26.5 tIDx\_Assign

Subroutine tIDx\_Assign assigns the time index pointer of the file data object of the passed list container to the corresponding time index element of the time index collection. The time slice cycle interval is determined from the number of time slices (length of the data array vector) and the time difference (deltaT) between them.

Note: Scale factors read directly from the HEMCO configuration file become their delta T assigned upon reading from file (see subroutine Register\_Scal in hco\_config\_mod.F90).

#### **INTERFACE:**

```
SUBROUTINE tIDx_Assign( HcoState, Dct, RC )
```

#### **USES:**

```
USE HCO_State_Mod, ONLY : HCO_State USE HCO_Types_Mod, ONLY : DataCont
```

### INPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! Hemco state
TYPE(DataCont), POINTER :: Dct ! Data container
```

# INPUT/OUTPUT PARAMETERS:

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

#### REVISION HISTORY:

```
13 Jan 2014 - C. Keller - Initial version
```

## 1.26.6 tIDx\_IsInRange

Subroutine tIDx\_IsInRange returns true if the passed datetime is within the range of the date ranges of the data container.

#### INTERFACE:

```
FUNCTION tIDx_IsInRange ( Lct, Yr, Mt, Dy, Hr ) RESULT ( InRange )
USES:
```

```
USE HCO_TYPES_MOD, ONLY : ListCont
```

### **INPUT PARAMETERS:**

```
TYPE(ListCont), POINTER :: Lct ! File data object
INTEGER, INTENT(IN) :: Yr
INTEGER, INTENT(IN) :: Mt
INTEGER, INTENT(IN) :: Dy
INTEGER, INTENT(IN) :: Hr
```

# INPUT/OUTPUT PARAMETERS:

```
LOGICAL :: InRange
```

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

## 1.26.7 HCO\_GetPrefTimeAttr

Subroutine HCO\_GetPrefTimeAttr returns the preferred time reading attributes for a given field, based upon the specs set in the HEMCO configuration file and the current simulation date. This routine is used to select the proper time slice to be read at the given time.

The time reading attributes are set to the value that is closest (or equal) to the current datetime but within the range provided in the configuration file. If the year, month, or day is not specified, the current simulation date values are taken. For unspecified hours, a value of -1 is returned (this allows to read all hourly slices at once).

## **INTERFACE:**

```
SUBROUTINE HCO_GetPrefTimeAttr( am_I_Root, HcoState, Lct, & readYr, readMt, readDy, & readHr, readMn, RC )
```

#### **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_State

USE HCO_TYPES_MOD, ONLY : ListCont

USE HCO_TYPES_MOD, ONLY : HCO_CFLAG_RANGE, HCO_CFLAG_EXACT

USE HCO_CLOCK_MOD ONLY : HcoClock_Get
```

USE HCO\_CLOCK\_MOD, ONLY : HcoClock\_Get
USE HCO\_TIMESHIFT\_MOD, ONLY : TimeShift\_Apply

#### **INPUT PARAMETERS:**

```
LOGICAL, INTENT(IN ) :: am_I_Root ! preferred year TYPE(HCO_State), POINTER :: HcoState ! List container TYPE(ListCont), POINTER :: Lct ! List container
```

#### **OUTPUT PARAMETERS:**

```
INTENT( OUT) :: readYr
                                             ! preferred year
INTEGER,
INTEGER,
                 INTENT(
                          OUT) :: readMt
                                             ! preferred month
                                             ! preferred day
INTEGER,
                 INTENT(
                         OUT) :: readDy
                                            ! preferred hour
INTEGER,
                 INTENT(
                          OUT) :: readHr
INTEGER,
                 INTENT( OUT) :: readMn
                                             ! preferred minute
```

# INPUT/OUTPUT PARAMETERS:

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

```
13 Jan 2014 - C. Keller - Initial version
29 Feb 2016 - C. Keller - Added time shift option
```

## 1.26.8 HCO\_ExtractTime

Subroutine HCO\_ExtractTime extracts the time stamp (ranges) from the passed character string. The string is expected to be in format Yr/Mt/Dy/Hr. Valid values for Yr, Mt, Dy and Hr are:

- 1. Range of values, separated by sign: e.g. 2000-2010.
- 2. Single value: 2000
- 3. Wildcard character (default = \*). In this case, the data interval is determined automatically by HEMCO based on the number of time slices found in the data set.
- 4. Time tokens: YYYY,MM, DD,HH. When reading the data, these values will be substituted by the current simulation date.
- 5. String 'WD'. Denotes that the data contains weekday data. It is expected that the first slice represents Sunday. Weekday data can be used in combination with annual or monthly data. In that case, there need to be seven entries for every year and/or month, respectively.

The extracted time stamp is written into the arrays ncYrs, ncMts, ncDys and ncHrs of the passed data structure Dta.

## **INTERFACE:**

```
SUBROUTINE HCO_ExtractTime ( HcoConfig, CharStr, Dta, RC )
```

#### **USES:**

```
USE CHARPAK_MOD, ONLY: STRSPLIT

USE HCO_TYPES_MOD, ONLY: FileData

USE HCO_TYPES_MOD, ONLY: ConfigObj

USE HCO_TYPES_MOD, ONLY: HCO_UFLAG_ALWAYS

USE HCO_EXTLIST_MOD, ONLY: HCO_GetOpt

USE HCO_TIMESHIFT_MOD, ONLY: TimeShift_Set
```

#### INPUT PARAMETERS:

```
TYPE(ConfigObj), POINTER :: HcoConfig ! config obj
CHARACTER(LEN=*), INTENT(IN ) :: CharStr
TYPE(FileData), POINTER :: Dta
```

#### **OUTPUT PARAMETERS:**

```
INTEGER, INTENT(INOUT) :: RC
```

```
18 Sep 2013 - C. Keller - Initial version (update)
29 Feb 2016 - C. Keller - Added time shift option
```

#### 1.27 Fortran: Module Interface hco\_timeshift\_mod.F90

Module hco\_timeshift\_mod.F90 contains routines to shift the file reference time by a given value. Time stamps shifts can be provided as optional fifth element to the time stamp attribute in the HEMCO configuration file.

For instance, consider the case where 3-hourly averages are provided in individual files with centered time stamps, e.g.: file.yyyymmdd\_0130z.nc, file.yyyymmdd\_0430z.nc, ..., file.yyymmdd\_2230z.nc To read these files \*at the beginning\* of their time intervals, the time stamp can be shifted by 90 minutes, e.g. the file name, variable, and time attribute section reads: ... file.\$yyyymmdd\_\$hh\$mnz.nc VARNAME 2000-2016/1-12/1-31/0-23/+90minutes ...

At time 00z, HEMCO will then read file 0130z and keep using this file until 03z, when it switches to file 0430z. Similarly, it is possible to shift the file reference time by any number of years, months, days, or hours. Time shifts can be forward or backward in time (use - sign to shift backwards).

This module contains subroutines to determine the time to be shifted (stored in filedata variable tshift) and shifts the desired reference time as needed.

#### **INTERFACE:**

```
MODULE HCO_TIMESHIFT_MOD
```

## **USES:**

```
USE HCO_Error_Mod
USE HCO_State_Mod, ONLY : HCO_State
IMPLICIT NONE
PRIVATE
```

#### PUBLIC MEMBER FUNCTIONS:

PUBLIC :: TimeShift\_Set
PUBLIC :: TimeShift\_Apply

#### **REMARKS:**

#### **REVISION HISTORY:**

```
29 Feb 2016 - C. Keller - Initial version
```

#### 1.27.1 TimeShift\_Set

Subroutine TimeShift\_Set sets the time shift values. The time shift attribute tshift contains two entries: the first entry denotes the number of months to be shifted (integer value), while the second entry denotes then number of seconds to be shifted.

#### **INTERFACE:**

```
SUBROUTINE TimeShift_Set( HcoConfig, Dta, shift, RC )
```

#### **USES:**

```
USE HCO_TYPES_MOD, ONLY : ListCont
USE HCO_TYPES_MOD, ONLY : FileData
USE HCO_TYPES_MOD, ONLY : ConfigObj
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(ConfigObj), POINTER :: HcoConfig ! HEMCO config TYPE(FileData), POINTER :: Dta ! file container CHARACTER(LEN=*), INTENT(IN ) :: shift ! time shift INTEGER, INTENT(INOUT) :: RC ! Return code
```

#### REVISION HISTORY:

```
29 Feb 2016 - C. Keller - Initial version
```

# 1.27.2 TimeShift\_Apply

Subroutine TimeShift\_Apply shifts the reference time (provided through arguments yr, mt, dy, hr, and mn, by the time shift specified in the HEMCO configuration file (if specified at all).

#### INTERFACE:

```
SUBROUTINE TimeShift_Apply( am_I_Root, HcoState, Lct, & yr, mt, dy, hr, mn, RC)
```

## **USES:**

```
USE Julday_Mod
USE HCO_TYPES_MOD, ONLY : ListCont
```

# INPUT/OUTPUT PARAMETERS:

```
LOGICAL,
                 INTENT(IN
                             ) :: am_I_Root ! Root CPU
TYPE(HCO_State), POINTER
                                 :: HcoState ! Hemco state
TYPE(ListCont),
                 POINTER
                                :: Lct
                                             ! List container
INTEGER,
                 INTENT(INOUT) :: yr
                                             ! year
INTEGER,
                 INTENT(INOUT) :: mt
                                             ! month
INTEGER,
                 INTENT(INOUT) :: dy
                                             ! day
INTEGER,
                 INTENT(INOUT) :: hr
                                             ! hour
                 INTENT(INOUT) :: mn
                                             ! minute
INTEGER,
                 INTENT(INOUT) :: RC
INTEGER,
                                             ! Return code
```

```
29 Feb 2016 - C. Keller - Initial version
```

# 1.28 Fortran: Module Interface hco\_types\_mod.F90

Module HCO\_Types\_Mod contains HEMCO derived type definitions and global parameters. The here derived types become all bundled into the HEMCO state object, which is defined in module hco\_state\_mod.F90. Specific routines for the various derived types defined below can be found in the respective HEMCO modules (e.g. hco\_datacont\_mod.F90 for handling of HEMCO data containers and data container lists).

Prior to HEMCO v2.0, the derived type definitions were placed within the corresponding modules. Collecting them here breaks unnecessary dependencies amongst the various modules and consequently gives greater flexibility in using the modules independently.

#### **INTERFACE:**

```
MODULE HCO_TYPES_MOD
 USES:
 USE HCO_Error_Mod
 USE HCO_Arr_Mod
  IMPLICIT NONE
 PUBLIC
  !PUBLIC PARAMETERS:
  ! Maximum length of option name
  INTEGER, PARAMETER
                         :: OPTLEN = 1023
  ! Cycle flags. Used to determine the temporal behavior of data
  ! fields. For example, data set to 'cycle' will be recycled if
  ! the simulation date is outside of the datetime range of the
  ! source data. See data reading routine (hcoio_dataread_mod.F90)
  ! for more details.
  INTEGER, PARAMETER, PUBLIC :: HCO_CFLAG_CYCLE
                                                    = 1
  INTEGER, PARAMETER, PUBLIC :: HCO_CFLAG_RANGE
  INTEGER, PARAMETER, PUBLIC :: HCO_CFLAG_EXACT
  INTEGER, PARAMETER, PUBLIC :: HCO_CFLAG_INTER
  INTEGER, PARAMETER, PUBLIC
                             :: HCO_CFLAG_AVERG
  INTEGER, PARAMETER, PUBLIC :: HCO_CFLAG_RANGEAVG = 6
  ! Data container update flags. At the moment, those only indicate
  ! if a container gets updated every time step or based upon the
  ! details specifications ('srcTime') in the HEMCO configuration file.
  INTEGER, PARAMETER, PUBLIC :: HCO_UFLAG_FROMFILE = 1
  INTEGER, PARAMETER, PUBLIC :: HCO_UFLAG_ALWAYS
  ! Data container types. These are used to distinguish between
  ! base emissions, scale factors and masks.
  INTEGER, PARAMETER, PUBLIC :: HCO_DCTTYPE_BASE = 1
  INTEGER, PARAMETER, PUBLIC :: HCO_DCTTYPE_SCAL = 2
  INTEGER, PARAMETER, PUBLIC :: HCO_DCTTYPE_MASK = 3
```

```
! PBL level flag
INTEGER, PARAMETER, PUBLIC :: HCO_EMISL_PBL = 0
INTEGER, PARAMETER, PUBLIC :: HCO_EMISL_LEV = 1
INTEGER, PARAMETER, PUBLIC :: HCO_EMISL_M = 2
PUBLIC TYPES:
```

```
! HcoSpc: Derived type for HEMCO species
! **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.
TYPE :: HcoSpc
                                  ! HEMCO species ID
  INTEGER
                       :: HcoID
                       :: ModID ! Model species ID
  INTEGER
  CHARACTER(LEN= 31) :: SpcName ! species names
  REAL(hp)
                       :: MW_g ! species molecular wt.
                       :: EmMW_g ! emission molecular wt.**1 (g/mol)
  REAL(hp)
  REAL(hp)
                       :: MolecRatio ! molecule emission ratio**2 (-)
  REAL(hp)
                       :: HenryKO ! liq. over gas Henry const [M/atm]
                       :: HenryCR ! KO temp. dependency [K]
  REAL(hp)
                       :: HenryPKA ! pKa for Henry const. correction
  REAL(hp)
  TYPE(Arr2D_HP), POINTER :: Depv
                                  ! Deposition velocity [1/s] ! Emission flux [kg/m2/s]
  TYPE(Arr3D_HP), POINTER :: Emis
  TYPE(Arr3D_HP), POINTER :: Conc ! Concentration [v/v]
END TYPE HcoSpc
! HcoOpt: Derived type for HEMCO run options
TYPE :: HcoOpt
  INTEGER :: ExtNr
                          ! ExtNr to be used
  INTEGER :: SpcMin
                          ! Smallest HEMCO species ID to be considered
  INTEGER :: SpcMax
                          ! Highest HEMCO species ID to be considered
  INTEGER :: CatMin
                         ! Smallest category to be considered
  INTEGER :: CatMax
                       ! Highest category to be considered
  LOGICAL :: HcoWritesDiagn ! If set to .TRUE., HEMCO will schedule the
                           ! output of the default HEMCO diagnostics
                           ! (in hco_driver_mod.F90).
  LOGICAL :: AutoFillDiagn ! Write into AutoFill diagnostics?
  LOGICAL :: FillBuffer
                           ! Write calculated emissions into buffer
                           ! instead of emission array?
```

```
! Negative value flag (from configfile):
  INTEGER :: NegFlag
                           ! 2 = allow negative values
                           ! 1 = set neg. values to zero and prompt warning
                          ! 0 = return w/ error if neg. value
  LOGICAL :: PBL_DRYDEP
                          ! If true, dry deposition frequencies will
                          ! be calculated over the full PBL. If false,
                           ! they are calculated over the first layer only.
  REAL(hp) :: MaxDepExp
                          ! Maximum value of deposition freq. x time step.
  LOGICAL :: MaskFractions
                          ! If TRUE, masks are treated as binary, e.g.
                          ! grid boxes are 100% inside or outside of a
                          ! mask.
  LOGICAL :: Field2Diagn
                          ! When reading fields from disk, check if there
                          ! is a diagnostics with the same name and write
                          ! field to that diagnostics? Defaults to yes in
                           ! standalone mode and no in other setups.
  LOGICAL :: VertWeight
                          ! if spreading 2D fields across multiple vert.
                          ! levels, weight vertical dilution factors based
                          ! upon level depths?
END TYPE HcoOpt
! VertGrid: Description of vertical grid
TYPE :: VertGrid
  INTEGER
                        :: ZTYPE
                                         ! Grid type
  REAL(hp),
                POINTER :: Ap(:) => NULL() ! Hybrid sigma Ap values
  REAL(hp),
                POINTER :: Bp(:) => NULL() ! Hybrid sigma Bp values
END TYPE VertGrid
! -----
! HcoGrid: Derived type for HEMCO grid. The grid edges are used for data
! interpolation. The pressure midpoints are not needed by HEMCO core but
! can be specified for the extensions through ExtList.
! NOTES:
! * Not used in ESMF environment
! ** Only used by some extensions
!-----
TYPE :: HcoGrid
  TYPE(Arr2D_Hp), POINTER :: XMID
                                    ! mid-points in x-direction (lon)
  TYPE(Arr2D_Hp), POINTER :: YMID
                                    ! mid-points in y-direction (lat)
  TYPE(Arr2D_Hp), POINTER :: XEDGE
                                    ! grid edges in x-direction (lon)*
  TYPE(Arr2D_Hp), POINTER :: YEDGE
                                    ! grid edges in y-direction (lat)*
  TYPE(Arr3D_Hp), POINTER :: PEDGE
                                    ! pressure edges (Pa)
  TYPE(Arr2D_Hp), POINTER :: YSIN
                                    ! sin of y-direction grid edges*
  TYPE(Arr2D_Hp), POINTER :: AREA_M2
                                    ! grid box areas (m2)
  TYPE(Arr2D_Hp), POINTER :: ZSFC
                                    ! surface geopotential height (m) **
  TYPE(Arr2D_Hp), POINTER :: PSFC
                                    ! surface pressure (Pa)
  TYPE(Arr2D_Hp), POINTER :: PBLHEIGHT ! PBL height in m
```

```
TYPE(Arr3D_Hp), POINTER :: BXHEIGHT_M ! grid box heights (m) **
  TYPE(VertGrid), POINTER :: ZGRID ! vertical grid description
END TYPE HcoGrid
! HcoClock: Derived type definition for the HEMCO clock object
TYPE :: HcoClock
  ! Current time stamp (UTC)
  INTEGER :: ThisYear
                                  ! year
                 :: ThisMonth
  INTEGER
                                  ! month
                 :: ThisDay
  INTEGER
                                 ! day
                 :: ThisHour
  INTEGER
                                 ! hour
                 :: ThisMin
  INTEGER
                                 ! minute
                 :: ThisSec
                                ! second
  INTEGER
                 :: ThisDOY ! day of year
:: ThisWD ! weekday (0=Sun,...,6=Sat)
  INTEGER
  INTEGER
                 :: MonthLastDay ! Last day of month: 28,29,30,31
  INTEGER
  ! Current local times
  INTEGER
          :: ntz
                                  ! number of time zones
  INTEGER, POINTER :: ThisLocYear(:) ! local year
  INTEGER, POINTER :: ThisLocMonth(:) ! local month
  INTEGER, POINTER :: ThisLocDay(:) ! local day
  INTEGER, POINTER :: ThisLocWD(:) ! local weekday
  REAL(sp), POINTER :: ThisLocHour(:) ! local hour
  ! Previous time stamp (UTC)
           :: PrevYear
  INTEGER
  INTEGER
                 :: PrevMonth
  INTEGER
                 :: PrevDav
                 :: PrevHour
  INTEGER
  INTEGER
                 :: PrevMin
  INTEGER
                 :: PrevSec
  INTEGER
                 :: PrevDOY
                 :: PrevWD
  INTEGER
  ! Current emission time stamp
  INTEGER
                  :: ThisEYear
  INTEGER
                 :: ThisEMonth
  INTEGER
                 :: ThisEDay
                 :: ThisEHour
  INTEGER
                 :: ThisEMin
  INTEGER
                 :: ThisESec
  INTEGER
  ! Previous emission time stamp
  INTEGER
           :: PrevEYear
```

```
INTEGER
                  :: PrevEMonth
  INTEGER
                  :: PrevEDay
  TNTEGER.
                  :: PrevEHour
  INTEGER
                  :: PrevEMin
                  :: PrevESec
  INTEGER
  ! Simulation year, month, day, hour, minute, second. Will only
  ! be different from current time stamp in special cases, e.g.
  ! if emission year shall be fixed.
  INTEGER
                  :: SimYear
                                  ! year
                  :: SimMonth
  INTEGER
                                 ! month
                                 ! day
  INTEGER
                  :: SimDay
                  :: SimHour
  INTEGER
                                 ! hour
                  :: SimMin
                                 ! minute
  INTEGER
  INTEGER
                  :: SimSec
                                ! second
  ! total number of elapsed time steps and emission time steps
  ! LastEStep denotes the last nEmisSteps values for which
  ! emissions have been calculated.
  INTEGER
                  :: nSteps
  INTEGER
                  :: nEmisSteps
  INTEGER
                  :: LastEStep
  ! Pointer to gridded time zones. Will only hold data if a field 'TIMEZONES'
  ! is provided in the HEMCO configuration file.
  ! NOTE: This pointer is initialized by a call to HcoClock_InitTzPtr
  ! from the HEMCO run routine (HCO_Run, in hco_driver_mod.F90).
  ! This is necessary to avoid segmentation faults when running with
  ! OpenMP turned on. (bmy, 2/23/15)
  TYPE(Arr2D_Sp), POINTER :: TIMEZONES
  ! Fixed dates to be used for simulation dates
  INTEGER
                   :: FixYY = -1
  INTEGER
                   :: FixMM = -1
  INTEGER
                   :: Fixdd = -1
  INTEGER
                   :: Fixhh = -1
  ! Last time step?
  LOGICAL
                 :: isLast
END TYPE HcoClock
! HcoPhys: Derived type for HEMCO physical constants
TYPE :: HcoPhys
  REAL(dp) :: Avgdr ! Avogadro number (mol-1)
```

```
REAL(dp) :: PI_180 ! Pi / 180
  REAL(dp) :: Re
                  ! Earth radius [m]
  REAL(dp) :: AIRMW   ! Molecular weight of air (g/mol)
  REAL(dp) :: g0 ! Gravity at surface of earth (m/s2)
  REAL(dp) :: Rd ! Gas Constant (R) in dry air (J/K/kg)
  REAL(dp) :: Rdg0 ! Rd/g0
  REAL(dp) :: RSTARG ! Universal gas constant [J/K/mol]
END TYPE HcoPhys
! HcoMicroPhys: Derived type for aerosol microphysics settings
TYPE :: HcoMicroPhys
                                    ! # of size-resolved bins
  INTEGER
                 :: nBins
  INTEGER
                  :: nActiveModebins ! # of active mode bins
  REAL(dp), POINTER :: BinBound(:) ! Size bin boundaries
END TYPE HcoMicroPhys
! RdList contains lists to all ReadLists
TYPE :: RdList
  TYPE(ListCont), POINTER :: Once
  TYPE(ListCont), POINTER :: Always
  TYPE(ListCont), POINTER :: Year
  TYPE(ListCont), POINTER :: Month
  TYPE(ListCont), POINTER :: Day
  TYPE(ListCont), POINTER :: Hour
  INTEGER
                      :: FileLun
                                    = -1 ! LUN of file in archive
  CHARACTER(LEN=2023) :: FileInArchive = '' ! name of file in archive
END TYPE RdList
!-----
! DataCont: Derived type definition for HEMCO data container
TYPE :: DataCont
  ! Container information
  CHARACTER(LEN= 63)
                                        ! Cont. name
                         :: cName
                                         ! Cont. ID
  INTEGER
                          :: cID
                                        ! target ID
  INTEGER
                          :: targetID
                          :: DctType
                                         ! Data type
  INTEGER
  TYPE(FileData), POINTER :: Dta
                                         ! data information
                          :: DtaHome
                                         ! Home cont for Dta?
  INTEGER
                          :: SpcName
  CHARACTER(LEN= 31)
                                         ! Species Name
  INTEGER
                          :: HcoID
                                         ! HEMCO species ID
                                         ! Extension #
  INTEGER
                          :: ExtNr
                          :: Cat
                                         ! Category
  INTEGER
                          :: Hier
  INTEGER
                                         ! Hierarchy
                          :: ScalID
                                        ! Scale factor ID
  INTEGER
```

```
:: nScalID
  INTEGER
                                            ! Operator
                 :: Uper ! Uperator
:: nScalID ! # of scale factor IDs
POINTER :: Scal_cID(:) ! assoc. scalefactor IDs
  INTEGER
  INTEGER,
                       :: Scal_cID_set ! cIDs or scalIDs
  LOGICAL
END TYPE DataCont
I-----
! ListCont: Derived type definition for HEMCO list object
!-----
TYPE :: ListCont
  TYPE(DataCont),
                   POINTER :: Dct
  TYPE(ListCont),
                   POINTER :: NextCont
END TYPE ListCont
T-----
! FileData: Derived type definition for HEMCO filetype object
I-----
TYPE :: FileData
  CHARACTER(LEN=255) :: ncFile ! file path+name CHARACTER(LEN= 31) :: ncPara ! file parameter
                          :: ncYrs(2) ! year range
  INTEGER
                           :: ncMts(2) ! month range
  INTEGER
  INTEGER
                          :: ncDys(2) ! day range
                          :: ncHrs(2) ! hour range
  INTEGER
                           :: tShift(2) ! time stamp shift in months & seconds
  INTEGER
                          :: CycleFlag ! cycle flag
  INTEGER
  LOGICAL
                           :: MustFind ! file must be found
  INTEGER
                           :: UpdtFlag ! update flag
                           :: ncRead ! read from source?
  LOGICAL
  TYPE(Arr3D_SP), POINTER :: V3(:)
                                      ! vector of 3D fields
  TYPE(Arr2D_SP), POINTER :: V2(:) ! vector of 2D fields
TYPE(TimeIdx), POINTER :: tIDx ! for time slice indexing
                     :: OrigUnit ! original data units
  CHARACTER(LEN= 31)
  CHARACTER(LEN= 63)
                          :: ArbDimName! name of additional dimension
                          :: ArbDimVal ! desired value of additional dimension
  CHARACTER(LEN= 63)
  INTEGER
                           :: Cover ! data coverage
                           :: SpaceDim ! space dimension: 1, 2 or 3
  INTEGER
                                     ! vertical level handling
  INTEGER
                           :: Levels
                                      ! level to use for 2D data
   INTEGER
                            :: Lev2D
                           :: EmisL1
  REAL(hp)
                                       ! emission level 1
  REAL(hp)
                           :: EmisL2
                                       ! emission level 2
  INTEGER
                           :: EmisL1Unit ! emission level 1 unit
                           :: EmisL2Unit ! emission level 2 unit
  INTEGER
  INTEGER
                           :: nt
                                       ! time dimension: length of Arr
                                       ! temp. resolution of array [h]
  INTEGER
                           :: DeltaT
                           :: IsLocTime ! local time?
  LOGICAL
  LOGICAL
                           :: IsConc
                                       ! concentration data?
                           :: DoShare ! shared object?
  LOGICAL
```

```
LOGICAL
                     :: IsInList ! is in emissions list?
  LOGICAL
                     :: IsTouched ! Has container been touched yet?
END TYPE FileData
!-----
! TimeIdx: Derived type definition for the object that points to the
! current time slices of data within a file. Used by hco_tidx_mod.F90.
1-----
TYPE :: TimeIdx
  INTEGER
                     :: TypeID
                    :: TempRes
  CHARACTER (LEN=31)
END TYPE TimeIdx
! The TimeIdxCollection derived type contains the pointers with the
! current valid vector indices for all defined cycling intervals.
TYPE :: TimeIdxCollection
  TYPE(TimeIdx), POINTER :: CONSTANT
  TYPE(TimeIdx), POINTER :: HOURLY
  TYPE(TimeIdx), POINTER :: HOURLY_GRID
  TYPE(TimeIdx), POINTER :: WEEKDAY
  TYPE(TimeIdx), POINTER :: MONTHLY
END TYPE TimeIdxCollection
!-----
! cIdListPnt: Derived type definition for pointing to list containers
!-----
TYPE :: cIDListPnt
  TYPE(DataCont),
               POINTER :: PNT ! Pointer to list container
END TYPE cIDListPnt
!-----
! Variables to store (unique) scale factor IDs and species names
!-----
TYPE :: ScalIDCont
  INTEGER
                   :: ScalID
  TYPE(ScalIDCont), POINTER :: NEXT
END TYPE ScalIDCont
TYPE :: SpecNameCont
  CHARACTER(LEN=31)
                     :: SpecName
  TYPE(SpecNameCont), POINTER :: NEXT
END TYPE SpecNameCont
!-----
! Derived type to store options
!-----
TYPE :: Opt
  CHARACTER(LEN=OPTLEN) :: OptName
```

```
:: OptValue
  CHARACTER (LEN=OPTLEN)
  TYPE(Opt), POINTER :: NextOpt => NULL()
END TYPE Opt
!-----
! Derived type to manage list of extensions and associated options
!-----
TYPE :: Ext
  CHARACTER(LEN=255) :: ExtName ! Name
  CHARACTER(LEN=OPTLEN) :: Spcs ! Species
                     :: ExtNr ! Ext. number
  INTEGER
  TYPE(Opt), POINTER :: Opts ! Options linked list
  TYPE(Ext), POINTER :: NextExt ! next list item
END TYPE Ext
!-----
! Configuration object
<u>|------</u>
TYPE :: ConfigObj
  CHARACTER (LEN=OPTLEN)
                        :: ROOT
  CHARACTER (LEN=255)
                         :: ConfigFileName = ''
  TYPE(ScalIDCont), POINTER :: ScalIDList => NULL()
  TYPE(SpecNameCont), POINTER :: SpecNameList => NULL()
  TYPE(Ext), POINTER :: ExtList
TYPE(HcoErr), POINTER :: Err
                 POINTER :: ExtList
                                        => NULL()
                                        => NULL()
  LOGICAL
                        :: ConfigFileRead = .FALSE.
END TYPE ConfigObj
1-----
! DiagnCont: Diagnostics container derived type declaration
!-----
TYPE :: DiagnCont
  CHARACTER(LEN= 63)
                       :: cName ! Cont. name
                       :: long_name ! ncdf long_name attribute
:: cID ! Cont. ID
  CHARACTER (LEN=255)
  INTEGER
                                       ! Extension #
                        :: ExtNr
  INTEGER
                                     ! Category
! Hierarchy
! HEMCO species ID
! fill automatically?
! Space dimension (1-3)
! 1D scalar
                        :: Cat
  INTEGER
  INTEGER
                        :: Hier
                         :: HcoID
  INTEGER
  INTEGER
                         :: AutoFill
  INTEGER
                         :: SpaceDim
                         :: Scalar
  REAL(sp)
                         :: Scalar    ! 1D scalar
:: Arr2D     ! 2D array
:: Arr3D     ! 3D array
:: Total     ! Diagnostics total
:: DtaIsPtr     ! Is data just a pointer?
:: LevIdx     ! Level index to be used
  TYPE(Arr2D_SP), POINTER :: Arr2D
  TYPE(Arr3D_SP),
                 POINTER :: Arr3D
  REAL(sp)
                        :: Total
  LOGICAL
                        :: LevIdx
  INTEGER
```

```
CHARACTER(LEN= 31) :: OutUnit ! Output unit

INTEGER :: AreaFlag ! 2=per area, 3=per volume, 0 otherwise

REAL(hp) :: AreaScal ! Scale factor for area

REAL(hp) :: MassScal ! Scale factor for mass

REAL(hp) :: ScaleFact ! Uniform scale factor

INTEGER :: TimeAvg ! Scale flag for time unit

INTEGER :: Counter ! time steps since

! last output
                                             ! Output averaging operation ! Averaging flag for
   CHARACTER(LEN= 31) :: AvgName
   INTEGER
                             :: AvgFlag
                                               ! non-standard units
                           :: LastUpdateID ! Last update time
   INTEGER
                            :: nnGetCalls ! # of Diagn_Get calls w/o update
:: IsOutFormat ! Data is in output format?
   INTEGER
  LOGICAL
                         :: CollectionID ! Collection diagnostics belongs to
   INTEGER
  TYPE(DiagnCont), POINTER :: NextCont ! Ptr to next item in list
END TYPE DiagnCont
1-----
! Diagnostcs collection derived type.
! DiagnList : Linked list with all diagnostics container of
!
                 this collection.
! nnDiag : Number of diagnostics in this collection.
! AF_LevelDefined: Set to true if there is at least one autofill
                 diagnostics at the given level (1-4).
! PREFIX : Prefix to be used for diagnostics output file name.
! NX, NY, NZ
               : Grid dimensions.
! TS
               : Time step. This is only of relevance for emission
                diagnostics that are internally converted from kg/m2/s to kg/m2.
              : Surface grid box areas. May be required for unit
                 conversions.
!-----
TYPE :: DiagnCollection
  :: nnDiagn = 0
   INTEGER
                                :: AF_LevelDefined(4) = .FALSE.
  LOGICAL
                                :: CollectionID = -1
   INTEGER
                                                      = ,,
   CHARACTER (LEN=255)
                                :: PREFIX
                                :: NX
                                                     = 0
   INTEGER
   INTEGER
                                :: NY
:: NZ
                                :: NY
                                                     = 0
   INTEGER
                                :: deltaYMD
                                                     = 0
   INTEGER
                                :: deltaHMS
   INTEGER
                                                     = 0
                                :: lastYMD
                                                     = -1
   INTEGER
                                :: lastHMS
                                                     = -1
   INTEGER
                                                   = -1
   INTEGER
                                :: OutTimeStamp
                                :: TS
                                                     = 0 ! Time step
   REAL(sp)
```

REAL(hp), POINTER :: AREA\_M2(:,:) => NULL()
TYPE(DiagnCollection), POINTER :: NextCollection => NULL()
END TYPE DiagnCollection

TYPE :: DiagnBundle

TYPE(DiagnCollection), POINTER :: Collections => NULL()
INTEGER :: HcoDiagnIDDefault = -999
INTEGER :: HcoDiagnIDMestart = -999
INTEGER :: HcoDiagnIDManual = -999
INTEGER :: nnCollections = 0

END TYPE DiagnBundle

#### **REVISION HISTORY:**

15 Feb 2016 - C. Keller - Initial version (collected from various modules)

# 1.29 Fortran: Module Interface hco\_unit\_mod.F90

Module HCO\_Unit\_Mod contains routines to check/convert units.

#### INTERFACE:

MODULE HCO\_Unit\_Mod

#### **USES:**

USE HCO\_Error\_Mod

IMPLICIT NONE PRIVATE

# PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCO\_Unit\_Change
PUBLIC :: HCO\_Unit\_GetMassScal
PUBLIC :: HCO\_Unit\_GetAreaScal
PUBLIC :: HCO\_Unit\_GetTimeScal
PUBLIC :: HCO\_Unit\_ScalCheck
PUBLIC :: HCO\_IsUnitLess
PUBLIC :: HCO\_IsIndexData
PUBLIC :: HCO\_UnitTolerance

# PRIVATE MEMBER FUNCTIONS:

PRIVATE :: HCO\_Unit\_Change\_SP
PRIVATE :: HCO\_Unit\_Change\_DP

```
15 May 2012 - C. Keller - Initialization

08 Jul 2014 - R. Yantosca - Cosmetic changes in ProTeX headers

08 Jul 2014 - R. Yantosca - Now use F90 free-format indentation

24 Jul 2014 - C. Keller - Now define unitless & 'standard' units as parameter

13 Aug 2014 - C. Keller - Interface for sp & dp arrays

13 Mar 2015 - R. Yantosca - Add m and m2 to the "unitless" list

16 Mar 2015 - R. Yantosca - Also allow "kg m-2 s-1" and similar units

16 Mar 2015 - R. Yantosca - Add dobsons and dobsons/day units

16 Jun 2015 - R. Yantosca - Add % and percent to the unitless list

17 Jan 2016 - E. Lundgren - Update Avogadro's # to NIST 2014 value

19 Sep 2016 - R. Yantosca - Make sure all strings are the same length in the array constructor or Gfortran will choke
```

# 1.29.1 HCO\_Unit\_Change\_sp

Subroutine HCO\_UNIT\_CHANGE\_SP is a wrapper routine to convert the values of the passed single precision array to units of (emitted) kg/m2/s.

#### **INTERFACE:**

```
SUBROUTINE HCO_Unit_Change_SP( HcoConfig, ARRAY, UNITS, MW_IN, MW_OUT, & MOLEC_RATIO, YYYY, MM, AreaFlag, & TimeFlag, FACT, RC, KeepSpec )
```

#### **USES:**

```
USE HCO_TYPES_MOD, ONLY : ConfigObj
```

## INPUT PARAMETERS:

```
TYPE(ConfigObj), POINTER
                                          :: HcoConfig
CHARACTER(LEN=*), INTENT(IN )
                                          :: UNITS
                                                            ! Data unit
REAL(hp),
                 INTENT(IN )
                                          :: MW_IN
                                                            ! MW g/mol
                                          :: MW_OUT
                                                            ! MW g/mol
REAL(hp),
                 INTENT(IN )
REAL(hp),
                                          :: MOLEC_RATIO
                                                            ! molec. ratio
                 INTENT(IN )
INTEGER,
                 INTENT(IN )
                                          :: YYYY
                                                            ! Data year
INTEGER,
                 INTENT(IN)
                                          :: MM
                                                            ! Data month
LOGICAL,
                 INTENT(IN ), OPTIONAL
                                          :: KeepSpec
                                                            ! Keep input species?
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: AreaFlag ! 2 if per area, 3 if per volume integer, INTENT(INOUT) :: TimeFlag ! 1 if per time, 0 otherwise REAL(sp), POINTER :: ARRAY(:,:,:) ! Data
INTEGER, INTENT(INOUT) :: RC
```

#### **OUTPUT PARAMETERS:**

```
REAL(hp), INTENT( OUT), OPTIONAL :: FACT ! Applied factor
```

## **REVISION HISTORY:**

```
13 Aug 2014 - C. Keller - Initial Version
```

# 1.29.2 HCO\_Unit\_Change\_dp

Subroutine HCO\_UNIT\_CHANGE\_DP is a wrapper routine to convert the values of the passed double precision array to units of (emitted) kg/m2/s.

#### **INTERFACE:**

```
SUBROUTINE HCO_Unit_Change_DP( HcoConfig, ARRAY, UNITS, MW_IN, MW_OUT, & MOLEC_RATIO, YYYY, MM, AreaFlag, & TimeFlag, FACT, RC, KeepSpec )
```

#### **USES:**

```
USE HCO_TYPES_MOD, ONLY : ConfigObj
```

# INPUT PARAMETERS:

```
TYPE(ConfigObj), POINTER
                                             :: HcoConfig
CHARACTER(LEN=*), INTENT(IN )
                                             :: UNITS
                                                                ! Data unit
             INTENT(IN )
INTENT(IN )
INTENT(IN )
INTENT(IN )
INTENT(IN )
REAL(hp),
                                             :: MW_IN
                                                                ! MW g/mol
REAL(hp),
                                                                ! MW g/mol
                                             :: MW_OUT
REAL(hp),
                                             :: MOLEC_RATIO ! molec. ratio
                                             :: YYYY
                                                                 ! Data year
INTEGER,
INTEGER,
                                             :: MM
                                                                 ! Data month
LOGICAL,
                   INTENT(IN ), OPTIONAL
                                             :: KeepSpec
                                                                 ! Keep input species?
```

# INPUT/OUTPUT PARAMETERS:

#### **OUTPUT PARAMETERS:**

```
REAL(hp), INTENT( OUT), OPTIONAL :: FACT ! Applied factor
```

# **REVISION HISTORY:**

```
13 Aug 2014 - C. Keller - Initial Version
```

#### 1.29.3 HCO\_Unit\_Factor

Subroutine HCO\_UNIT\_Factor calculates the conversion factor needed to conver unit UNIT to HEMCO units.

The mass is in units of kg and refers to mass of emitted species. For most compounds, this corresponds to the molecular mass of the species, but e.g. for VOCs this can be mass of carbon instead. The mass and area/volume conversion is always performed, but the time conversion is only done if a valid time string is provided. For example, if the input unit is kg/cm3 it will be converted to kg/m3, while ug/m2/year is converted to kg/m2/s. If no (valid) area/volume is given in the unit string, the return flag PerArea is set to False (True otherwise).

The input argument UNITS refers to the unit of the input data. Argument MW\_IN denotes the molecular weight of the input unit (g/mol), while MW\_OUT is the molecular weight of the output unit. They can differ e.g. for VOCs whose output units are in mass carbon instead of mass species. The argument MOLEC\_RATIO is the coefficient used for the conversion of molecules of species to molecules of carbon. For example, MOLEC\_RATIO should be set to 2 for C2H6, which will properly convert kg species (or molec species) to kg C. If the input unit is already on a per carbon basis (e.g. kgC, or molecC), no species coefficients will be applied!

## Supported unit values:

#### MASSES:

- molec (includes molecC; molec(C); molec tracer; molecN, molec(N))
- atom or atoms (incl. atomC, etc.)
- kg, g, mg, ug, ng (incl. kgC, etc.)

## TIMES:

- s, sec, hr, hour, d, day, mt, month, y, year.
- Valid formats: s, s-1, s-1.

## **VOLUMES/AREAS:**

- cm2, m2, km2, cm3, dm3, m3, l.
- Valid formats: cm3, cm-3, cm3, cm-3.

The following units will be ignored (no unit conversion is applied):

- unitless
- fraction
- factor
- hours
- degC
- 1

#### **INTERFACE:**

```
SUBROUTINE HCO_Unit_Factor( HcoConfig, UNITS, MW_IN, MW_OUT, MOLEC_RATIO, YYYY, & MM, AreaFlag, TimeFlag, Factor, RC, KeepSpec )
```

## **USES:**

```
USE HCO_TYPES_MOD, ONLY : ConfigObj
USE CharPak_Mod, ONLY : CStrip
```

#### INPUT PARAMETERS:

```
TYPE(ConfigObj), POINTER
                                        :: HcoConfig
CHARACTER(LEN=*), INTENT(IN)
                                        :: UNITS
                                                       ! Data unit
REAL(hp),
                 INTENT(IN )
                                        :: MW_IN
                                                       ! MW g/mol
                                                       ! MW g/mol
REAL(hp),
                                        :: MW_OUT
                 INTENT(IN )
REAL(hp),
                 INTENT(IN)
                                        :: MOLEC_RATIO ! molec. ratio
INTEGER,
                 INTENT(IN )
                                        :: YYYY
                                                       ! Data year
INTEGER,
                 INTENT(IN )
                                                       ! Data month
                                        :: MM
LOGICAL,
                 INTENT(IN ), OPTIONAL :: KeepSpec
                                                       ! Keep input species?
```

## **OUTPUT PARAMETERS:**

```
INTEGER, INTENT( OUT) :: AreaFlag
INTEGER, INTENT( OUT) :: TimeFlag
REAL(hp), INTENT( OUT) :: Factor ! Conversion factor
```

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

#### REVISION HISTORY:

# $1.29.4 \quad HCO\_Unit\_GetMassScal$

Returns the mass scale factors for the given unit. This is the scale factor required to convert from input units to HEMCO units (i.e. kg). If KeepSpec is set to true, the molecular weight of the input data is preserved, e.g. data in kgC is kept in kgC, data in molecC is converted to kgC, etc.

#### **INTERFACE:**

```
SUBROUTINE HCO_UNIT_GetMassScal( HcoConfig, unt, MW_IN, MW_OUT, & MOLEC_RATIO, Scal, KeepSpec )
```

#### **USES:**

```
USE HCO_CharTools_Mod
USE HCO_TYPES_MOD, ONLY : ConfigObj
```

## INPUT PARAMETERS:

```
TYPE(ConfigObj), POINTER
                                   :: HcoConfig
 CHARACTER(LEN=*), INTENT(IN)
                                                 ! Input units
                                   :: unt
                                                 ! MW g/mol
 REAL(hp),
                INTENT(IN)
                                   :: MW_IN
 REAL(hp),
                                                ! MW g/mol
               INTENT(IN)
                                   :: MW_OUT
                                   :: MOLEC_RATIO ! molec. ratio
 REAL(hp),
               INTENT(IN)
          INTENT(IN), OPTIONAL :: KeepSpec ! Keep input species?
 LOGICAL,
!OUTPUT PARAMETER:
 REAL(hp),
                INTENT(OUT)
                            :: Scal ! Scale factor
```

## **REVISION HISTORY:**

```
13 Mar 2013 - C. Keller - Initial version
17 Sep 2014 - C. Keller - Now accept '1' as mass unit (e.g. 1/m3/s)
```

#### 1.29.5 HCO\_Unit\_GetTimeScal

Returns the time scale factors for the given unit. This is the scale factor required to convert from unit 'Unit' to HEMCO units (i.e. per second).

#### **INTERFACE:**

```
SUBROUTINE HCO_Unit_GetTimeScal( unt, MM, YYYY, Scal, Flag )
```

## **USES:**

USE HCO\_CharTools\_Mod

## **INPUT PARAMETERS:**

```
CHARACTER(LEN=*), INTENT(IN) :: unt ! This unit
INTEGER, INTENT(IN) :: MM ! Current month
INTEGER, INTENT(IN) :: YYYY ! Current year
```

# **OUTPUT PARAMETERS:**

```
REAL(hp), INTENT(OUT) :: Scal ! Scale factor
INTEGER, INTENT(OUT) :: Flag ! 1=per time, 0 otherwise
```

```
13 Mar 2013 - C. Keller - Initial version
```

## 1.29.6 HCO\_Unit\_GetAreaScal

Returns the area/volume scale factors for the given unit. This is the scale factor required to convert from unit 'Unit' to HEMCO units (i.e. per m2 or per m3).

## **INTERFACE:**

```
SUBROUTINE HCO_Unit_GetAreaScal( unt, Scal, Flag )
```

#### **USES:**

USE HCO\_CharTools\_Mod

#### **INPUT PARAMETERS:**

```
CHARACTER(LEN=*), INTENT(IN) :: unt ! This unit
```

## **OUTPUT PARAMETERS:**

```
REAL(hp), INTENT(OUT) :: Scal ! scale factor
```

INTEGER, INTENT(OUT) :: Flag ! 2=per area, 3= per volume, 0 otherwise

#### **REVISION HISTORY:**

```
13 Mar 2013 - C. Keller - Initial version
```

#### 1.29.7 HCO\_Unit\_ScalCheck

Check if the provided unit is unitless. Returns 0 if Unit is unitless, 1 if it's not unitless but in correct HEMCO emission units (i.e. kg/m2/s), 2 if it's in HEMCO concentration units (kg/m3), -1 otherwise.

## **INTERFACE:**

```
FUNCTION HCO_Unit_ScalCheck( Unit ) Result ( Flag )
```

# **USES:**

```
USE CharPak_Mod, ONLY : TRANLC
```

#### INPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(IN) :: Unit
```

# **OUTPUT PARAMETERS:**

```
INTEGER :: Flag ! O=ok, 1=warning, 2=error
```

```
13 Mar 2013 - C. Keller - Initial version
```

## 1.29.8 HCO\_IsUnitless

Returns TRUE if the passed string corresponds to the HEMCO unitless data unit string.

#### **INTERFACE:**

```
FUNCTION HCO_IsUnitless( Unt ) Result ( Bool )
```

#### INPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(IN) :: Unt
```

#### **OUTPUT PARAMETERS:**

```
LOGICAL :: Bool
```

#### **REVISION HISTORY:**

```
24 Jul 2014 - C. Keller - Initial version
```

#### 1.29.9 HCO\_IsIndexData

Returns TRUE if the passed string corresponds to the HEMCO index data unit string.

#### **INTERFACE:**

```
FUNCTION HCO_IsIndexData( Unt ) Result ( Bool )
```

### **INPUT PARAMETERS:**

```
CHARACTER(LEN=*), INTENT(IN) :: Unt
```

# **OUTPUT PARAMETERS:**

LOGICAL :: Bool

#### REVISION HISTORY:

```
24 Jul 2014 - C. Keller - Initial version
```

#### 1.29.10 HCO\_UnitTolerance

Returns the HEMCO unit tolerance as defined in the HEMCO configuration file (under settings). Returns a default value of 0 (no tolerance) if no value is set in the configuration file.

## **INTERFACE:**

```
FUNCTION HCO_UnitTolerance( HcoConfig ) Result ( UnitTolerance )
```

#### **USES:**

```
USE HCO_TYPES_MOD, ONLY : ConfigObj
```

USE HCO\_EXTLIST\_MOD, ONLY : GetExtOpt, CoreNr

#### INPUT PARAMETERS:

TYPE(ConfigObj), POINTER :: HcoConfig

# **OUTPUT PARAMETERS:**

INTEGER :: UnitTolerance

#### **REVISION HISTORY:**

24 Jul 2014 - C. Keller - Initial version

# 1.30 Fortran: Module Interface hco\_vertgrid\_mod.F90

Module HCO\_VERTGRID\_Mod contains routines and variables for the definition of the vertical grid and related calculations.

#### **INTERFACE:**

MODULE HCO\_VertGrid\_Mod

#### **USES:**

```
USE HCO_Error_Mod
USE HCO_Arr_Mod
USE HCO_Types_Mod, ONLY: VertGrid
```

IMPLICIT NONE PRIVATE

## PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCO\_VertGrid\_Init
PUBLIC :: HCO\_VertGrid\_Define
PUBLIC :: HCO\_VertGrid\_Cleanup

#### PRIVATE MEMBER FUNCTIONS:

## **PARAMETERS:**

```
1.091817e+04_hp, 1.189586e+04_hp, 1.286959e+04_hp, 1.429100e+04_hp, &
            1.562600e+04_hp, 1.696090e+04_hp, 1.816190e+04_hp, 1.930970e+04_hp, &
            2.032590e+04_hp, 2.121500e+04_hp, 2.187760e+04_hp, 2.238980e+04_hp, &
            2.243630e+04_hp, 2.168650e+04_hp, 2.011920e+04_hp, 1.769300e+04_hp, &
            1.503930e+04_hp, 1.278370e+04_hp, 1.086630e+04_hp, 9.236572e+03_hp, &
            7.851231e+03_hp, 5.638791e+03_hp, 4.017541e+03_hp, 2.836781e+03_hp, &
            1.979160e+03_hp, 9.292942e+02_hp, 4.076571e+02_hp, 1.650790e+02_hp, &
            6.167791e+01_hp, 2.113490e+01_hp, 6.600001e+00_hp, 1.000000e+00_hp &
                                                                    /)
! Bp [unitless] for 47 levels (48 edges)
REAL(hp), PARAMETER
                             :: Bp47(48) = (/
            1.000000e+00_hp, 9.849520e-01_hp, 9.634060e-01_hp, 9.418650e-01_hp, &
            9.203870e-01_hp, 8.989080e-01_hp, 8.774290e-01_hp, 8.560180e-01_hp, &
            8.346609e-01_hp, 8.133039e-01_hp, 7.919469e-01_hp, 7.706375e-01_hp, &
            7.493782e-01_hp, 7.211660e-01_hp, 6.858999e-01_hp, 6.506349e-01_hp, &
            6.158184e-01_hp, 5.810415e-01_hp, 5.463042e-01_hp, 4.945902e-01_hp, &
            4.437402e-01_hp, 3.928911e-01_hp, 3.433811e-01_hp, 2.944031e-01_hp, &
            2.467411e-01_hp, 2.003501e-01_hp, 1.562241e-01_hp, 1.136021e-01_hp, &
            6.372006e-02_hp, 2.801004e-02_hp, 6.960025e-03_hp, 8.175413e-09_hp, &
            0.000000e+00_hp, 0.000000e+00_hp, 0.000000e+00_hp, 0.000000e+00_hp, &
            0.000000e+00_hp, 0.000000e+00_hp, 0.000000e+00_hp, 0.000000e+00_hp, &
            0.000000e+00_hp, 0.000000e+00_hp, 0.000000e+00_hp, 0.000000e+00_hp, &
            0.000000e+00_hp, 0.000000e+00_hp, 0.000000e+00_hp, 0.000000e+00_hp &
                                                                    /)
! Ap [Pa] for 72 levels (73 edges)
                             :: Ap72(73) = (/
REAL(hp), PARAMETER
            0.000000e+00_hp, 4.804826e+00_hp, 6.593752e+02_hp, 1.313480e+03_hp, &
            1.961311e+03_hp, 2.609201e+03_hp, 3.257081e+03_hp, 3.898201e+03_hp, &
            4.533901e+03_hp, 5.169611e+03_hp, 5.805321e+03_hp, 6.436264e+03_hp, &
            7.062198e+03_hp, 7.883422e+03_hp, 8.909992e+03_hp, 9.936521e+03_hp, &
            1.091817e+04_hp, 1.189586e+04_hp, 1.286959e+04_hp, 1.429100e+04_hp, &
            1.562600e+04_hp, 1.696090e+04_hp, 1.816190e+04_hp, 1.930970e+04_hp, &
            2.032590e+04_hp, 2.121500e+04_hp, 2.187760e+04_hp, 2.238980e+04_hp, &
            2.243630e+04_hp, 2.168650e+04_hp, 2.011920e+04_hp, 1.769300e+04_hp, &
            1.503930e+04_hp, 1.278370e+04_hp, 1.086630e+04_hp, 9.236572e+03_hp, &
            7.851231e+03_hp, 6.660341e+03_hp, 5.638791e+03_hp, 4.764391e+03_hp, &
            4.017541e+03_hp, 3.381001e+03_hp, 2.836781e+03_hp, 2.373041e+03_hp, &
            1.979160e+03_hp, 1.645710e+03_hp, 1.364340e+03_hp, 1.127690e+03_hp, &
            9.292942e+02_hp, 7.619842e+02_hp, 6.216801e+02_hp, 5.046801e+02_hp, &
            4.076571e+02_hp, 3.276431e+02_hp, 2.620211e+02_hp, 2.084970e+02_hp, &
            1.650790e+02_hp, 1.300510e+02_hp, 1.019440e+02_hp, 7.951341e+01_hp, &
            6.167791e+01_hp, 4.758061e+01_hp, 3.650411e+01_hp, 2.785261e+01_hp, &
            2.113490e+01_hp, 1.594950e+01_hp, 1.197030e+01_hp, 8.934502e+00_hp, &
            6.600001e+00_hp, 4.758501e+00_hp, 3.270000e+00_hp, 2.000000e+00_hp, &
            1.000000e+00_hp /)
```

```
! Bp [unitless] for 72 levels (73 edges)
REAL(hp), PARAMETER
                             :: Bp72(73) = (/
                                                                     &
            1.000000e+00_hp, 9.849520e-01_hp, 9.634060e-01_hp, 9.418650e-01_hp, &
            9.203870e-01_hp, 8.989080e-01_hp, 8.774290e-01_hp, 8.560180e-01_hp, &
            8.346609e-01_hp, 8.133039e-01_hp, 7.919469e-01_hp, 7.706375e-01_hp, &
            7.493782e-01_hp, 7.211660e-01_hp, 6.858999e-01_hp, 6.506349e-01_hp, &
            6.158184e-01_hp, 5.810415e-01_hp, 5.463042e-01_hp, 4.945902e-01_hp, &
            4.437402e-01_hp, 3.928911e-01_hp, 3.433811e-01_hp, 2.944031e-01_hp, &
            2.467411e-01_hp, 2.003501e-01_hp, 1.562241e-01_hp, 1.136021e-01_hp, &
            6.372006e-02_hp, 2.801004e-02_hp, 6.960025e-03_hp, 8.175413e-09_hp, &
            0.000000e+00_hp, 0.000000e+00_hp, 0.000000e+00_hp, 0.000000e+00_hp, &
            0.000000e+00\_hp,\ 0.000000e+00\_hp,\ 0.000000e+00\_hp,\ 0.000000e+00\_hp,\ \&
            0.000000e+00_hp, 0.000000e+00_hp, 0.000000e+00_hp, 0.000000e+00_hp, &
            0.000000e+00_hp /)
```

PUBLIC TYPES:

#### **REVISION HISTORY:**

28 Sep 2015 - C. Keller - Initialization

#### 1.30.1 HCO\_VertGrid\_Init

Function HCO\_VertGrid\_Init initializes the vertical grid.

## **INTERFACE:**

```
SUBROUTINE HCO_VertGrid_Init( am_I_Root, zGrid, RC )
```

#### INPUT PARAMETERS:

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

# INPUT/OUTPUT PARAMETERS:

```
TYPE(VertGrid), POINTER :: zGrid ! vertical grid INTEGER, INTENT(INOUT) :: RC ! Return code
```

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

## 1.30.2 HCO\_VertGrid\_Define

Function HCO\_VertGrid\_Define initializes the vertical grid.

#### **INTERFACE:**

```
SUBROUTINE HCO_VertGrid_Define( am_I_Root, HcoConfig, zGrid, nz, Ap, Bp, RC )
```

#### **USES:**

```
USE HCO_TYPES_MOD, ONLY : ConfigObj
```

#### INPUT PARAMETERS:

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

INTEGER, INTENT(IN ) :: nz ! # of vertical levels

REAL(hp), INTENT(IN ), OPTIONAL :: Ap(nz+1) ! Ap values

REAL(hp), INTENT(IN ), OPTIONAL :: Bp(nz+1) ! Bp values
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(ConfigObj),POINTER :: HcoConfig ! HEMCO config obj
TYPE(VertGrid), POINTER :: zGrid ! vertical grid
INTEGER, INTENT(INOUT) :: RC ! Return code
```

## **REVISION HISTORY:**

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

#### 1.30.3 HCO\_VertGrid\_Cleanup

Function HCO\_VertGrid\_Cleanup cleans up the vertical grid.

## **INTERFACE:**

```
SUBROUTINE HCO_VertGrid_Cleanup( zGrid )
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(VertGrid), POINTER :: zGrid ! vertical grid
```

#### **REVISION HISTORY:**

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

# 2 HEMCO "Extensions" modules

These modules define the HEMCO Extensions. These are emissions that rely on environmental variables (e.g. temperature, pressure, sunlight, boundary layer height, etc.) supplied by GEOS-Chem.

# 2.1 Fortran: Module Interface drydep\_toolbox\_mod.F90

Module DryEep\_ToolBox\_Mod contains routines used for dry deposition (and soil NOx emissions) calculations, as implemented into! the GEOS-Chem model.

#### **INTERFACE:**

```
MODULE DryDep_ToolBox_Mod
```

## **USES:**

```
USE HCO_ERROR_MOD, ONLY : hp    ! Precision (hp)
```

IMPLICIT NONE PRIVATE

#### PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: BIOFIT
```

INTERFACE BIOFIT

MODULE PROCEDURE BIOFIT\_R4

MODULE PROCEDURE BIOFIT\_R8

END INTERFACE

#### PRIVATE MEMBER FUNCTIONS:

PRIVATE :: SUNPARAM\_R4
PRIVATE :: SUNPARAM\_R8

# **REVISION HISTORY:**

```
14 Nov 2013 - C. Keller - Created from BIOFIT.F and SUNPARAM.F
09 Jul 2014 - R. Yantosca - Now use F90 free-format indentation
09 Jul 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
11 Dec 2014 - M. Yannetti - Split BIOFIT into R4 and R8 versions
Split SUNPARAM into R4 and R8 versions
```

#### 2.1.1 BIOFIT\_R4

Function BioFit computes the light correction used in the dry deposition and canopy NOx modules.

# **INTERFACE:**

```
FUNCTION BIOFIT_R4( COEFF1, XLAI1, SUNCOS1, CFRAC1, NPOLY ) RESULT ( BIO_FIT )
```

## **INPUT PARAMETERS:**

```
REAL*4, INTENT(IN) :: COEFF1(NPOLY) ! Baldocchi drydep coefficients
REAL*4, INTENT(IN) :: XLAI1 ! Leaf area index [cm2/cm2]
REAL*4, INTENT(IN) :: SUNCOS1 ! Cosine( Solar Zenith Angle )
REAL*4, INTENT(IN) :: CFRAC1 ! Cloud fraction [unitless]
INTEGER, INTENT(IN) :: NPOLY ! # of drydep coefficients
```

#### RETURN VALUE:

REAL\*4 :: BIO\_FIT ! Resultant light correction

#### **REMARKS:**

This routine is ancient code from Yuhang Wang. It was part of the old Harvard-GISS CTM and was ported into GEOS-Chem. See this reference for more information:

Wang, Y., D.J. Jacob, and J.A. Logan, "Global simulation of tropospheric O3-NOx-hydrocarbon chemistry, 1. Model formulation", J. Geophys. Res., 103/D9, 10,713-10,726, 1998.

#### **REVISION HISTORY:**

```
13 Dec 2012 - R. Yantosca - Added ProTeX headers
09 Dec 2014 - R. Yantosca - Now use BIO_FIT as the return value
11 Dec 2014 - M. Yannetti - Split from BIO_FIT
```

## 2.1.2 **BIOFIT\_R8**

Function BioFit computes the light correction used in the dry deposition and canopy NOx modules.

### INTERFACE:

FUNCTION BIOFIT\_R8( COEFF1, XLAI1, SUNCOS1, CFRAC1, NPOLY ) RESULT ( BIO\_FIT )

#### INPUT PARAMETERS:

```
REAL*8, INTENT(IN) :: COEFF1(NPOLY) ! Baldocchi drydep coefficients
REAL*8, INTENT(IN) :: XLAI1 ! Leaf area index [cm2/cm2]
REAL*8, INTENT(IN) :: SUNCOS1 ! Cosine( Solar Zenith Angle )
REAL*8, INTENT(IN) :: CFRAC1 ! Cloud fraction [unitless]
INTEGER, INTENT(IN) :: NPOLY ! # of drydep coefficients
```

#### RETURN VALUE:

REAL\*8 :: BIO\_FIT ! Resultant light correction

## **REMARKS:**

This routine is ancient code from Yuhang Wang. It was part of the old Harvard-GISS CTM and was ported into GEOS-Chem. See this reference for more information:

Wang, Y., D.J. Jacob, and J.A. Logan, "Global simulation of tropospheric O3-NOx-hydrocarbon chemistry, 1. Model formulation", J. Geophys. Res., 103/D9, 10,713-10,726, 1998.

#### REVISION HISTORY:

```
13 Dec 2012 - R. Yantosca - Added ProTeX headers
09 Dec 2014 - R. Yantosca - Now use BIO_FIT as the return value
11 Dec 2014 - M. Yannetti - Split from BIO_FIT
```

#### 2.1.3 SunParam\_r4

Subroutine SUNPARAM is called by BIOFIT to perform the light correction used in the dry deposition and canopy NOx modules.

#### INTERFACE:

SUBROUTINE SUNPARAM\_R4( X )

#### **DEFINED PARAMETERS:**

INTEGER, PARAMETER :: NN = 3 ! # of variables (LAI, SUNCOS, CLDFRC)

## INPUT/OUTPUT PARAMETERS:

REAL\*4, INTENT(INOUT) :: X(NN) ! LAI, SUNCOS, or cloud fraction

## **REMARKS:**

This routine is ancient code from Yuhang Wang. It was part of the old Harvard-GISS CTM and was ported into GEOS-Chem. See this reference for more information:

Wang, Y., D.J. Jacob, and J.A. Logan, "Global simulation of tropospheric O3-NOx-hydrocarbon chemistry, 1. Model formulation", J. Geophys. Res., 103/D9, 10,713-10,726, 1998.

```
13 Dec 2012 - R. Yantosca - Added ProTeX headers
11 Dec 2014 - M. Yannetti - Split into R4 and R8 versions.
```

## 2.1.4 SunParam\_r8

Subroutine SUNPARAM is called by BIOFIT to perform the light correction used in the dry deposition and canopy NOx modules.

#### **INTERFACE:**

```
SUBROUTINE SUNPARAM_R8( X )
```

# **DEFINED PARAMETERS:**

```
INTEGER, PARAMETER :: NN = 3 ! # of variables (LAI, SUNCOS, CLDFRC)
```

# INPUT/OUTPUT PARAMETERS:

```
REAL*8, INTENT(INOUT) :: X(NN) ! LAI, SUNCOS, or cloud fraction
```

#### **REMARKS:**

This routine is ancient code from Yuhang Wang. It was part of the old Harvard-GISS CTM and was ported into GEOS-Chem. See this reference for more information:

```
Wang, Y., D.J. Jacob, and J.A. Logan, "Global simulation of tropospheric 03-NOx-hydrocarbon chemistry, 1. Model formulation", J. Geophys. Res., 103/D9, 10,713-10,726, 1998.
```

## **REVISION HISTORY:**

```
13 Dec 2012 - R. Yantosca - Added ProTeX headers
11 Dec 2014 - M. Yannetti - Split into R4 and R8 versions.
```

#### 2.2 Fortran: Module Interface hcox\_aerocom\_mod.F90

Module HCOX\_AeroCom\_Mod.F90 is a HEMCO extension to use AeroCom volcano emissions from ascii tables. This module reads the daily AeroCom tables and emits the emissions according to the information in this file.

# **INTERFACE:**

```
MODULE HCOX_AeroCom_Mod
```

#### **USES:**

```
USE HCO_Error_MOD

USE HCO_Diagn_MOD

USE HCOX_TOOLS_MOD

USE HCOX_State_MOD, ONLY: Ext_State

USE HCO_State_MOD, ONLY: HCO_State

IMPLICIT NONE

PRIVATE
```

## PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCOX\_AeroCom\_Run
PUBLIC :: HCOX\_AeroCom\_Init
PUBLIC :: HCOX\_AeroCom\_Final

#### PRIVATE MEMBER FUNCTIONS:

PRIVATE :: ReadVolcTable
PRIVATE :: EmitVolc

#### **REMARKS:**

Each AeroCom table is expected to list the volcano location, sulfur emissions (in kg S/s), and the volcano elevation as well as the volcano plume column height. These entries need be separated by space characters. For example:

### LAT (-90,90), LON (-180,180), SULFUR [kg S/s], ELEVATION [m], CLOUD\_COLUMN\_HEIGHT [m]

### If elevation=cloud\_column\_height, emit in layer of elevation

### else, emit in top 1/3 of cloud\_column\_height

volcano:: 50.170 6.850 3.587963e-03 600. 600.

: :

The sulfur read from table is emitted as the species defined in the AeroCom settings section. More than one species can be provided. Mass sulfur is automatically converted to mass of emitted species (using the emitted molecular weight and molecular ratio of the corresponding HEMCO species). Additional scale factors can be defined in the settings section by using the (optional) setting 'Scaling\_<SpecName>'.

For example, to emit SO2 and BrO from volcanoes, with an additional scale factor of 1e-4 kg BrO / kgS for BrO, use the following setting:

115 AeroCom\_Volcano : on SO2/BrO --> Scaling\_BrO : 1.0e-4

--> AeroCom\_Table : /path/to/Aerocom.so2\_volcanic.\$YYYY\$MM\$DD.rc

This extension was primarily added for usage within GEOS-5.

When using this extension, you should turn off any other volcano emission inventories!

#### **REVISION HISTORY:**

04 Jun 2015 - C. Keller - Initial version

## 2.2.1 HCOX\_AeroCom\_Run

Subroutine HCOX\_AeroCom\_Run is the driver routine for the customizable HEMCO extension.

#### **INTERFACE:**

SUBROUTINE HCOX\_AeroCom\_Run( am\_I\_Root, ExtState, HcoState, RC )

#### **USES:**

USE HCO\_FluxArr\_Mod, ONLY: HCO\_EmisAdd

## INPUT PARAMETERS:

LOGICAL, INTENT(IN ) :: am\_I\_Root ! Are we on the root CPU?

TYPE(Ext\_State), POINTER :: ExtState ! Module options

# INPUT/OUTPUT PARAMETERS:

TYPE(HCO\_State), POINTER :: HcoState ! Hemco state

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

#### **REMARKS:**

#### **REVISION HISTORY:**

```
04 Jun 2015 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

## 2.2.2 HCOX\_AeroCom\_Init

Subroutine HCOX\_AeroCom\_Init initializes the HEMCO CUSTOM extension.

# **INTERFACE:**

```
SUBROUTINE HCOX_AeroCom_Init( am_I_Root, HcoState, ExtName, & ExtState, RC )
```

#### **USES:**

```
USE HCO_ExtList_Mod, ONLY : GetExtNr
USE HCO_ExtList_Mod, ONLY : GetExtOpt
USE HCO_ExtList_Mod, ONLY : GetExtSpcVal
USE HCO_STATE_MOD, ONLY : HCO_GetExtHcoID
```

## INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
```

CHARACTER(LEN=\*), INTENT(IN ) :: ExtName ! Extension name TYPE(Ext\_State), POINTER :: ExtState ! Module options

## INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! Hemco state
```

INTEGER, INTENT(INOUT) :: RC

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

## 2.2.3 HCOX\_AeroCom\_Final

Subroutine HCOX\_AeroCom\_Final finalizes the HEMCO AeroCom extension.

#### **INTERFACE:**

```
SUBROUTINE HCOX_AeroCom_Final ( ExtState )
```

#### INPUT PARAMETERS:

```
TYPE(Ext_State), POINTER :: ExtState ! Module options
```

#### REVISION HISTORY:

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

#### 2.2.4 ReadVolcTable

Subroutine ReadVolcTable reads the AeroCom volcano table of the current day.

#### INTERFACE:

```
SUBROUTINE ReadVolcTable ( am_I_Root, HcoState, ExtState, Inst, RC )
```

### **USES:**

```
USE HCO_CharTools_Mod
USE inquireMod, ONLY : find
```

USE inquireMod, ONLY : findfreeLun

USE HCO\_CLOCK\_MOD, ONLY : HcoClock\_NewDay

USE HCO\_CLOCK\_MOD, ONLY : HcoClock\_Get

USE HCO\_GeoTools\_MOD, ONLY : HCO\_GetHorzIJIndex

USE HCO\_EXTLIST\_MOD, ONLY : HCO\_GetOpt

#### INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
```

TYPE(Ext\_State), POINTER :: ExtState ! Module options

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! Hemco state
```

TYPE(MyInst), POINTER :: Inst INTEGER, INTENT(INOUT) :: RC

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

#### 2.2.5 EmitVolc

Subroutine EmitVolc reads the AeroCom volcano table of the current day.

#### **INTERFACE:**

```
SUBROUTINE EmitVolc (am_I_Root, HcoState, ExtState, Inst, SO2d, SO2e, RC)
USES:
```

#### INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root

TYPE(Ext_State), POINTER :: ExtState ! Module options
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! Hemco state
TYPE(MyInst), POINTER :: Inst
INTEGER, INTENT(INOUT) :: RC
```

## **OUTPUT PARAMETERS:**

```
REAL(sp), INTENT( OUT) :: SO2e(HcoState%NX, HcoState%NY, HcoState%NZ)
REAL(sp), INTENT( OUT) :: SO2d(HcoState%NX, HcoState%NY, HcoState%NZ)
```

#### REVISION HISTORY:

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

#### 2.2.6 InstGet

Subroutine InstGet returns a poiner to the desired instance.

# **INTERFACE:**

```
SUBROUTINE InstGet (Instance, Inst, RC, PrevInst)
```

#### INPUT PARAMETERS:

```
18 Feb 2016 - C. Keller - Initial version
```

# 2.2.7 InstCreate

Subroutine InstCreate creates a new instance.

# **INTERFACE:**

```
SUBROUTINE InstCreate (ExtNr, Instance, Inst, RC)
```

# INPUT PARAMETERS:

INTEGER, INTENT(IN) :: ExtNr

# **OUTPUT PARAMETERS:**

INTEGER, INTENT( OUT) :: Instance TYPE(MyInst), POINTER :: Inst

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

# REVISION HISTORY:

```
18 Feb 2016 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

#### 2.2.8 InstRemove

Subroutine InstRemove creates a new instance.

#### **INTERFACE:**

```
SUBROUTINE InstRemove (Instance)
```

#### INPUT PARAMETERS:

INTEGER :: Instance

# **REVISION HISTORY:**

```
18 Feb 2016 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 2.3 Fortran: Module Interface hcox\_ch4wetland\_mod.F90

Module HCOX\_CH4Wetland\_Mod contains routines to calculate methane emissions (including rice) from wetlands. This code is adapted from the GEOS-Chem CH4 offline simulation.

This is a HEMCO extension module that uses many of the HEMCO core utilities.

This code can be used to calculate emissions from wetlands, from rice, or both. Both

sources can be enabled/disabled in the HEMCO configuration file.

This extension can calculate emissions for as many species as desired. Those can be listed in the extensions settings (see below), together with individual scale factors and masks. For example, to calculate emissions for total CH4 and two tagged CH4 species (CH4\_NA and CH4\_EU) with NA emissions scaled by a factor of 1.1, as well as applying the gridded factors NAFIELD and EUFIELD to CH4\_NA and CH4\_EU, respectively:

121 CH4\_WETLANDS : on CH4/CH4\_NA/CH4\_EU  $-\dot{\iota}$  Wetlands : true  $-\dot{\iota}$  Rice : true  $-\dot{\iota}$  ScaleField\_CH4\_NA : 1.10  $-\dot{\iota}$  ScaleField\_CH4\_NA: NAFIELD  $-\dot{\iota}$  ScaleField\_CH4\_EU: EU-FIELD

The fields NAFIELD and EUFIELD must be defined in the base emission section of the HEMCO configuration file. You can apply any scale factors/masks to that field.

#### References:

 Pickett-Heaps CA, Jacob DJ, Wecht KJ, et al. Magnitude and seasonality of wetland methane emissions from the Hudson Bay Lowlands (Canada). ACP, 11, 3773-3779, 2011.

# **INTERFACE:**

```
MODULE HCOX_CH4WETLAND_Mod
```

#### **USES:**

```
USE HCO_Error_MOD

USE HCO_Diagn_MOD

USE HCOX_TOOLS_MOD

USE HCO_State_MOD, ONLY: HCO_State

USE HCOX_State_MOD, ONLY: Ext_State

IMPLICIT NONE

PRIVATE
```

# PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: HCOX_CH4WETLAND_RUN

PUBLIC :: HCOX_CH4WETLAND_RUN

PUBLIC :: HCOX_CH4WETLAND_FINAL
```

#### PRIVATE MEMBER FUNCTIONS:

```
PRIVATE :: WETLAND_EMIS
PRIVATE :: RICE_EMIS
```

# **REVISION HISTORY:**

```
11 Sep 2014 - C. Keller - Initial version
01 Oct 2013 - C. Keller - Now a HEMCO extension module
11 Dec 2013 - C. Keller - Now define container name during initialization
01 Jul 2014 - R. Yantosca - Now use F90 free-format indentation
01 Jul 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
```

```
11 Jun 2015 - C. Keller - Update to support multiple species with individual scale factors and mask regions.

14 Oct 2016 - C. Keller - Now use HCO_EvalFld instead of HCO_GetPtr.
```

#### 2.3.1 HCOX\_CH4WETLAND\_Run

Subroutine HcoX\_CH4WETLAND\_Run is the run routine to calculate oceanic emissions for the current time step.

# **INTERFACE:**

```
SUBROUTINE HCOX_CH4WETLAND_Run( am_I_Root, ExtState, HcoState, RC )
```

# **USES:**

```
USE HCO_CALC_MOD, ONLY : HCO_EvalFld
USE HCO_EMISLIST_MOD, ONLY : HCO_GetPtr
USE HCO_FLUXARR_MOD, ONLY : HCO_EmisAdd
USE HCO_TYPES_MOD, ONLY : DiagnCont
USE HCO_CLOCK_MOD, ONLY : HcoClock_First
```

# INPUT PARAMETERS:

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

TYPE(HCO_State), POINTER :: HcoState ! Output obj

TYPE(Ext_State), POINTER :: ExtState ! Module options
```

# INPUT/OUTPUT PARAMETERS:

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

# REVISION HISTORY:

```
11 Sep 2014 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 2.3.2 WETLAND\_EMIS

Subroutine WETLAND\_EMIS is the driver routine for the CH4 wetland emissions. It calculates wetland emissions and writes them into the passed array CH4wtl.

# INTERFACE:

```
SUBROUTINE WETLAND_EMIS ( am_I_Root, HcoState, ExtState, Inst, CH4wtl, RC )
USES:
```

#### INPUT PARAMETERS:

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

TYPE(HCO_State), POINTER :: HcoState ! Output obj

TYPE(Ext_State), POINTER :: ExtState ! Module options
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(MyInst), POINTER :: Inst

REAL(hp), INTENT(INOUT) :: CH4wtl(HcoState%NX, HcoState%NY) ! CH4 emis

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

# **REVISION HISTORY:**

- (1) Adapted by Jrme Drevet (3/06) from the BIOME-TG Wetland-Methane scheme provided by Jed O. Kaplan.
- (2) CH4 Emissions from Wetland depend on:
  - a Soil Carbon content.
  - b Vegetation type
  - c Wetland area (%)
  - d Soil moisture.
  - a, b, c are taken from the LPJ, a vegetation model. Data are provided by J.O.Kaplan. Soil moisture is read from GEOS Met input files.
- (3) Corrected order of DO loops (bmy, 10/1/09)
- 08 Feb 2012 R. Yantosca Treat GEOS-5.7.x in the same way as MERRA
- 01 Mar 2012 R. Yantosca Now use GET\_AREA\_M2(I,J,L) from grid\_mod.F90
- 07 Mar 2012 M. Payer Added ProTeX headers
- 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
- 23 Jan 2014 M. Sulprizio- Now zero wetland emissions if snow covers the ground. Also updated MOIST\_SCALE and EMIT\_FACT.
  - (K. Wecht, C. Pickett-Heaps)
- 12 Feb 2014 K. Wecht Updated for 0.25 x 0.3125 NA grid
- 09 Apr 2014 R. Yantosca Bug fix, extend #ifdef for MERRA met fields
- 11 Sep 2014 C. Keller Now a HEMCO extension
- 12 Aug 2015 R. Yantosca Extend #ifdef for MERRA2 met fields

# 2.3.3 RICE\_EMIS

Subroutine RICE\_EMIS is the driver routine for the CH4 rice emissions. It calculates rice emissions and writes them into the passed array CH4.

# **INTERFACE:**

```
SUBROUTINE RICE_EMIS ( am_I_Root, HcoState, ExtState, Inst, CH4rce, RC )
USES:
```

#### INPUT PARAMETERS:

```
LOGICAL,
               INTENT(IN ) :: am_I_Root ! root CPU?
TYPE(HCO_State), POINTER
                          :: HcoState ! Output obj
TYPE(Ext_State), POINTER :: ExtState ! Module options
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(MyInst),
              POINTER
                         :: Inst
```

INTENT(INOUT) :: CH4rce(HcoState%NX, HcoState%NY) ! CH4 emis REAL(hp),

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

# **REMARKS:**

Rice Emissions are scaled to GEOS soil wetness. Scaling sceme developed and implemented by Jerome Drevet.

Wetland emissions are modified by the presence of rice emissions. Sceme developed by Jerome Drevet.

# **REVISION HISTORY:**

- (1) CH4 emissions from rice calculated with a routine created by Jerome Drevet. Adapted as its own subroutine by Kevin Wecht (6/03/09)
- (2) Corrected ordering of DO loops (bmy, 10/1/09)
- 07 Mar 2012 M. Payer - Added ProTeX headers
- 25 Mar 2013 R. Yantosca Now accept am\_I\_Root, Input\_Opt, State\_Chm, RC
- 09 Apr 2014 R. Yantosca Bug fix, extend #ifdef for MERRA met fields
- 11 Sep 2014 C. Keller Now a HEMCO extension

# 2.3.4 HCOX\_CH4WETLAND\_INIT

Subroutine HCOX\_CH4WETLAND\_INIT initializes all module variables.

# **INTERFACE:**

```
SUBROUTINE HCOX_CH4WETLAND_INIT( am_I_Root, HcoState, ExtName, ExtState, RC )
```

#### **USES:**

```
USE HCO_ExtList_Mod,
                             ONLY : GetExtNr
USE HCO_ExtList_Mod,
USE HCO STATE YOU
USE HCO_ExtList_Mod,
                             ONLY : GetExtOpt
                             ONLY : GetExtSpcVal
                             ONLY : HCO_GetExtHcoID
USE HCO_STATE_MOD,
```

#### INPUT PARAMETERS:

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

:: HcoState ! Hemco State obj.
) :: ExtName ! Extension name CHARACTER(LEN=\*), INTENT(IN

TYPE(Ext\_State), POINTER :: ExtState ! Ext. obj.

# INPUT/OUTPUT PARAMETERS:

INTENT(INOUT) :: RC ! Return status INTEGER.

# **REVISION HISTORY:**

```
11 Sep 2014 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 2.3.5 HCOX\_CH4WETLAND\_Final

Subroutine HCOX\_CH4WETLAND\_Final deallocates all module arrays.

# **INTERFACE:**

```
SUBROUTINE HCOX_CH4WETLAND_Final( ExtState )
```

# INPUT PARAMETERS:

```
TYPE(Ext_State), POINTER :: ExtState ! Module options
```

# **REVISION HISTORY:**

```
11 Sep 2014 - C. Keller - Initial version
```

# 2.3.6 InstGet

Subroutine InstGet returns a poiner to the desired instance.

# **INTERFACE:**

```
SUBROUTINE InstGet (Instance, Inst, RC, PrevInst)
```

# **INPUT PARAMETERS:**

# REVISION HISTORY:

```
18 Feb 2016 - C. Keller - Initial version
```

# 2.3.7 InstCreate

Subroutine InstCreate creates a new instance.

# **INTERFACE:**

```
SUBROUTINE InstCreate (ExtNr, Instance, Inst, RC)
```

# INPUT PARAMETERS:

INTEGER, INTENT(IN) :: ExtNr

#### **OUTPUT PARAMETERS:**

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

# **REVISION HISTORY:**

```
18 Feb 2016 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 2.3.8 InstRemove

Subroutine InstRemove creates a new instance.

# **INTERFACE:**

```
SUBROUTINE InstRemove (Instance)
```

# INPUT PARAMETERS:

INTEGER :: Instance

#### REVISION HISTORY:

18 Feb 2016 - C. Keller - Initial version

# 2.4 Fortran: Module Interface hcox\_custom\_mod.F90

Customizable HEMCO emission extension.

# INTERFACE:

MODULE HCOX\_Custom\_Mod

#### **USES:**

USE HCO\_Error\_MOD
USE HCO\_Diagn\_MOD

USE HCOX\_State\_MOD, ONLY : Ext\_State
USE HCO\_State\_MOD, ONLY : HCO\_State

IMPLICIT NONE

PRIVATE

# PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: HCOX_Custom_Run
PUBLIC :: HCOX_Custom_Init
PUBLIC :: HCOX_Custom_Final
```

#### **REVISION HISTORY:**

```
13 Dec 2013 - C. Keller - Initial version
06 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
06 Jun 2014 - R. Yantosca - Now indented with F90 free-format
```

# 2.4.1 HCOX\_Custom\_Run

Subroutine HCOX\_Custom\_Run is the driver routine for the customizable HEMCO extension.

# **INTERFACE:**

```
SUBROUTINE HCOX_Custom_Run( am_I_Root, ExtState, HcoState, RC )
```

# **USES:**

```
USE HCO_FluxArr_Mod, ONLY : HCO_EmisAdd USE HCO_GeoTools_Mod, ONLY : HCO_LANDTYPE
```

# INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root ! Are we on the root CPU? TYPE(Ext_State), POINTER :: ExtState ! Module options
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! Hemco state INTEGER, INTENT(INOUT) :: RC ! Success or failure
```

# **REMARKS:**

# **REVISION HISTORY:**

```
13 Dec 2013 - C. Keller - Initial version
05 Jun 2014 - R. Yantosca - Now store the results of HCO_LANDTYPE
in a PRIVATE variable for the !OMP loop
05 Jun 2014 - R. Yantosca - Cosmetic changes
06 Jun 2014 - R. Yantosca - Now indented with F90 free-format
```

# 2.4.2 HCOX\_Custom\_Init

Subroutine HCOX\_Custom\_Init initializes the HEMCO CUSTOM extension.

# **INTERFACE:**

```
SUBROUTINE HCOX_Custom_Init( am_I_Root, HcoState, ExtName, & ExtState, RC )
```

#### **USES:**

```
USE HCO_ExtList_Mod, ONLY : GetExtNr
```

USE HCO\_STATE\_MOD, ONLY : HCO\_GetExtHcoID

# INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
```

CHARACTER(LEN=\*), INTENT(IN ) :: ExtName ! Extension name TYPE(Ext\_State), POINTER :: ExtState ! Module options

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! Hemco state
```

INTEGER, INTENT(INOUT) :: RC

#### **REVISION HISTORY:**

```
13 Dec 2013 - C. Keller - Now a HEMCO extension
```

06 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers

06 Jun 2014 - R. Yantosca - Now indented using F90 free-format

# 2.4.3 HCOX\_Custom\_Final

Subroutine HCOX\_Custom\_Final finalizes the HEMCO CUSTOM extension.

# INTERFACE:

SUBROUTINE HCOX\_Custom\_Final

# **REVISION HISTORY:**

```
13 Dec 2013 - C. Keller - Now a HEMCO extension
```

06 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers

06 Jun 2014 - R. Yantosca - Now indended with F90 free-format

# 2.5 Fortran: Module Interface hcox\_driver\_mod.F90

Module hcox\_driver\_mod.F90 contains the driver routines (INIT, RUN, FINAL) for the HEMCO extensions. It determines the extensions to be used (based on the settings specified in the configuration file) and invokes the respective extension module calls.

Call this module at the HEMCO - model interface level to execute the HEMCO extensions.

# **INTERFACE:**

```
MODULE HCOX_Driver_Mod
```

# **USES:**

```
USE HCO_Error_Mod
USE HCO_State_Mod, ONLY: HCO_State
USE HCOX_State_Mod, ONLY: Ext_State
IMPLICIT NONE
PRIVATE
```

# PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCOX\_Init
PUBLIC :: HCOX\_Run
PUBLIC :: HCOX\_Final

PRIVATE :: HCOX\_DiagnDefine
PRIVATE :: HCOX\_DiagnFill

#### **REMARKS:**

- (1) The extension option objects (e.g. meteorological variables) are defined in the HEMCO - model interface module and passed to this module.
- (2) To add/remove HEMCO extensions from a model application, just add/remove the corresponding initialize, run, and finalize calls in the respective driver routines!

# **REVISION HISTORY:**

```
15 Dec 2013 - C. Keller - Initial version
01 Jul 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
01 Jul 2014 - R. Yantosca - Now use F90 free-format indentation
```

#### 2.5.1 HCOX\_Init

Subroutine HCOX\_Init is the driver routine to initialize all enabled HEMCO extensions. INTERFACE:

SUBROUTINE HCOX\_Init( amIRoot, HcoState, ExtState, RC )

# **USES:**

USE HCOX\_State\_MOD, ONLY : ExtStateInit USE HCOX\_Custom\_Mod, ONLY : HCOX\_Custom\_Init USE HCOX\_SeaFlux\_Mod, ONLY : HCOX\_SeaFlux\_Init USE HCOX\_ParaNOx\_Mod, ONLY : HCOX\_ParaNOx\_Init USE HCOX\_LightNox\_Mod, ONLY : HCOX\_LightNox\_Init USE HCOX\_SoilNox\_Mod, ONLY : HCOX\_SoilNox\_Init USE HCOX\_DustDead\_Mod, ONLY : HCOX\_DustDead\_Init USE HCOX\_DustGinoux\_Mod, ONLY : HCOX\_DustGinoux\_Init USE HCOX\_SeaSalt\_Mod, ONLY : HCOX\_SeaSalt\_Init USE HCOX\_GFED\_Mod, ONLY : HCOX\_GFED\_Init USE HCOX\_MEGAN\_Mod, ONLY : HCOX\_MEGAN\_Init USE HCOX\_Finn\_Mod, ONLY : HCOX\_FINN\_Init USE HCOX\_GC\_RnPbBe\_Mod, ONLY : HCOX\_GC\_RnPbBe\_Init USE HCOX\_GC\_POPs\_Mod, ONLY : HCOX\_GC\_POPs\_Init USE HCOX\_CH4WetLand\_MOD, ONLY : HCOX\_CH4WETLAND\_Init USE HCOX\_AeroCom\_Mod, ONLY : HCOX\_AeroCom\_Init #if defined( TOMAS ) USE HCOX\_TOMAS\_Jeagle\_Mod, ONLY : HCOX\_TOMAS\_Jeagle\_Init USE HCOX\_TOMAS\_DustDead\_Mod, ONLY : HCOX\_TOMAS\_DustDead\_Init #endif

# **INPUT PARAMETERS:**

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

# INPUT/OUTPUT PARAMETERS:

TYPE(HCO\_State), POINTER :: HcoState ! HEMCO state object
TYPE(Ext\_State), POINTER :: ExtState ! HEMCO extension object
INTEGER, INTENT(INOUT) :: RC ! Failure or success

# REMARKS:

By default we will call routine ExtStateInit, which initializes the ExtState object. In some instances, we may want to call ExtStateInit from a higher-level routine. For example, this allows us to pass via ExtState additional scalar quantities from the driving model to HEMCO. To do this, you will need to (1) call ExtStateInit separately, and (2) set the optional argument NoExtStateInit=.FALSE. flag in the call to HCOX\_INIT.

# **REVISION HISTORY:**

```
12 Sep 2013 - C. Keller - Initial version
07 Jul 2014 - R. Yantosca - Now init GEOS-Chem Rn-Pb-Be emissions module
20 Aug 2014 - M. Sulprizio- Now init GEOS-Chem POPs emissions module
01 Oct 2014 - R. Yantosca - Now init TOMAS sea salt emissions module
```

01 Nov 2016 - M. Sulprizio- Rename TOMAS sea salt to TOMAS Jeagle (J. Kodros)

# 2.5.2 HCOX Run

Subroutine HCOX\_Run is the driver routine to run the HEMCO extensions. All enabled emission extensions are executed, and the emissions calculated therein become added to the respective flux arrays in HcoState.

### **INTERFACE:**

```
SUBROUTINE HCOX_Run( amIRoot, HcoState, ExtState, RC )
```

# **USES:**

```
ONLY : HcoClock_Get
   USE HCO_Clock_Mod,
   USE HCOX_Custom_Mod,
                                ONLY : HCOX_Custom_Run
   USE HCOX_SeaFlux_Mod,
                                ONLY : HCOX_SeaFlux_Run
   USE HCOX_ParaNox_Mod,
                                ONLY : HCOX_ParaNox_Run
   USE HCOX_LightNox_Mod,
                                ONLY : HCOX_LightNox_Run
   USE HCOX_SoilNox_Mod,
                                ONLY : HCOX_SoilNox_Run
   USE HCOX_DustDead_Mod,
                                ONLY : HCOX_DustDead_Run
   USE HCOX_DustGinoux_Mod,
                                ONLY : HCOX_DustGinoux_Run
   USE HCOX_SeaSalt_Mod,
                                ONLY : HCOX_SeaSalt_Run
   USE HCOX_Megan_Mod,
                                ONLY : HCOX_Megan_Run
   USE HCOX_GFED_Mod,
                                ONLY: HCOX_GFED_Run
   USE HcoX_FINN_Mod,
                                ONLY: HcoX_FINN_Run
   USE HCOX_GC_RnPbBe_Mod,
                                ONLY : HCOX_GC_RnPbBe_Run
   USE HCOX_GC_POPs_Mod,
                                ONLY: HCOX_GC_POPs_Run
   USE HCOX_CH4WetLand_mod,
                                ONLY: HCOX_CH4Wetland_Run
   USE HCOX_AeroCom_Mod,
                                ONLY : HCOX_AeroCom_Run
#if defined( TOMAS )
   USE HCOX_TOMAS_Jeagle_Mod,
                                 ONLY: HCOX_TOMAS_Jeagle_Run
   USE HCOX_TOMAS_DustDead_Mod, ONLY : HCOX_TOMAS_DustDead_Run
#endif
```

# **INPUT PARAMETERS:**

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

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object
TYPE(Ext_State), POINTER :: ExtState ! Extension options object
INTEGER, INTENT(INOUT) :: RC ! Failure or success
!NOTE:
```

The ExtState object contains all extension option objects. In particular, it contains the pointers to all met fields used by the extensions. These pointers have to be set in the HEMCO-model interface module beforehand!

# REVISION HISTORY:

```
15 Dec 2013 - C. Keller - Initial version
07 Jul 2014 - R. Yantosca - Now Run GEOS-Chem Rn-Pb-Be emissions module
```

```
20 Aug 2014 - M. Sulprizio- Now run GEOS-Chem POPs emissions module
01 Oct 2014 - R. Yantosca - Now run TOMAS sea salt emissions module
01 Nov 2016 - M. Sulprizio- Rename TOMAS sea salt to TOMAS Jeagle (J. Kodros)
```

# 2.5.3 HCOX\_Final

Subroutine HCOX\_Final finalizes all HEMCO extensions.

#### INTERFACE:

```
SUBROUTINE HCOX_Final( am_I_Root, HcoState, ExtState, RC )
```

### **USES:**

```
USE HCOX_State_Mod,
                                ONLY : ExtStateFinal
   USE HCOX_Custom_Mod,
                                ONLY : HCOX_Custom_Final
   USE HCOX_SeaFlux_Mod,
                                ONLY : HCOX_SeaFlux_Final
   USE HCOX_ParaNOx_Mod,
                                ONLY : HCOX_PARANOX_Final
   USE HCOX_LightNox_Mod,
                                ONLY : HCOX_LightNox_Final
   USE HCOX_SoilNox_Mod,
                                ONLY : HCOX_SoilNox_Final
   USE HCOX_DustDead_Mod,
                                ONLY : HCOX_DustDead_Final
   USE HCOX_DustGinoux_Mod,
                                ONLY : HCOX_DustGinoux_Final
   USE HCOX_SeaSalt_Mod,
                                ONLY : HCOX_SeaSalt_Final
   USE HCOX_MEGAN_Mod,
                                ONLY : HCOX_MEGAN_Final
   USE HCOX_GFED_Mod,
                                ONLY : HCOX_GFED_Final
   USE HcoX_FINN_Mod,
                                ONLY : HcoX_FINN_Final
   USE HCOX_GC_RnPbBe_Mod,
                                ONLY : HCOX_GC_RnPbBe_Final
   USE HCOX_GC_POPs_Mod,
                                ONLY : HCOX_GC_POPs_Final
   USE HCOX_CH4WetLand_Mod,
                                ONLY : HCOX_CH4Wetland_Final
   USE HCOX_AeroCom_Mod,
                                ONLY : HCOX_AeroCom_Final
#if defined( TOMAS )
   USE HCOX_TOMAS_Jeagle_Mod, ONLY : HCOX_TOMAS_Jeagle_Final
   USE HCOX_TOMAS_DustDead_Mod, ONLY : HCOX_TOMAS_DustDead_Final
#endif
```

#### INPUT PARAMETERS:

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

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object
TYPE(Ext_State), POINTER :: ExtState ! Extension options object
INTEGER, INTENT(INOUT) :: RC ! Failure or success
```

# **REVISION HISTORY:**

```
12 Sep 2013 - C. Keller - Initial version
07 Jul 2014 - R. Yantosca - Now finalize GEOS-Chem Rn-Pb-Be emissions pkg
20 Aug 2014 - M. Sulprizio- Now finalize GEOS-Chen POPs emissions module
```

```
01 Oct 2014 - R. Yantosca - Now finalize TOMAS sea salt emissions module
09 Mar 2015 - C. Keller - Now pass HcoState since it is needed by some
finalization calls.
01 Nov 2016 - M. Sulprizio- Rename TOMAS sea salt to TOMAS Jeagle (J. Kodros)
```

# 2.5.4 HCOX\_DiagnDefine

Subroutine HCOX\_DiagnDefine creates custom-defined diagnostics. This is very preliminary and for testing only.

# INTERFACE:

```
SUBROUTINE HCOX_DiagnDefine( am_I_Root, HcoState, ExtState, RC )
USES:
```

#### INPUT PARAMETERS:

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

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object
TYPE(Ext_State), POINTER :: ExtState ! Extension options object
```

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

# **REVISION HISTORY:**

```
19 Feb 2015 - C. Keller - Initial version
```

# 2.5.5 DgnDefine

Helper routine to define a target diagnostics.

# **INTERFACE:**

```
SUBROUTINE DgnDefine ( am_I_Root, HcoState, DgnName, Trgt2D, RC )
```

# **USES:**

```
USE HCO_DIAGN_MOD, ONLY : Diagn_Create
```

# INPUT PARAMETERS:

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

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State),
                  POINTER
                                  :: HcoState
                                                ! HEMCO state object
CHARACTER(LEN=*), INTENT(IN
                               )
                                  :: DgnName
                                                  ! diagnostics name
REAL(sp),
                                  :: Trgt2D(HcoState%NX,HcoState%NY)
                  INTENT(IN
                               )
INTEGER,
                  INTENT(INOUT)
                                  :: RC
                                                ! Failure or success
```

# **REVISION HISTORY:**

```
19 Feb 2015 - C. Keller - Initial version
```

# 2.5.6 HCOX\_DiagnFill

Subroutine HCOX\_DiagnFill fills custom-defined diagnostics.

#### **INTERFACE:**

```
SUBROUTINE HCOX_DiagnFill( am_I_Root, HcoState, ExtState, RC )
USES:
```

#### INPUT PARAMETERS:

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

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object
TYPE(Ext_State), POINTER :: ExtState ! Extension options object
INTEGER, INTENT(INOUT) :: RC ! Failure or success
```

# **REVISION HISTORY:**

```
19 Feb 2015 - C. Keller - Initial version
```

# 2.6 Fortran: Module Interface hcox\_dust\_dead\_mod.F

Module hcox\_dust\_dead\_mod.F contains routines and variables from Charlie Zender's DEAD dust mobilization model. Most routines are from Charlie Zender, but have been modified and/or cleaned up for inclusion into GEOS-Chem.

This is a HEMCO extension module that uses many of the HEMCO core utilities.

NOTE: The current (dust) code was validated at 2 x 2.5 resolution. We have found that running at 4x5 we get much lower (50emissions than at 2x2.5. Recommend we either find a way to scale the U\* computed in the dust module, or run a 1x1 and store the the dust emissions, with which to drive lower resolution runs. – Duncan Fairlie, 1/25/07

(We'll) implement the [dust] code in the standard [GEOS-Chem] model and put a warning about expected low bias when the simulation is run at 4x5. Whoever is interested in running dust at 4x5 in the future can deal with making the fix. – Daniel Jacob, 1/25/07

#### !REFERENCES:

• Zender, C. S., Bian, H., and Newman, D.: Mineral Dust Entrainment and Deposition (DEAD) model: Description and 1990s dust climatology, Journal of Geophysical Research: Atmospheres, 108, 2003.

# **INTERFACE:**

MODULE HCOX\_DUSTDEAD\_MOD

### **USES:**

USE HCO\_ERROR\_MOD

USE HCO\_DIAGN\_MOD

USE HCOX\_State\_MOD, ONLY : Ext\_State

USE HCO\_STATE\_MOD, ONLY : HCO\_State

IMPLICIT NONE

PRIVATE

# PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCOX\_DustDead\_Run
PUBLIC :: HCOX\_DustDead\_Init
PUBLIC :: HCOX\_DustDead\_Final
PUBLIC :: HCOX\_DustDead\_GetFluxTun

#### REVISION HISTORY:

- (1 ) Added parallel DO loop in GET\_ORO (bmy, 4/14/04)
- (2) Now references "directory\_mod.f" (bmy, 7/20/04)
- (3) Fixed typo in ORO\_IS\_LND for PGI compiler (bmy, 3/1/05)
- (4) Modified for GEOS-5 and GCAP met fields (swu, bmy, 8/16/05)
- (5 ) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (6) Now uses GOCART source function (tdf, bmy, 1/25/07)
- (7) Modifications for 0.5 x 0.667 grid (yxw, dan, bmy, 11/6/08)
- (8) Updates for nested grids (amv, bmy, 12/18/09)
- 01 Mar 2012 R. Yantosca Now reference new grid\_mod.F90
- 25 Nov 2013 C. Keller Now a HEMCO extension
- 06 Oct 2014 C. Keller Allow mass flux tuning factor be set in configuration file.
- 08 Jul 2015 M. Sulprizio- Now include dust alkalinity source (tdf 04/10/08)
- 07 Jan 2016 E. Lundgren Change dry air gas constant and molec wt to match GC values and update acc due to gravity and universal gas constant to NIST 2014 values
- 14 Oct 2016 C. Keller Now use HCO\_EvalFld instead of HCO\_GetPtr.

# 2.6.1 HCOX\_DustDead\_Run

Subroutine HcoX\_DustDead\_Run is the driver routine for the HEMCO DEAD dust extension.

SUBROUTINE HCOX\_DustDead\_Run( am\_I\_Root, ExtState, HcoState, RC )

### **USES:**

```
USE HCO_CALC_MOD, ONLY : HCO_EvalFld
USE HCO_FLUXARR_MOD, ONLY : HCO_EmisAdd
USE HCO_CLOCK_MOD, ONLY : HcoClock_Get
USE HCO_CLOCK_MOD, ONLY : HcoClock_First
```

# INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
```

TYPE(Ext\_State), POINTER :: ExtState ! Module options
TYPE(HCO\_State), POINTER :: HcoState ! Hemco state

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

#### **REVISION HISTORY:**

- 08 Apr 2004 T. D. Fairlie Initial version
- (1) Added OpenMP parallelization, added comments (bmy, 4/8/04)
- (2) Bug fix: DSRC needs to be held PRIVATE (bmy, 4/14/04)
- (3) Now references DATA\_DIR from "directory\_mod.f" (bmy, 7/20/04)
- (4) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (5 ) Bug fix: It should be SNOW/1d3 not SNOW\*1d3 (tdf, bmy, 11/18/05)
- (6) Updated output statement (bmy, 1/23/07)
- (7) Use SNOMAS (m H2O) for GEOS-5 (bmy, 1/24/07)
- 25 Aug 2010 R. Yantosca Treat MERRA in the same way as for GEOS-5
- 25 Aug 2010 R. Yantosca Added ProTeX headers
- 03 Sep 2010 R. Yantosca Bug fix, SNOMAS was mislabled in GEOS-5 and has units of mm H2O instead of m H2O so we need to convert to m H2O.
- 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\_R(I,J,L) from grid\_mod.F90
- 09 Nov 2012 M. Payer Replaced all met field arrays with State\_Met derived type object
- 25 Nov 2013 C. Keller  $\,$  Now a HEMCO extension
- 06 Oct 2014 C. Keller Now calculate pressure center from edges.
- 26 Jun 2015 E. Lundgren Add L. Zhang new dust size distribution scheme
- 08 Jul 2015 M. Sulprizio- Now include dust alkalinity source (tdf 04/10/08)
- 26 Oct 2016 R. Yantosca Don't nullify local ptrs in declaration stmts

#### 2.6.2 HCOX\_DustDead\_Init

Subroutine HcoX\_DustDead\_Init initializes the HEMCO DUST\_DEAD extension.

```
SUBROUTINE HCOX_DustDead_Init ( am_I_Root, HcoState, ExtName, & ExtState, RC )
```

# **USES:**

```
USE HCO_ExtList_Mod, ONLY : GetExtNr, GetExtOpt
USE HCO_STATE_MOD, ONLY : HCO_GetExtHcoID
```

# INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
```

TYPE(HCO\_State), POINTER :: HcoState ! Hemco state
CHARACTER(LEN=\*), INTENT(IN ) :: ExtName ! Extension name
TYPE(Ext\_State), POINTER :: ExtState ! Module options

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

# **REVISION HISTORY:**

```
25 Nov 2013 - C. Keller - Now a HEMCO extension
14 Aug 2014 - R. Yantosca - Now always print out extension info
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 2.6.3 HCOX\_DustDead\_Final

Subroutine HcoX\_DustDead\_Final finalizes the HEMCO DUST\_DEAD extension.

# **INTERFACE:**

```
SUBROUTINE HCOX_DustDead_Final ( ExtState )
```

# INPUT PARAMETERS:

```
TYPE(Ext_State), POINTER :: ExtState ! Module options
```

# **REVISION HISTORY:**

```
25 Nov 2013 - C. Keller - Now a HEMCO extension !NOTES:
```

# 2.6.4 InstGet

Subroutine InstGet returns a pointer to the desired instance.

```
SUBROUTINE InstGet (Instance, Inst, RC, PrevInst)
```

# INPUT PARAMETERS:

INTEGER :: Instance
TYPE(MyInst), POINTER :: Inst
INTEGER :: RC

TYPE(MyInst), POINTER, OPTIONAL :: PrevInst

# REVISION HISTORY:

18 Feb 2016 - C. Keller - Initial version

# 2.6.5 InstCreate

Subroutine InstCreate creates a new instance.

# **INTERFACE:**

SUBROUTINE InstCreate (ExtNr, Instance, Inst, RC)

### INPUT PARAMETERS:

INTEGER, INTENT(IN) :: ExtNr

# **OUTPUT PARAMETERS:**

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

# **REVISION HISTORY:**

18 Feb 2016 - C. Keller - Initial version 26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts

# 2.6.6 InstRemove

Subroutine InstRemove creates a new instance.

# **INTERFACE:**

SUBROUTINE InstRemove (Instance)

# INPUT PARAMETERS:

INTEGER :: Instance

# REVISION HISTORY:

18 Feb 2016 - C. Keller - Initial version

26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts

# 2.7 Fortran: Module Interface hemcox\_dustginoux\_mod.F90

Paul GINOUX dust source function. This subroutine updates the surface mixing ratio of dust aerosols for NDSTBIN size bins. The uplifting of dust depends in space on the source function, and in time and space on the soil moisture and surface wind speed (10 meters). Dust is uplifted if the wind speed is greater than a threshold velocity which is calculated with the formula of Marticorena et al. (JGR, v.102, pp 23277-23287, 1997). To run this subroutine you need the source function which can be obtained by contacting Paul Ginoux at ginoux@rondo.gsfc.nasa.gov/ If you are not using GEOS DAS met fields, you will most likely need to adapt the adjusting parameter.

This is a HEMCO extension module that uses many of the HEMCO core utilities.

#### References:

- Ginoux, P., M. Chin, I. Tegen, J. Prospero, B. Hoben, O. Dubovik, and S.-J. Lin, "Sources and distributions of dust aerosols simulated with the GOCART model", J. Geophys. Res., 2001
- 2. 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.

# **AUTHOR:**

```
Paul Ginoux (ginoux@rondo.gsfc.nasa.gov)
```

# **INTERFACE:**

MODULE HCOX\_DustGinoux\_Mod

# **USES:**

```
USE HCO_Error_Mod
USE HCO_Diagn_Mod
USE HCO_State_Mod, ONLY: HCO_State
USE HCOX_State_Mod, ONLY: Ext_State
IMPLICIT NONE
PRIVATE
```

#### PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: HcoX_DustGinoux_Run

PUBLIC :: HcoX_DustGinoux_Init

PUBLIC :: HcoX_DustGinoux_Final

PUBLIC :: HcoX_DustGinoux_GetChDust
```

# **REVISION HISTORY:**

```
08 Apr 2004 - T. D. Fairlie - Initial version
(1 ) Added OpenMP parallelization (bmy, 4/8/04)
(2) Now references DATA_DIR from "directory_mod.f" (bmy, 7/20/04)
25 Aug 2010 - R. Yantosca - Added ProTeX headers
01 Mar 2012 - R. Yantosca - Now use GET_AREA_M2(I,J,L) from 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
                          - Replaced all met field arrays with State_Met
09 Nov 2012 - M. Payer
                            derived type object
26 Feb 2013 - R. Yantosca - Now accept Input_Opt via the arg list
11 Dec 2013 - C. Keller - Now a HEMCO extension.
29 Sep 2014 - R. Yantosca - Now make NBINS a variable and not a parameter
29 Sep 2014 - R. Yantosca - Now use F90 free-format indentation
08 Jul 2015 - M. Sulprizio- Now include dust alkalinity source (tdf 04/10/08)
14 Oct 2016 - C. Keller - Now use HCO_EvalFld instead of HCO_GetPtr.
```

# 2.7.1 HCOX\_DustGinoux\_Run

Subroutine HcoX\_DustGinoux\_Run is the driver routine for the Paul Ginoux dust source function HEMCO extension.

#### **INTERFACE:**

```
SUBROUTINE HcoX_DustGinoux_Run( am_I_Root, ExtState, HcoState, RC )
```

#### **USES:**

```
USE HCO_Calc_Mod, ONLY : HCO_EvalFld
USE HCO_EmisList_Mod, ONLY : HCO_GetPtr
USE HCO_FluxArr_Mod, ONLY : HCO_EmisAdd
USE HCO_Clock_Mod, ONLY : HcoClock_First
```

# INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root ! Are we on the root CPU? TYPE(Ext_State), POINTER :: ExtState ! Options for this ext
```

# INPUT/OUTPUT PARAMETERS:

SRCE\_FUNK Source function

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object INTEGER, INTENT(INOUT) :: RC ! Success or failure?
```

#### **REMARKS:**

```
for 1: Sand, 2: Silt, 3: Clay

DUSTDEN Dust density (kg/m3)

DUSTREFF Effective radius (um)

AD Air mass for each grid box (kg)
```

(-)

```
NTDT Time step (s)
W10m Velocity at the anemometer level (10meters) (m/s)
GWET Surface wetness (-)
```

Dust properties used in GOCART

Size classes: 01-1, 1-1.8, 1.8-3, 3-6 (um)

Radius: 0.7, 1.5, 2.5, 4 (um)

Density: 2500, 2650, 2650, 2650 (kg/m3)

# REVISION HISTORY:

```
08 Apr 2004 - T. D. Fairlie - Initial version
(1 ) Added OpenMP parallelization (bmy, 4/8/04)
(2) Now references DATA_DIR from "directory_mod.f" (bmy, 7/20/04)
25 Aug 2010 - R. Yantosca - Added ProTeX headers
01 Mar 2012 - R. Yantosca - Now use GET_AREA_M2(I,J,L) from 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
09 Nov 2012 - M. Payer
                         - Replaced all met field arrays with State_Met
                            derived type object
26 Feb 2013 - R. Yantosca - Now accept Input_Opt via the arg list
11 Dec 2013 - C. Keller - Now a HEMCO extension
29 Sep 2014 - R. Yantosca - Bug fix: SRCE_CLAY should have been picked when
                            M=3 but was picked when M=2. Now corrected.
26 Jun 2015 - E. Lundgren - Add L. Zhang new dust size distribution scheme
08 Jul 2015 - M. Sulprizio- Now include dust alkalinity source (tdf 04/10/08)
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 2.7.2 HCOX\_DustGinoux\_Init

Subroutine HcoX\_DustGinoux\_Init initializes the HEMCO DUSTGINOUX extension.

# **INTERFACE:**

```
SUBROUTINE HcoX_DustGinoux_Init( am_I_Root, HcoState, ExtName, ExtState, RC )
USES:
```

```
USE HCO_ExtList_Mod, ONLY : GetExtNr, GetExtOpt
USE HCO_State_Mod, ONLY : HCO_GetExtHcoID
```

# INPUT PARAMETERS:

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

TYPE(HCO_State), POINTER :: HcoState ! HEMCO State object

CHARACTER(LEN=*), INTENT(IN ) :: ExtName ! Extension name

TYPE(Ext_State), POINTER :: ExtState ! Extension options
```

# INPUT/OUTPUT PARAMETERS:

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

#### **REVISION HISTORY:**

```
11 Dec 2013 - C. Keller - Now a HEMCO extension
26 Sep 2014 - R. Yantosca - Updated for TOMAS
29 Sep 2014 - R. Yantosca - Now initialize NBINS from HcoState%N_DUST_BINS
```

# 2.7.3 HCOX\_DustGinoux\_Final

Subroutine HcoX\_DustGinoux\_Final finalizes the HEMCO DUSTGINOUX extension.

### **INTERFACE:**

SUBROUTINE HcoX\_DustGinoux\_Final()

#### **REVISION HISTORY:**

```
11 Dec 2013 - C. Keller - Now a HEMCO extension
```

# 2.7.4 HCOX\_DustGinoux\_GetChDust

Function HCOX\_DustGinoux\_GetChDust returns the CH\_DUST parameter for the current simulation type.

#### **INTERFACE:**

```
FUNCTION HCOX_DustGinoux_GetChDust() RESULT( CH_DUST )
```

# **RETURN VALUE:**

```
REAL*8 :: CH_DUST
```

# **REMARKS:**

The logic in the #ifdefs may need to be cleaned up later on. We have just replicated the existing code in pre-HEMCO versions of dust\_mod.F.

# REVISION HISTORY:

```
11 Dec 2013 - C. Keller - Initial version
25 Sep 2014 - R. Yantosca - Updated for TOMAS
```

# 2.8 Fortran: Module Interface hcox\_finn\_mod.F90

Module HCOX\_FINN\_MOD contains routines and variables to calculate FINN biomass burning emissions in HEMCO. **INTERFACE:** 

```
MODULE HcoX_FINN_Mod
```

# **USES:**

```
USE HCO_Error_Mod
USE HCO_Diagn_Mod
USE HCOX_TOOLS_MOD
USE HCO_State_Mod, ONLY: HCO_State
USE HCOX_State_Mod, ONLY: Ext_State
IMPLICIT NONE
PRIVATE
```

#### PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCOX\_FINN\_Init
PUBLIC :: HCOX\_FINN\_Run
PUBLIC :: HCOX\_FINN\_Final

#### **REMARKS:**

Emissions of biomass burning species are read at monthly or daily resolution. Note: no emission factors are used here - emissions of individual species are given in input files. Emissions on the FINN 0.5x0.5 degree grid are regridded to the current model grid.

FINN biomass burning emissions are computed for the following gas-phase and aerosol-phase species:

```
[kgC/m2/s]
(1) NOx [kg/m2/s]
                         (13) BC
(2 ) CO
          [kg/m2/s]
                                   [kgC/m2/s]
                         (14) OC
(3 ) ALK4 [kgC/m2/s]
                         (15) MGLY [ kg/m2/s]
                         (16) BENZ [kgC/m2/s]
(4) ACET [kgC/m2/s]
                         (17) TOLU [kgC/m2/s]
(5) MEK [kgC/m2/s]
(6 ) ALD2 [kgC/m2/s]
                         (18) C2H4 [kgC/m2/s]
                         (19) C2H2 [kgC/m2/s]
(7 ) PRPE [kgC/m2/s]
(8) C3H8 [kgC/m2/s]
                         (20) GLYC [ kg/m2/s]
(9) CH20 [kg/m2/s]
                         (21) HAC [ kg/m2/s]
(10) C2H6 [kgC/m2/s]
                         (22) CO2
                                   [kg/m2/s]
(11) SO2 [ kg/m2/s]
                         (23) CH4
                                   [kg/m2/s]
(12) NH3 [ kg/m2/s]
                         (24)
```

All species to be used must be listed in the settings section of the HEMCO configuration file. For every listed species, individual scale factors as well as masks can be defined. For example, to scale FINN CO emissions by a factor of 1.05 and restrict them to North America, as well as to scale NO emissions by a factor of 1.5:

```
emissions by a factor of 1.5:
                                  NO/CO/ALK4/ACET/MEK/ALD2/PRPE/C3H8/CH2O/C2H6/SO2/NH3/BCPI/I
114
        FINN
                          : on
    --> FINN_daily
                          :
                                   false
    --> hydrophilic BC
                                  0.2
                          :
    --> hydrophilic OC
                                  0.5
                          :
    --> Mask_CO
                                  NAMASK
```

--> Scaling\_CO : 1.05

```
--> Scaling_NO : 1.5
```

Field NAMASK must be defined in section mask of the HEMCO configuration file.

#### References:

\_\_\_\_\_\_

- (1 ) Original FINN database from Christine Wiedinmyer http://bai.acd.ucar.edu/Data/fire/
- (2) Wiedinmyer, C., Akagi, S.K., Yokelson, R.J., Emmons, L.K., Al-Saadi, J.A., Orlando, J.J., and Soja, A.J.: The Fire Inventory from NCAR (FINN): a high resolution global model to estimate the emissions from open burning, Geoscientific Model Development, 4, 625-641, doi:10.5194/gmd-4-625-2011, 2011.

# **REVISION HISTORY:**

```
02 Jan 2013 - J. Mao & J.A. Fisher - Initial version, based on GFED3
01 Oct 2013 - J.A. Fisher - Update to only use one input file
05 May 2014 - J.A. Fisher - Replace NOx emissions with NO emissions as part of removal of NOx-Ox partitioning
18 Jun 2014 - C. Keller - Now a HEMCO extension.
03 Jul 2014 - C. Keller - Added 13 new FINN species
11 Aug 2014 - R. Yantosca - Now get emission factors and NMOC ratios from hard-coded statements in hcox_finn_include.H
11 Aug 2014 - R. Yantosca - Now use F90 free-form indentation
11 Aug 2014 - R. Yantosca - Cosmetic changes to ProTeX subroutine headers
11 Jun 2015 - C. Keller - Update to include individual scale factors and masks.
```

14 Oct 2016 - C. Keller - Now use HCO\_EvalFld instead of HCO\_GetPtr.

# 2.8.1 HCOX\_FINN\_Run

Subroutine HCOX\_FINN\_Run computes the FINN biomass burning emissions for the current date.

# **INTERFACE:**

```
SUBROUTINE HCOX_FINN_Run( am_I_Root, ExtState, HcoState, RC )
```

#### **USES:**

```
USE HCO_EmisList_mod, ONLY: HCO_GetPtr

USE HCO_Calc_Mod, ONLY: HCO_EvalFld

USE HCO_FluxArr_mod, ONLY: HCO_EmisAdd

USE HCO_State_mod, ONLY: HCO_GetHcoID

USE HCO_Clock_mod, ONLY: HcoClock_Get

USE HCO_Clock_mod, ONLY: HcoClock_First

USE HCO_Clock_mod, ONLY: HcoClock_NewMonth, HcoClock_NewDay
```

#### INPUT PARAMETERS:

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

TYPE(Ext_State), POINTER :: ExtState ! Module options
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! Output obj
```

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

#### REVISION HISTORY:

```
02 Jan 2012 - J. Mao & J. Fisher - Initial version, based on GFED3
```

18 Jun 2014 - C. Keller - Now a HEMCO extension.

26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts

#### 2.8.2 HCOX\_FINN\_Init

Subroutine HCOX\_FINN\_INIT initializes all module arrays and variables.

# **INTERFACE:**

```
SUBROUTINE HCOX_FINN_Init( am_I_Root, HcoState, ExtName, ExtState, RC )
```

# USES:

```
USE HCO_State_Mod, ONLY : HCO_GetHcoID
USE HCO_State_Mod, ONLY : HCO_GetExtHcoID
USE HCO_ExtList_Mod, ONLY : GetExtNr, GetExtOpt
USE HCO_ExtList_Mod, ONLY : GetExtSpcVal
```

# INPUT PARAMETERS:

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

TYPE(HCO\_State), POINTER :: HcoState ! HEMCO state object CHARACTER(LEN=\*), INTENT(IN ) :: ExtName ! Extension name TYPE(Ext\_State), POINTER :: ExtState ! Extensions object

# INPUT/OUTPUT PARAMETERS:

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

# **REVISION HISTORY:**

```
02 Jan 2013 - J. Mao & J. Fisher - Initial version, based on GFED3
```

05 May 2014 - J.A. Fisher - Replace NOx emissions with NO emissions as part of removal of NOx-Ox partitioning

18 Jun 2014 - C. Keller - Now a HEMCO extension.

11 Aug 2014 - R. Yantosca - Now get FINN emission factors and species names

from include file hcox\_finn\_include.H.

11 Nov 2014 - C. Keller - Now get hydrophilic fractions through config file

# 2.8.3 HCOX\_FINN\_Final

Subroutine HCOX\_FINN\_FINAL deallocates all module arrays.

# **INTERFACE:**

```
SUBROUTINE HCOX_FINN_FINAL()
```

# **REVISION HISTORY:**

```
02 Jan 2013 - J. Mao & J. Fisher - Initial version, based on GFED3
18 Jun 2014 - C. Keller - Now a HEMCO extension.
```

# 2.9 Fortran: Module Interface hcox\_gc\_POPs\_mod.F90

Defines the HEMCO extension for the GEOS-Chem persistent organic pollutants (POPs) specialty simulation.

# **INTERFACE:**

```
MODULE HCOX_GC_POPs_Mod
```

#### **USES:**

```
USE HCO_Error_Mod

USE HCO_Diagn_Mod

USE HCO_State_Mod, ONLY: HCO_State ! Derived type for HEMCO state

USE HCOX_State_Mod, ONLY: Ext_State ! Derived type for External state

IMPLICIT NONE

PRIVATE
```

#### PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: HcoX_GC_POPs_Run
PUBLIC :: HcoX_GC_POPs_Init
PUBLIC :: HcoX_Gc_POPs_Final
```

# PRIVATE MEMBER FUNCTIONS:

```
PRIVATE :: VEGEMISPOP
PRIVATE :: LAKEEMISPOP
PRIVATE :: SOILEMISPOP
PRIVATE :: IS_LAND
PRIVATE :: IS_ICE
```

# **REMARKS:**

#### References:

\_\_\_\_\_\_\_

(1) Zhang, Y., and S. Tao, Global atmospheric emission inventory of polycyclic aromatic hydrocarbons (PAHs) for 2004. Atm Env, 43, 812-819,

2009.

- (2) Friedman, C.L, and N.E. Selin, Long-Range Atmospheric Transport of Polycyclic Aromatic Hydrocarbons: A Global 3-D Model Analysis Including Evaluation of Arctic Sources, Environ. Sci. Technol., 46(17), 9501-9510, 2012.
- (3) Friedman, C.L., Y. Zhang, and N.E. Selin, Climate change and emissions impacts on atmospheric PAH transport to the Arctic, Environ. Sci. Technol., 48, 429-437, 2014.
- (4) Friedman, C.L., J.R. Pierce, and N.E. Selin, Assessing the influence of secondary organic versus primary carbonaceous aerosols on long-range atmospheric polycyclic aromatic hydrocarbon transport, Environ. Sci. Technol., 48(6), 3293-3302, 2014.

# **REVISION HISTORY:**

```
20 Sep 2010 - N.E. Selin - Initial Version
04 Jan 2011 - C.L. Friedman - Expansion on initial version
19 Aug 2014 - M. Sulprizio - Now a HEMCO extension
18 Aug 2015 - M. Sulprizio - Add VEGEMISPOP, LAKEEMISPOP, and SOILEMISPOP routines from new land_pops_mod.F written by C.L. Friedman.
```

# 2.9.1 HCOX\_GC\_POPs\_run

Subroutine HcoX\_Gc\_POPs\_Run computes emissions of OC-phase, BC-phase, and gas-phase POPs for the GEOS-Chem POPs specialty simulation.

# **INTERFACE:**

```
SUBROUTINE HCOX_GC_POPs_Run( am_I_Root, ExtState, HcoState, RC )
```

# **USES:**

```
! HEMCO modules
USE HCO_EmisList_Mod, ONLY : HCO_GetPtr
USE HCO_FluxArr_Mod, ONLY : HCO_EmisAdd
USE HCO_Clock_Mod, ONLY : HcoClock_First
```

# INPUT PARAMETERS:

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

TYPE(Ext_State), POINTER :: ExtState ! Options for POPs sim

TYPE(HCO_State), POINTER :: HcoState ! HEMCO state
```

# INPUT/OUTPUT PARAMETERS:

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

#### **REMARKS:**

This code is based on routine EMISSPOPS in prior versions of GEOS-Chem.

# **REVISION HISTORY:**

# 2.9.2 soilemispop

Subroutine SOILEMISPOP is the subroutine for secondary POP emissions from soils.

# **INTERFACE:**

```
SUBROUTINE SOILEMISPOP( POP_SURF, F_OC_SOIL, EPOP_SOIL, & HcoState, ExtState )
```

#### INPUT PARAMETERS:

```
REAL(sp), DIMENSION(:,:), INTENT(IN) :: POP_SURF ! POP sfc conc [kg]
REAL(sp), DIMENSION(:,:), INTENT(IN) :: F_OC_SOIL ! Frac C in soil [g/g]
TYPE(HCO_STATE), POINTER :: HcoState ! Hemco state
TYPE(Ext_State), POINTER :: ExtState ! Module options
```

# **OUTPUT PARAMETERS:**

```
REAL(hp), DIMENSION(:,:), INTENT(OUT) :: EPOP_SOIL ! POP emissions from ! soil [kg/m2/s]
```

# **REMARKS:**

# **REVISION HISTORY:**

```
21 Aug 2012 - C.L. Friedman - Initial version based on LAND_MERCURY_MOD 25 Aug 2015 - M. Sulprizio - Moved to hcox_gc_POPs_mod.F90 02 Oct 2015 - E. Lundgren - ExtState%POPG is now kg/kg dry air (prev kg) 07 Jan 2016 - E. Lundgren - Update molar gas constant to NIST 2014
```

# 2.9.3 lakeemispop

Subroutine LAKEEMISPOP is the subroutine for secondary POP emissions from lakes.

SUBROUTINE LAKEEMISPOP( POP\_SURF, EPOP\_LAKE, HcoState, ExtState )

#### **USES:**

#### INPUT PARAMETERS:

### **OUTPUT PARAMETERS:**

```
REAL(hp), DIMENSION(:,:), INTENT(OUT) :: EPOP_LAKE ! POP emissions from ! lakes [kg/m2/s]
```

#### **REMARKS:**

# **REVISION HISTORY:**

```
21 Aug 2012 - C.L. Friedman - Initial version based on LAND_MERCURY_MOD 25 Aug 2015 - M. Sulprizio - Moved to hcox_gc_POPs_mod.F90 02 Oct 2015 - E. Lundgren - ExtState%POPG is now kg/kg dry air (prev kg) 07 Jan 2016 - E. Lundgren - Update molar gas constant to NIST 2014
```

# 2.9.4 vegemispop

Subroutine VEGEMISPOP is the subroutine for secondary POP emissions from soils.

#### INTERFACE:

```
SUBROUTINE VEGEMISPOP( POP_SURF, EPOP_VEG, HcoState, ExtState )
```

#### **USES:**

# INPUT PARAMETERS:

```
REAL(sp), DIMENSION(:,:), INTENT(IN) :: POP_SURF ! POP sfc conc [kg] TYPE(HCO_State), POINTER :: HcoState ! Hemco state TYPE(Ext_State), POINTER :: ExtState ! Module options
```

# **OUTPUT PARAMETERS:**

#### **REMARKS:**

#### **REVISION HISTORY:**

```
21 Aug 2012 - C.L. Friedman - Initial version based on LAND_MERCURY_MOD 25 Aug 2015 - M. Sulprizio - Moved to hcox_gc_POPs_mod.F90 02 Oct 2015 - E. Lundgren - ExtState%POPG is now kg/kg dry air (prev kg) 07 Jan 2016 - E. Lundgren - Update molar gas constant to NIST 2014
```

# 2.9.5 is\_land

Function IS\_LAND returns TRUE if surface grid box (I,J) is a land box.

#### INTERFACE:

**USES:** 

```
FUNCTION IS_LAND( I, J, ExtState ) RESULT ( LAND )
```

#### INPUT PARAMETERS:

# RETURN VALUE:

LOGICAL :: LAND ! =T if it is a land box

# **REVISION HISTORY:**

- 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
                          - Replaced all met field arrays with State_Met
09 Nov 2012 - M. Payer
                            derived type object
```

# 2.9.6 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, ExtState ) RESULT ( ICE )
```

#### **USES:**

#### INPUT PARAMETERS:

```
! Longitude index of grid box
INTEGER,
               INTENT(IN) :: I
INTEGER,
               INTENT(IN) :: J
                                       ! Latitude index of grid box
```

:: ExtState ! Module options TYPE(Ext\_State), POINTER

# RETURN VALUE:

LOGICAL 

# **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

# 2.9.7 HCOX\_GC\_POPs\_Init

Subroutine HcoX\_GC\_POPs\_Init initializes the HEMCO GC\_POPs extension.

```
SUBROUTINE HCOX_GC_POPs_Init( am_I_Root, HcoState, ExtName, ExtState, RC )
```

# **USES:**

```
USE HCO_ExtList_Mod, ONLY : GetExtNr
```

USE HCO\_STATE\_MOD, ONLY : HCO\_GetExtHcoID

# INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
```

CHARACTER(LEN=\*), INTENT(IN ) :: ExtName ! Extension name TYPE(Ext\_State), POINTER :: ExtState ! Module options TYPE(HCO\_State), POINTER :: HcoState ! Hemco state

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

# **REVISION HISTORY:**

```
19 Aug 2014 - M. Sulprizio- Initial version
01 May 2015 - R. Yantosca - Bug fix: need to zero arrays after allocating
```

### 2.9.8 HCOX\_GC\_POPs\_Final

Subroutine HcoX\_GC\_POPs\_Final finalizes the HEMCO extension for the GEOS-Chem POPs specialty simulation. All module arrays will be deallocated.

# **INTERFACE:**

```
SUBROUTINE HCOX_GC_POPs_Final()
```

### **REVISION HISTORY:**

```
19 Aug 2014 - M. Sulprizio- Initial version
```

# 2.10 Fortran: Module Interface hcox\_gc\_RnPbBe\_mod.F90

Defines the HEMCO extension for the GEOS-Chem Rn-Pb-Be specialty simulation.

This extension parameterizes emissions of Rn and/or Pb based upon the literature given below. The emission fields become automatically added to the HEMCO emission array of the given species. It is possible to select only one of the two species (Rn or Pb) in the HEMCO configuration file. This may be useful if a gridded data inventory shall be applied to one of the species (through the standard HEMCO interface).

# **INTERFACE:**

```
MODULE HCOX_GC_RnPbBe_Mod
```

# **USES:**

```
USE HCO_Error_Mod

USE HCO_Diagn_Mod

USE HCO_State_Mod, ONLY: HCO_State ! Derived type for HEMCO state

USE HCOX_State_Mod, ONLY: Ext_State ! Derived type for External state

IMPLICIT NONE

PRIVATE
```

# PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HcoX\_GC\_RnPbBe\_Run
PUBLIC :: HcoX\_GC\_RnPbBe\_Init
PUBLIC :: HcoX\_Gc\_RnPbBe\_Final

# PRIVATE MEMBER FUNCTIONS:

PRIVATE :: Init\_7Be\_Emissions

#### **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.

# **REVISION HISTORY:**

```
07 Jul 2014 - R. Yantosca - Initial version
15 Aug 2014 - C. Keller - Targets now in hp precision. Cosmetic changes
21 Aug 2014 - R. Yantosca - Add Pb as a species
21 Aug 2014 - R. Yantosca - Add HEMCO species indices as module variables
04 Sep 2014 - R. Yantosca - Remove IDTPb; Pb210 only has a chemical source
04 Sep 2014 - R. Yantosca - Modified for GCAP simulation
05 Nov 2014 - C. Keller - Now allow Rn or Pb to be not specified.
07 Jan 2016 - E. Lundgren - Update Avogadro's # to NIST 2014 value
```

# 2.10.1 HCOX\_Gc\_RnPbBe\_run

Subroutine HcoX\_Gc\_RnPbBe\_Run computes emissions of 222Rn and 7Be for the GEOS-Chem Rn-Pb-Be specialty simulation.

SUBROUTINE HCOX\_Gc\_RnPbBe\_Run( am\_I\_Root, ExtState, HcoState, RC )

# **USES:**

```
! HEMCO modules
```

USE HCO\_FluxArr\_Mod, ONLY : HCO\_EmisAdd

# INPUT PARAMETERS:

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

TYPE(Ext_State), POINTER :: ExtState ! Options for Rn-Pb-Be sim

TYPE(HCO_State), POINTER :: HcoState ! HEMCO state
```

# INPUT/OUTPUT PARAMETERS:

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

# **REMARKS:**

This code is based on routine EMISSRnPbBe in prior versions of GEOS-Chem.

# **REVISION HISTORY:**

```
07 Jul 2014 - R. Yantosca - Initial version
03 Sep 2014 - R. Yantosca - Bug fix: Prevent div-by-zero errors
06 Oct 2014 - C. Keller - Now calculate pressure centers from edges.
29 Oct 2014 - R. Yantosca - Use latitude centers of the grid box to
facilitate running in ESMF/MPI environment
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 2.10.2 HCOX\_Gc\_RnPbBe\_Init

Subroutine HcoX\_Gc\_RnPbBe\_Init initializes the HEMCO GC\_Rn-Pb-Be extension.

# **INTERFACE:**

```
SUBROUTINE HCOX_Gc_RnPbBe_Init( am_I_Root, HcoState, ExtName, ExtState, RC )
```

#### **USES:**

```
USE HCO_ExtList_Mod, ONLY : GetExtNr
USE HCO_State_Mod, ONLY : HCO_GetExtHcoID
```

# INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
CHARACTER(LEN=*), INTENT(IN ) :: ExtName ! Extension name
TYPE(Ext_State), POINTER :: ExtState ! Module options
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! Hemco state INTEGER, INTENT(INOUT) :: RC
```

# **REVISION HISTORY:**

```
07 Jul 2014 - R. Yantosca - Initial version
21 Aug 2014 - R. Yantosca - Now define HEMCO indices as well
04 Sep 2014 - R. Yantosca - Activate ExtState%TROPP for GCAP simulation
```

# 2.10.3 HCOX\_Gc\_RnPbBe\_Final

Subroutine HcoX\_Gc\_RnPbBe\_Final finalizes the HEMCO extension for the GEOS-Chem Rn-Pb-Be specialty simulation. All module arrays will be deallocated.

#### **INTERFACE:**

```
SUBROUTINE HCOX_Gc_RnPbBe_Final()
```

# REVISION HISTORY:

```
13 Dec 2013 - C. Keller - Now a HEMCO extension
06 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
06 Jun 2014 - R. Yantosca - Now indended with F90 free-format
```

# 2.10.4 Init\_7Be\_Emissions

Subroutine Init\_7Be\_Emissions initializes the 7Be emissions from Lal & Peters on 33 pressure levels. This data used to be read from a file, but we have now hardwired it to facilitate I/O in the ESMF environment.

# **INTERFACE:**

```
SUBROUTINE Init_7Be_Emissions()
```

#### **REMARKS:**

- (1) Reference: 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.
- (2) In prior versions of GEOS-Chem, this routine was named READ\_7BE, and it read the ASCII file "7Be.Lal". Because this data set is not placed on a lat/lon grid, ESMF cannot regrid it. To work around this, we now hardwire this data in module arrays rather than read it from disk.
- (3) Units of 7Be emissions are [stars/g air/s].
  Here, "stars" = # of nuclear disintegrations of cosmic rays
- (4) Original data from Lal & Peters (1967), w/ these modifications:(a) Replace data at (OhPa, 70S) following Koch 1996:(i ) old value = 3000

```
(ii) new value = 1900
```

(b) Copy data from 70S to 80S and 90S at all levels

### **REVISION HISTORY:**

```
07 Aug 2002 - H. Liu - Initial version
(1) This code was split off from routine EMISSRnPbBe below. (bmy, 8/7/02)
(2 ) Now reference DATA_DIR from "directory_mod.f" (bmy, 7/19/04)
08 Dec 2009 - R. Yantosca - Added ProTeX headers
01 Aug 2012 - R. Yantosca - Add reference to findFreeLUN from inqure_mod.F90
02 Jul 2014 - R. Yantosca - Now hardwire the data instead of reading it
                            from an ASCII file. This facilitates ESMF I/O.
07 Jul 2014 - R. Yantosca - Now renamed to INIT_7Be_Emissions and added
                            as a HEMCO extension
07 Jul 2014 - R. Yantosca - Now use F90 free-format indentation
8 Aug 2014 - R. Yantosca - Now split off into hcox_gc_RnPbBe_include.H
05 Nov 2014 - C. Keller - Converted from double-precision to flexible
                            (HEMCO) precision hp.
26 Feb 2015 - R. Yantosca - Now inline the code that used to be in the
                            include file hcox_gc_RnPbBe_include.H.
                            will result in faster compilation.
08 Jan 2016 - R. Yantosca - Change 54_hp to 54.0_hp to avoid error
```

### 2.10.5 SLQ

Subroutine SLQ is an interpolation subroutine from a Chinese reference book (says Hongyu Liu).

### INTERFACE:

```
SUBROUTINE SLQ( X, Y, Z, N, M, U, V, W)
```

### **INPUT PARAMETERS:**

```
INTEGER :: N     ! First dimension of Z
INTEGER :: M     ! Second dimension of Z
REAL(hp) :: X(N)     ! X-axis coordinate on original grid
REAL(hp) :: Y(M)     ! Y-axis coordinate on original grid
REAL(hp) :: Z(N,M)     ! Array of data on original grid
REAL(hp) :: U     ! X-axis coordinate for desired interpolated value
REAL(hp) :: V     ! Y-axis coordinate for desired interpolated value
```

## **OUTPUT PARAMETERS:**

```
REAL(hp) :: W ! Interpolated value of Z array, at coords (U,V)
```

### **REMARKS:**

This routine was taken from the old RnPbBe\_mod.F.

# **REVISION HISTORY:**

```
17 Mar 1998 - H. Liu - Initial version
(1 ) Added to "RnPbBe_mod.f" (bmy, 7/16/01)
(2 ) Removed duplicate definition of IQ. Added comments. (bmy, 11/15/01)
08 Dec 2009 - R. Yantosca - Added ProTeX headers
7 Jul 2014 - R. Yantosca - Now use F90 free-format indentation
04 Dec 2014 - M. Yannetti - Added PRECISION_MOD
```

# 2.11 Fortran: Module Interface hcox\_gfed\_mod.F90

Module HCOX\_GFED\_MOD contains routines to calculate GFED biomass burning emissions in HEMCO. This can be GFED-3 or GFED-4, depending on the input data selected in the HEMCO configuration file.

!NOTES:

!REFERENCES: INTERFACE:

MODULE HCOX\_GFED\_MOD

#### **USES:**

```
USE HCO_ERROR_MOD

USE HCO_DIAGN_MOD

USE HCOX_TOOLS_MOD

USE HCO_STATE_MOD, ONLY: HCO_State

USE HCOX_State_MOD, ONLY: Ext_State

IMPLICIT NONE

PRIVATE
```

### PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCOX\_GFED\_Init
PUBLIC :: HCOX\_GFED\_Run
PUBLIC :: HCOX\_GFED\_Final

# **REMARKS:**

```
Monthly emissions of DM are read from disk, multiplied by daily and 3hourly fractions (if necessary), and then multiplied by the appropriate emission factors to produce biomass burning emissions.
```

All species to be used must be listed in the settings section of the HEMCO configuration file. For every listed species, individual scale factors as well as masks can be defined. For example, to scale FINN CO emissions by a factor of 1.05 and restrict them to North America, as well as to scale NO emissions by a factor of 1.5:

```
111 GFED : on NO/CO/ALK4/ACET/MEK/ALD2/PRPE/C3H8/CH2O/C2H6/SO2/NH3/BCPI/I
--> GFED3 : false
```

```
--> GFED4
                            true
--> GFED_daily
                   :
                            false
--> GFED_3hourly
                   :
                            false
--> hydrophilic BC :
                           0.2
--> hydrophilic OC :
                           0.5
--> Mask_CO
                           NAMASK
--> Scaling_CO
                           1.05
--> Scaling_NO
                            1.5
```

Field NAMASK must be defined in section mask of the HEMCO configuration file.

### For SOA\_SVPOA mechanism:

- \* If tracers POG1 and POG2 are specified, emissions are calculated from OC, multiplied by a POG scale factor (Scaling\_POG1, Scaling\_POG2) that must be specified in the HEMCO configuration file.
- \* If tracer NAP is specified, emissions are calculated from CO, multiplied by a NAP scale factor (Scaling\_NAP) that must be specified in the HEMCO configuration file.

#### References:

\_\_\_\_\_\_

- (1 ) Original GFED3 database from Guido van der Werf http://www.falw.vu/~gwerf/GFED/GFED3/emissions/
- (2) Giglio, L., Randerson, J. T., van der Werf, G. R., Kasibhatla, P. S., Collatz, G. J., Morton, D. C., and DeFries, R. S.: Assessing variability and long-term trends in burned area by merging multiple satellite fire products, Biogeosciences, 7, 1171-1186, doi:10.5194/bg-7-1171-2010, 2010.
- (3 ) van der Werf, G. R., Randerson, J. T., Giglio, L., Collatz, G. J., Mu, M., Kasibhatla, P. S., Morton, D. C., DeFries, R. S., Jin, Y., and van Leeuwen, T. T.: Global fire emissions and the contribution of deforestation, savanna, forest, agricultural, and peat fires (1997~@~S2009), Atmos. Chem. Phys., 10, 11707-11735, doi:10.5194/acp-10-11707-2010, 2010.

```
07 Sep 2011 - P. Kasibhatla - Initial version, based on GFED2
07 Sep 2011 - R. Yantosca - Added ProTeX headers
14 Feb 2012 - M. Payer
                           - Add modifications for CH4 (K. Wecht)
01 Mar 2012 - R. Yantosca - Now reference new grid_mod.F90
06 Mar 2012 - P. Kasibhatla - Final version
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 Mar 2013 - M. Payer
                         - Replace NOx emissions with NO emissions as part
                            of removal of NOx-Ox partitioning
15 Dec 2013 - C. Keller - Now a HEMCO extension. Emissions in kg/m2/s,
                            emission factors in kg/kgDM.
01 Jul 2014 - R. Yantosca - Now use F90 free-format indentation
01 Jul 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
08 Aug 2014 - R. Yantosca - Now avoid ASCII file reads for ESMF
```

```
23 Sep 2014 - C. Keller - Increase N_SPEC to 26 (+Hg0)

12 Mar 2015 - C. Keller / P. Kasibhatla - Added GFED-4.

03 Jun 2015 - C. Keller / P. Kasibhatla - GFED-4 update: now use GFED-4

specific emission factors and DM data.

14 Oct 2016 - C. Keller - Now use HCO_EvalFld instead of HCO_GetPtr.
```

#### 2.11.1 HCOX\_GFED\_Run

Subroutine HcoX\_GFED\_Run is the driver run routine to calculate seasalt emissions in HEMCO.

### **INTERFACE:**

```
SUBROUTINE HCOX_GFED_Run( am_I_Root, ExtState, HcoState, RC )
```

#### **USES:**

```
USE HCO_Calc_Mod, ONLY : HCO_EvalFld
USE HCO_EmisList_Mod, ONLY : HCO_GetPtr
USE HCO_FluxArr_MOD, ONLY : HCO_EmisAdd
```

### INPUT PARAMETERS:

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

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! Output obj

TYPE(Ext_State), POINTER :: ExtState ! Module options
```

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

# **REVISION HISTORY:**

```
07 Sep 2011 - P. Kasibhatla - Initial version, based on GFED2
15 Dec 2013 - C. Keller - Now a HEMCO extension
03 Apr 2015 - C. Keller - Humid tropical forest mask is not binary any more but fraction (0.0 - 1.0).
21 Sep 2016 - R. Yantosca - Bug fix: move WHERE statement for HUMTROP into the GFED3 block to avoid segfault
```

# 2.11.2 HCOX\_GFED\_Init

Subroutine HcoX\_GFED\_Init initializes all extension variables.

# **INTERFACE:**

```
SUBROUTINE HCOX_GFED_Init ( am_I_Root, HcoState, ExtName, & ExtState, RC
```

#### **USES:**

```
USE HCO_STATE_MOD, ONLY : HCO_GetHcoID

USE HCO_STATE_MOD, ONLY : HCO_GetExtHcoID

USE HCO_ExtList_Mod, ONLY : GetExtNr, GetExtOpt
```

USE HCO\_ExtList\_Mod, ONLY : GetExtSpcVal

# INPUT/OUTPUT PARAMETERS:

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

CHARACTER(LEN=*), INTENT(IN ) :: ExtName ! Extension name

TYPE(Ext_State), POINTER :: ExtState ! Options object
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object INTEGER, INTENT(INOUT) :: RC ! Return status
```

#### REVISION HISTORY:

```
07 Sep 2011 - P. Kasibhatla - Initial version, based on GFED2
15 Dec 2013 - C. Keller - Now a HEMCO extension
08 Aug 2014 - R. Yantosca - Now include hcox_gfed_include.H, which defines GFED_SPEC_NAME and GFED_EMFAC arrays
11 Nov 2014 - C. Keller - Now get hydrophilic fractions via config file
22 Apr 2015 - R. Yantosca - Now explicitly test for "POA scale factor" and "NAP scale factor" to avoid search errors
07 Jan 2016 - M. Sulprizio - Change 'POA1' to 'POG1' to better reflect that SVOC emissions are added to the gas-phase species in carbon_mod.F
```

# 2.11.3 HCOX\_GFED\_Final

Subroutine HcoX\_GFED\_Final deallocates all module arrays.

### **INTERFACE:**

SUBROUTINE HCOX\_GFED\_Final

## **REVISION HISTORY:**

```
07 Sep 2011 - P. Kasibhatla - Initial version, based on GFED2
15 Dec 2013 - C. Keller - Now a HEMCO extension
```

# 2.12 Fortran: Module Interface hcox\_lightnox\_mod.F90

Module HCOX\_LightNOx\_Mod contains routines to compute NO lightning emissions, according to the GEOS-Chem lightning algorithms.

This is a HEMCO extension module that uses many of the HEMCO core utilities. In

particular, the LIS-OTD local redistribution factors are now read through the HEMCO framework, and the corresponding netCDF input file is specified in the HEMCO configuration file. The table of cumulative distribution functions used to vertically distribute lightning NOx emissions is specified in the extension switch section of the configuration file.

## References:

- Murray, L. T., Jacob, D. J., Logan, J. A., Hudman, R. C., and Koshak, W. J.: Optimized regional and interannual variability of lightning in a global chemical transport model con-strained by LIS/OTD satellite data, J. Geophys. Res., Atmospheres, 117, 2012.
- Ott, L. E., K. E. Pickering, G. L. Stenchikov, D. J. Allen, A. J. DeCaria, B. Ridley, R.-F. Lin, S. Lang, and W.-K. Tao, Production of lightning NOx and its vertical distribution calculated from three-dimensional cloud-scale chemical transport model simulations, J. Geophys. Res., 115, D04301, 2010.

### **INTERFACE:**

MODULE HCOX\_LightNOx\_Mod

# **USES:**

```
USE HCO_Error_Mod
USE HCO_Diagn_Mod
USE HCOX_TOOLS_MOD
USE HCO_State_Mod, ONLY: HCO_State
USE HCOX_State_MOD, ONLY: Ext_State
IMPLICIT NONE
PRIVATE
```

#### PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCOX\_LightNOX\_Run
PUBLIC :: HCOX\_LightNOX\_Final
PUBLIC :: HCOX\_LightNOX\_Init

### PRIVATE MEMBER FUNCTIONS:

PRIVATE :: LIGHTNOX
PRIVATE :: LIGHTDIST
PRIVATE :: FLASHES\_CTH
PRIVATE :: GET\_IC\_CG\_RATIO
PRIVATE :: GET\_OTD\_LIS\_SCALE

# **PUBLIC DATA MEMBERS:**

### **REMARKS:**

%%% NOTE: MFLUX and PRECON methods are now deprecated (1tm, bmy, 7/9/09)

#### References:

\_\_\_\_\_\_

- (1) Price & Rind (1992), JGR, vol. 97, 9919-9933.
- (2) Price & Rind (1994), M. Weather Rev, vol. 122, 1930-1939.
- (3) Allen & Pickering (2002), JGR, 107, D23, 4711, doi:10.1029/2002JD002066
- (4) Hudman et al (2007), JGR, 112, D12S05, doi:10.1029/2006JD007912
- (5 ) Sauvage et al, 2007, ACP, http://www.atmos-chem-phys.net/7/815/2007/acp-7-815-2007.pdf
- (6) Ott et al., (2010), JGR
- (7) Allen et al., (2010), JGR
- (8) Murray et al., (2011), in prep.

- 14 Apr 2004 L. Murray, R. Hudman Initial version
- (1 ) Based on "lightnox\_nox\_mod.f", but updated for near-land formulation and for CTH, MFLUX, PRECON parameterizations (ltm, bmy, 5/10/06)
- (2 ) Now move computation of IC/CG flash ratio out of routines FLASHES\_CTH, FLASHES\_MFLUX, FLASHES\_PRECON, and into routine GET\_IC\_CG\_RATIO. Added a fix in LIGHTDIST for pathological grid boxes. Set E\_IC\_CG=1 according to Allen & Pickering [2002]. Rename OTDSCALE array to OTD\_REG\_REDIST, and also add OTD\_LOC\_REDIST array. Now scale lightnox to 6 Tg N/yr for both 2x25 and 4x5. Rename routine GET\_OTD\_LIS\_REDIST to GET\_REGIONAL\_REDIST. Add similar routine GET\_LOCAL\_REDIST. Removed GET\_OTD\_LOCP AL\_REDIST. Bug fix: divide A\_M2 by 1d6 to get A\_KM2. (rch, ltm, bmy, 2/22/07)
- (3 ) Rewritten for separate treatment of LNOx emissions at tropics & midlatitudes, based on Hudman et al 2007. Removed obsolete variable E\_IC\_CG. (rch, ltm, bmy, 3/27/07)
- (4) Changes implemented in this version (ltm, bmy, 10/3/07)
  - \* Revert to not classifying near-land as land
  - \* Eliminate NOx emisisons per path length entirely
  - \* Scale tropics to 260 mol/fl constraint from Randall Martin's 4.4 Tg and OTD-LIS avg ann flash rate
  - \* Remove top-down scaling (remove the three functions)
  - \* Allow option of mid-level scaling to match global avg ann flash rate between G-C and OTD-LIS 11-year climatology (new function)
  - \* Local Redist now a la Murray et al, 2007 in preparation (monthly)
  - \* Replace GEMISNOX (from CMN\_NOX) with module variable EMIS\_LI\_NOx
- (5) Added MFLUX, PRECON redistribution options (ltm, bmy, 11/29/07)
- (6 ) Updated OTD/LIS scaling for GEOS-5 to get more realistic totals (ltm, bmy, 2/20/08)
- (7 ) Now add the proper scale factors for the GEOS-5 0.5 x 0.666 grid and the GEOS-3 1x1 nested N. America grid in routine GET\_OTD\_LIS\_SCALE. (yxw, dan, ltm, bmy, 11/14/08)
- (8) Added quick fix for GEOS-5 reprocessed met fields (ltm, bmy, 2/18/09)
- (9) Added quick fix for GEOS-5 years 2004, 2005, 2008 (ltm, bmy, 4/29/09)

```
(10) Updated OTD/LIS scaling for GEOS-5 reprocessed data (ltm, bmy, 7/10/09)
(11) Updated for GEOS-4 1 x 1.25 grid (lok, ltm, bmy, 1/13/10)
(12) Reprocessed for CLDTOPS calculation error; Updated Ott vertical
      profiles; Removal of depreciated options, e.g., MFLUX and PRECON;
      GEOS5 5.1.0 vs. 5.2.0 special treatment; MERRA; Other changes.
      Please see PDF on wiki page for full description of lightnox
      changes to v9-01-01. (ltm, 1/25/11)
13 Aug 2010 - R. Yantosca - Add modifications for MERRA
10 Nov 2010 - L. Murray - Updated OTD/LIS local scaling for MERRA 4x5
10 Nov 2010 - R. Yantosca - Added ProTeX headers
02 Feb 2012 - R. Yantosca - Added modifications for GEOS-5.7.x met fields
01 Mar 2012 - R. Yantosca - Now reference new grid_mod.F90
03 Aug 2012 - R. Yantosca - Move calls to findFreeLUN out of DEVEL block
22 Oct 2013 - C. Keller - Now a HEMCO extension.
22 Jul 2014 - R. Yantosca - Now hardwire the Lesley Ott et al CDF's in
                            lightning_cdf_mod.F90. This avoids having to
                            read an ASCII input in the ESMF environment.
13 Jan 2015 - L. Murray - Add most recent lightning updates to HEMCO version
26 Feb 2015 - R. Yantosca - Restore reading the lightning CDF's from an
                            ASCII file into the PROFILE array. This helps
                            to reduce compilation time.
                         - Added option to define scalar/gridded scale
31 Jul 2015 - C. Keller
                            factors via HEMCO configuration file.
14 Oct 2016 - C. Keller
                          - Now use HCO_EvalFld instead of HCO_GetPtr.
```

02 Dec 2016 - M. Sulprizio- Update WEST\_NS\_DIV from 23d0 to 35d0 (K. Travis)

# 2.12.1 HCOX\_LightNOx\_Run

Subroutine HCOX\_LIGHTNOX\_RUN is the driver routine to calculate lightnox NOx emissions and return them to the HEMCO driver routine.

### **INTERFACE:**

```
SUBROUTINE HCOX_LightNOx_Run( am_I_Root, ExtState, HcoState, RC )
```

# **USES:**

```
USE HCO_FluxArr_Mod, ONLY : HCO_EmisAdd
```

### INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root

TYPE(Ext_State), POINTER :: ExtState ! Module options

TYPE(HCO_State), POINTER :: HcoState ! Hemco options
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

# **REVISION HISTORY:**

```
09 Oct 1997 - R. Yantosca - Initial version
(1 ) Remove IOFF, JOFF from the argument list. Also remove references
      to header files "CMN_03" and "comtrid.h" (bmy, 3/16/00)
(2) Now use allocatable array for ND32 diagnostic (bmy, 3/16/00)
(3) Now reference BXHEIGHT from "dao_mod.f". Updated comments, cosmetic
      changes. Replace LCONVM with the parameter LLCONVM. (bmy, 9/18/02)
(4) Removed obsolete reference to "CMN". Now bundled into
      "lightnox_mod.f" (bmy, 4/14/04)
(5) Renamed from EMLIGHTNOX_NL to EMLIGHTNOX. Now replace GEMISNOX
      (from CMN_NOX) with module variable EMIS_LI_NOx. (ltm, bmy, 10/3/07)
10 Nov 2010 - R. Yantosca - 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 State_Chm
22 Oct 2013 - C. Keller - Now a HEMCO extension.
07 Oct 2013 - C. Keller - Now allow OTD-LIS scale factor to be set
                            externally. Check for transition to Sep 2008.
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 2.12.2 LightNOx

Subroutine LIGHTNOX uses Price & Rind's formulation for computing NOx emission from lightnox (with various updates).

### **INTERFACE:**

```
{\tt SUBROUTINE\ LightNOx(\ am\_I\_Root,\ HcoState,\ ExtState,\ Inst,\ RC\ )}
```

### **USES:**

```
USE HCO_Calc_Mod, ONLY : HCO_EvalFld
USE HCO_EmisList_Mod, ONLY : HCO_GetPtr
USE HCO_GeoTools_Mod, ONLY : HCO_LANDTYPE
USE HCO_Clock_Mod, ONLY : HcoClock_Get
USE HCO_Clock_Mod, ONLY : HcoClock_First
USE HCO_ExtList_Mod, ONLY : GetExtOpt
USE HCO_Types_Mod, ONLY : DiagnCont
```

#### INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root

TYPE(HCO_State), POINTER :: HcoState ! Output obj

TYPE(Ext_State), POINTER :: ExtState ! Module options

TYPE(MyInst ), POINTER :: Inst
```

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

### **REMARKS:**

### **REVISION HISTORY:**

- 10 May 2006 L. Murray Initial version
- (1) Now recompute the cold cloud thickness according to updated formula from Lee Murray. Rearranged argument lists to routines FLASHES\_CTH, FLASHES\_MFLUX, FLASHES\_PRECON. Now call READ\_REGIONAL\_REDIST and READ\_LOCAL\_REDIST. Updated comments accordingly. Now apply FLASH\_SCALE to scale the total lightnox NOx to 6 Tg N/yr. Now apply OTD/LIS regional or local redistribution (cf. B. Sauvage) to the ND56 diagnostic. lightnox redistribution to the ND56 diag. Renamed REGSCALE variable to REDIST. Bug fix: divide A\_M2 by 1d6 to get A\_KM2. (rch, ltm, bmy, 2/14/07)
- (2) Rewritten for separate treatment of LNOx emissions at tropics & midlatitudes (rch, ltm, bmy, 3/27/07)
- (3) Remove path-length algorithm. Renamed from LIGHTNOX\_NL to LIGHTNOX. Other improvements. (ltm, bmy, 9/24/07)
- (4) Remove depreciated options; Update to new Ott et al vertical profiles; Reprocessed for bug in CLDTOPS calculation. See PDF on wiki for full description of changes for v9-01-01. (ltm, bmy, 1/25,11)
- 10 Nov 2010 R. Yantosca Added ProTeX headers
- 09 Nov 2012 M. Payer Replaced all met field arrays with State\_Met derived type object
- 22 Oct 2013 C. Keller Now a HEMCO extension.
- 06 Oct 2014 C. Keller Now calculate pressure centers from edges.
- 16 Jan 2015 R. Yantosca Bug fix: TmpScale should be REAL(dp)
- 11 Mar 2015 C. Keller Now determine LTOP from buoyancy for grid boxes where convection is explicitly resolved. For now, this will only work in an ESMF environment.
- 31 Jul 2015 C. Keller Take into account scalar/gridded scale factors defined in HEMCO configuration file.
- 03 Mar 2016 C. Keller Use buoyancy in combination with convective fraction CNV\_FRC (ESMF only).
- 26 Oct 2016 R. Yantosca Don't nullify local ptrs in declaration stmts

# 2.12.3 LightDist

Subroutine LightDist reads in the CDF used to partition the column lightnox NOx into the GEOS-Chem vertical layers.

### **INTERFACE:**

```
SUBROUTINE LightDist( I, J, LTOP, HO, XLAT, TOTAL, VERTPROF, & ExtState, HcoState, SFCTYPE, cMt, MTYPE, Inst )
```

#### INPUT PARAMETERS:

```
INTENT(IN) :: I
                                        ! Longitude index
INTEGER,
INTEGER,
                INTENT(IN) :: J
                                        ! Latitude index
                INTENT(IN) :: LTOP
                                        ! Level of conv cloud top
INTEGER,
REAL*8,
                INTENT(IN) :: HO
                                        ! Conv cloud top height [m]
REAL*8,
                INTENT(IN) :: XLAT
                                        ! Latitude value [degrees]
                INTENT(IN) :: TOTAL
REAL*8,
                                       ! Column Total # of LNOx molec
TYPE(Ext_State), POINTER :: ExtState ! Module options
TYPE(HCO_State), POINTER :: HcoState ! Hemco state object
INTEGER,
               INTENT(IN) :: SFCTYPE ! Surface type
INTEGER,
                INTENT(IN) :: cMt
                                       ! Current month
TYPE(MyInst),
               POINTER :: Inst
                                       ! Hemco state object
```

# **OUTPUT PARAMETERS:**

REAL\*8, INTENT(OUT) :: VERTPROF(HcoState%NZ) ! Vertical profile INTEGER, INTENT(OUT) :: MTYPE ! lightning type

### **REMARKS:**

#### References:

\_\_\_\_\_\_

- (1 ) Pickering et al., JGR 103, 31,203 31,316, 1998.
- (2) Ott et al., JGR, 2010
- (3) Allen et al., JGR, 2010

- 18 Sep 2002 M. Evans Initial version (based on Yuhang Wang's code)
- (1) Use functions IS\_LAND and IS\_WATER to determine if the given grid box is over land or water. These functions work for all DAO met field data sets. (bmy, 4/2/02)
- (2 ) Renamed M2 to LTOP and THEIGHT to HO for consistency w/ variable names w/in "lightnox.f". Now read the "light\_dist.dat.geos3" file for GEOS-3 directly from the DATA\_DIR/lightnox\_NOx\_200203/ subdirectory. Now read the "light\_dist.dat" file for GEOS-1, GEOS-STRAT directly from the DATA\_DIR/lightnox\_NOx\_200203/ subdirectory. Added descriptive comment header. Now trap I/O errors across all platforms with subroutine "ioerror.f". Updated comments, cosmetic changes. Redimension FRAC(NNLIGHT) to FRAC(LLPAR). (bmy, 4/2/02)
- (3) Deleted obsolete code from April 2002. Now reference IU\_FILE and IOERROR from "file\_mod.f". Now use IU\_FILE instead of IUNIT as the file unit number. (bmy, 6/27/02)
- (4) Now reference BXHEIGHT from "dao\_mod.f" (bmy, 9/18/02)
- (5) Bug fix: add  $GEOS_4$  to the #if block (bmy, 3/4/04)
- (6 ) Now bundled into "lightnox\_mod.f". CDF's are now read w/in routine INIT\_LIGHTNOX to allow parallelization (bmy, 4/14/04)
- (7) Now references DATA\_DIR from "directory\_mod.f" (bmy, 7/20/04)
- (8) Now uses near-land formulation (ltm, bmy, 5/10/06)
- (9) Added extra safety check for pathological boxes (bmy, 12/11/06)

```
(10) Remove the near-land formulation, except for PRECON (ltm, bmy, 9/24/07)
```

```
(11) Now use the Ott et al. [2010] profiles, and apply consistently with GMI model [Allen et al., 2010] (ltm, bmy, 1/25/11).
```

```
10 Nov 2010 - R. Yantosca - Added ProTeX headers
```

```
01 Mar 2012 - R. Yantosca - Now use GET_AREA_CM2(I,J,L) from grid_mod.F90
```

- 15 Jun 2012 Nielsen INQUIRE finds free logical unit number for IU\_FILE
- 09 Nov 2012 M. Payer Replaced all met field arrays with State\_Met derived type object
- 22 Oct 2013 C. Keller Now a HEMCO extension.

#### 2.12.4 Flashes\_CTH

Subroutine Flashes\_CTH determines the rate of lightnox flashes per minute based on the height of convective cloud tops, and the intra-cloud to cloud-ground strike ratio.

## **INTERFACE:**

```
SUBROUTINE Flashes_CTH( I, J, HEIGHT, FLASHRATE, SFCTYPE )
```

#### INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I     ! Longitude index
INTEGER, INTENT(IN) :: J    ! Latitude index
```

REAL\*8, INTENT(IN) :: HEIGHT ! Height of conv cloud top [m]

INTEGER, INTENT(IN) :: SFCTYPE ! Surface type

# **OUTPUT PARAMETERS:**

```
REAL*8, INTENT(OUT) :: FLASHRATE ! LightNOX flash rate [flashes/min]
```

### **REVISION HISTORY:**

- 10 May 2006 L. Murray Initial version
- (1 ) Subroutine renamed from FLASHES (ltm, bmy, 5/10/06)
- (2 ) Remove CCTHICK, IC\_CG\_RATIO as arguments. Remove computation of IC\_CG\_RATIO and move that to GET\_IC\_CG\_RATIO. (ltm, bmy, 12/11/06)
- (3 ) Remove the near-land formulation (i.e. use function IS\_LAND instead of IS\_NEAR).(ltm, bmy, 9/24/07)
- 10 Nov 2010 R. Yantosca Added ProTeX headers
- 22 Oct 2013 C. Keller Now a HEMCO extension.

#### 2.12.5 Get\_IC\_CG\_Ratio

Function Get\_IC\_CG\_Ratio calculates the Intra-Cloud (IC) and Cloud-to-Ground (CG) lightnox flash ratio based on the method of Price and Rind 1993, which is calculated from the cold-cloud depth (CCTHICK).

#### **INTERFACE:**

FUNCTION Get\_IC\_CG\_ratio( CCTHICK ) RESULT( IC\_CG\_RATIO )

### INPUT PARAMETERS:

REAL\*8, INTENT(IN) :: CCTHICK ! Cold cloud thickness [m]

#### RETURN VALUE:

REAL\*8 :: IC\_CG\_RATIO ! Intra-cloud/cloud-ground ratio

#### REVISION HISTORY:

- 11 Dec 2006 R. Yantosca Initial version
- (1 ) Split off from FLASHES\_CTH, FLASHES\_MFLUX, FLASHES\_PRECON into this separate function (ltm, bmy, 12/11/06)
- (2 ) Bug fix for XLF compiler (morin, bmy, 7/8/09)
- 10 Nov 2010 R. Yantosca Added ProTeX headers
- 22 Oct 2013 C. Keller Now a HEMCO extension.

#### 2.12.6 Get\_OTD\_LIS\_Scale

Function GET\_OTD\_LIS\_SCALE returns a met-field dependent scale factor which is to be applied to the lightnox flash rate to bring the annual average flash rate to match that of the OTD-LIS climatology ( 45.9 flashes/sec ). Computed by running the model over the 11-year OTD-LIS campaign window and comparing the average flash rates, or as many years as are available.

### **INTERFACE:**

```
SUBROUTINE Get_OTD_LIS_Scale( am_I_Root, HcoState, BETA, RC )
```

# **USES:**

USE HCO\_Clock\_Mod, ONLY : HcoClock\_Get

#### INPUT PARAMETERS:

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

TYPE(HCO_State), POINTER :: HcoState ! HEMCO state obj

REAL*8, INTENT( OUT) :: BETA ! Scale factor
```

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC ! Suc

- 24 Sep 2007 L. Murray Initial version
- (1 ) Added MFLUX, PRECON scaling for GEOS-4. Also write messages for met field types/grids where scaling is not defined. (ltm, bmy, 11/29/07)
- (2) Now use different divisor for local redist (ltm, bmy, 2/20/08)
- (3 ) Now compute the proper scale factor for GEOS-5 0.5 x 0.666 grids

```
and the GEOS-3 1x1 nested NA grid (yxw, dan, ltm, bmy, 11/14/08)
(4 ) Added "quick fix" for reprocessed GEOS-5 met fields to be used when
      the IN_CLOUD_OD switch is turned on. (ltm, bmy, 2/18/09)
(5 ) Added "quick fix" for 2004, 2005, 2008 OTD/LIS (ltm, bmy, 4/29/09)
(6) Updated scale factors for GEOS-5 based on 4+ years of data. Remove
      temporary fixes. (bmy, 7/10/09)
(7) Modification for GEOS-4 1 x 1.25 grid (lok, ltm, bmy, 1/13/10)
(8) Reprocessed for error in CLDTOPS field; Updated for GEOS
      5.1.0 vs. 5.2.0; MERRA added; (ltm, bmy, 1/25/11)
10 Nov 2010 - R. Yantosca - Added ProTeX headers
02 Feb 2012 - R. Yantosca - Compute BETA for MERRA 2 x 2.5
02 Feb 2012 - R. Yantosca - Compute BETA for GEOS-5.7.x
22 Oct 2013 - C. Keller - Now a HEMCO extension.
04 Nov 2014 - Y. X. Wang - Define BETA, ANN_AVG_FLASHRATE for the
                            GEOS-FP 025x03125 NESTED_CH grid
14 Jan 2015 - L. Murray - Updated GEOS-FP files through Oct 2014
01 Apr 2015 - R. Yantosca - Cosmetic changes
01 Apr 2015 - R. Yantosca - Bug fix: GRID025x0325 should be GRID025x03125
01 Mar 2016 - L. Murray - Add preliminary values for MERRA-2 4x5, NA, CH
19 Jul 2016 - L. Murray - Add preliminary values for MERRA-2 2x2.5
```

# 2.12.7 HCOX\_LightNOx\_Init

Subroutine HCOX\_LIGHTNOX\_INIT allocates all module arrays. It also reads the lightnox CDF data from disk before the first lightnox timestep.

#### **INTERFACE:**

SUBROUTINE HCOX\_LightNOx\_Init( am\_I\_Root, HcoState, ExtName, ExtState, RC )
USES:

```
USE HCO_Chartools_Mod, ONLY : HCO_CharParse
USE HCO_ExtList_Mod, ONLY : GetExtNr
USE HCO_ExtList_Mod, ONLY : GetExtOpt
USE HCO_ExtList_Mod, ONLY : GetExtSpcVal
USE HCO_State_Mod, ONLY : HCO_GetHcoID
USE HCO_State_Mod, ONLY : HCO_GetExtHcoID
USE HCO_ReadList_Mod, ONLY : ReadList_Remove
USE inquireMod, ONLY : findfreeLUN
```

#### INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root

TYPE(HCO_State), POINTER :: HcoState ! Hemco options

CHARACTER(LEN=*), INTENT(IN ) :: ExtName ! Extension name

TYPE(Ext_State), POINTER :: ExtState ! Module options
```

#### **OUTPUT PARAMETERS:**

INTEGER, INTENT( OUT) :: RC

# **REVISION HISTORY:**

- 14 Apr 2004 R. Yantosca Initial version
- (1 ) Now reference DATA\_DIR from "directory\_mod.f"
- (2) Now call GET\_MET\_FIELD\_SCALE to initialize the scale factor for each met field type and grid resolution (bmy, 8/25/05)
- (3) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (4) Now get the box area at 30N for MFLUX, PRECON (1th, bmy, 5/10/06)
- (5) Rename OTDSCALE to OTD\_REG\_REDIST. Also add similar array
  OTD\_LOC\_REDIST. Now call GET\_FLASH\_SCALE\_CTH, GET\_FLASH\_SCALE\_MFLUX,
  GET\_FLASH\_SCALE\_PRECON depending on the type of lightnox param used.
  Updated comments. (ltm, bmy, 1/31/07)
- (6) Removed near-land stuff. Renamed from HCOX\_LightNOX\_Init\_NL to HCOX\_LightNOX\_Init. Now allocate EMIS\_LI\_NOx. (ltm, bmy, 10/3/07)
- (7 ) Also update location of PDF file to lightnox\_NOx\_200709 directory. (bmy, 1/24/08)
- (8) Read in new Ott profiles from lightnox\_NOx\_201101. Remove depreciated options. (ltm, bmy, 1/25/11)
- 10 Nov 2010 R. Yantosca Added ProTeX headers
- 01 Mar 2012 R. Yantosca Removed reference to GET\_YEDGE
- 22 Oct 2013 C. Keller Now a HEMCO extension.
- 26 Feb 2015 R. Yantosca Now re-introduce reading the CDF table from an ASCII file (reduces compilation time)
- 26 Oct 2016 R. Yantosca Don't nullify local ptrs in declaration stmts

# 2.12.8 hcox\_lightnox\_final

Subroutine HCOX\_LIGHTNOX\_FINAL deallocates all module arrays.

## **INTERFACE:**

SUBROUTINE HCOX\_LightNOx\_Final( ExtState )

### INPUT PARAMETERS:

TYPE(Ext\_State), POINTER :: ExtState ! Module options

- 14 Apr 2004 R. Yantosca Initial version
- (1) Now deallocates OTDSCALE (ltm, bmy, 5/10/06)
- (2) Rename OTDSCALE to OTD\_REG\_REDIST. Now deallocate OTD\_LOC\_REDIST. (bmy, 1/31/07)
- (3) Renamed from HCOX\_LightNOX\_Final\_NL to HCOX\_LightNOX\_Final.

  Now deallocate EMIS\_LI\_NOx. (ltm, bmy, 10/3/07)

#### 2.12.9 InstGet

Subroutine InstGet returns a pointer to the desired instance.

# **INTERFACE:**

```
SUBROUTINE InstGet ( Instance, Inst, RC, PrevInst )
```

### INPUT PARAMETERS:

### REVISION HISTORY:

```
18 Feb 2016 - C. Keller - Initial version
```

### 2.12.10 InstCreate

Subroutine InstCreate adds a new instance to the list of instances, assigns a unique instance number to this new instance, and archives this instance number to output argument Instance.

#### **INTERFACE:**

```
SUBROUTINE InstCreate (ExtNr, Instance, Inst, RC)
```

# INPUT PARAMETERS:

INTEGER, INTENT(IN) :: ExtNr

# **OUTPUT PARAMETERS:**

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

```
18 Feb 2016 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

### 2.12.11 InstRemove

Subroutine InstRemove removes an instance from the list of instances.

### **INTERFACE:**

```
SUBROUTINE InstRemove (Instance)
```

### **INPUT PARAMETERS:**

INTEGER :: Instance

#### REVISION HISTORY:

```
18 Feb 2016 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 2.13 Fortran: Module Interface hcox\_megan\_mod.F90

Module HCOX\_Megan\_Mod contains variables and routines specifying the algorithms that control the MEGAN inventory of biogenic emissions (as implemented into the GEOS-Chem model).

This is a HEMCO extension module that uses many of the HEMCO core utilities.

MEGAN calculates gamma activity factor based upon temperature and radiation information from the past. In the original GEOS-Chem code, the initial 10-d averages were explicitly calculated during initialization of MEGAN. This is not feasible in an ESMF environment, and the following restart variables can now be provided through the HEMCO configuration file:

- T\_DAVG: long-term historical temperature
- PARDR\_DAVG: long-term historical direct radiation
- PARDF\_DAVG: long-term historical diffuse radiation
- T\_PREVDAY: short-term historical temperature

These variables are automatically searched for on the first call of the run call. If not defined, default values will be used. The values of T\_DAVG, T\_PREVDAY, PARDR\_DAVG, and PARDF\_DAVG are continuously updated at the end of the run sequence, e.g. they represent the instantaneous running average. The e-folding times to be used when calculating the short=term and long-term running averages are defined as module parameter below (parameter TAU\_HOURS and TAU\_DAYS).

A similar procedure is also applied to the leaf area index variables. The original GEOS-Chem MEGAN code used three LAI variables: current month LAI (LAI\_CM), previous month LAI (LAI\_PM), and instantaneous LAI (LAI), which was a daily interpolation of LAI\_CM and next month' LAI, (LAI\_NM). The HEMCO implementation uses only the instantaneous LAI, assuming it is updated every day. The short term historical LAI is kept in

memory and used to determine the LAI change over time (used to calculate the gamma leaf age). It is also updated on every time step. For the first simulation day, the previous' day LAI is taken from the restart file (field LAI\_PREVDAY). If no restart variable is defined, a LAI change of zero is assumed (ckeller, 10/9/2014).

### !References:

- Guenther, A., et al., The Model of Emissions of Gases and Aerosols from Nature version 2.1 (MEGAN2.1): an extended and updated framework for modeling biogenic emissions, Geosci. Model Dev., 5, 1471-1792, 2012.
- Guenther, A., et al., A global model of natural volatile organic compound emissions, J.Geophys. Res., 100, 8873-8892, 1995.
- Wang, Y., D. J. Jacob, and J. A. Logan, Global simulation of tropospheric O3-Nox-hydrocarbon chemistry: 1. Model formulation, J. Geophys. Res., 103, D9, 10713-10726, 1998.
- Guenther, A., B. Baugh, G. Brasseur, J. Greenberg, P. Harley, L. Klinger, D. Serca, and L. Vierling, *Isoprene emission estimates and uncertanties for the Central African EXPRESSO study domain*, J. Geophys. Res., **104**, 30,625-30,639, 1999.
- Guenther, A. C., T. Pierce, B. Lamb, P. Harley, and R. Fall, Natural emissions of non-methane volatile organic compounds, carbon monoxide, and oxides of nitrogen from North America, Atmos. Environ., 34, 2205-2230, 2000.
- Guenther, A., and C. Wiedinmyer, *User's guide to Model of Emissions of Gases and Aerosols from Nature*. http://cdp.ucar.edu. (Nov. 3, 2004)
- Guenther, A., AEF for methyl butenol, personal commucation. (Nov. 2004)
- Sakulyanontvittaya, T., T. Duhl, C. Wiedinmyer, D. Helmig, S. Matsunaga, M. Potosnak, J. Milford, and A. Guenther, *Monoterpene and sesquiterpene emission estimates for the United States*, Environ. Sci. Technol, **42**, 1623-1629, 2008.

# **INTERFACE:**

MODULE HCOX\_MEGAN\_MOD

## **USES:**

USE HCO\_ERROR\_MOD USE HCO\_DIAGN\_MOD

USE HCOX\_State\_MOD, ONLY : Ext\_State USE HCO\_STATE\_MOD, ONLY : HCO\_STATE

IMPLICIT NONE PRIVATE

# PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCOX\_Megan\_Init
PUBLIC :: HCOX\_Megan\_Run
PUBLIC :: HCOX\_Megan\_Final

### PRIVATE MEMBER FUNCTIONS:

PRIVATE :: GET\_MEGAN\_EMISSIONS ! dbm, new MEGAN driver routine ! for all compounds (6/21/2012)

PRIVATE :: UPDATE\_T\_DAY
PRIVATE :: UPDATE\_T\_15\_AVG
PRIVATE :: GET\_MEGAN\_PARAMS
PRIVATE :: GET\_MEGAN\_AEF

PRIVATE :: GET\_GAMMA\_PAR\_PCEEA

PRIVATE :: GET\_GAMMA\_T\_LI
PRIVATE :: GET\_GAMMA\_T\_LD
PRIVATE :: GET\_GAMMA\_LAI
PRIVATE :: GET\_GAMMA\_AGE
PRIVATE :: GET\_GAMMA\_SM
PRIVATE :: CALC\_NORM\_FAC
PRIVATE :: SOLAR\_ANGLE

PRIVATE :: FILL\_RESTART\_VARS

PRIVATE :: CALC\_AEF

PRIVATE :: GET\_GAMMA\_CO2 ! (Tai, Jan 2013)

- (1) Original code (biogen\_em\_mod.f) by Dorian Abbot (6/2003). Updated to latest algorithm and modified for the standard code by May Fu (11/2004).
- (2 ) All emission are currently calculated using TS from DAO met field. TS is the surface air temperature, which should be carefully distinguished from TSKIN. (tmf, 11/20/2004)
- (3 ) In GEOS4, the TS used here are the T2M in the A3 files, read in 'a3\_read\_mod.f'.
- (4) Bug fix: change #if block to also cover GCAP met fields (bmy, 12/6/05)
- (5) Remove support for GEOS-1 and GEOS-STRAT met fields (bmy, 8/4/06)
- (6) Bug fix: Skip Feb 29th if GCAP in INIT\_MEGAN (phs, 9/18/07)
- (7) Added routine GET\_AEF\_05x0666 to read hi-res AEF data for the GEOS-5 0.5 x 0.666 nested grid simulations (yxw, dan, bmy, 11/6/08)
- 17 Dec 2009 R. Yantosca Added ProTeX headers
- 09 Mar 2010 R. Yantosca Minor bug fix in GET\_EMMONOT\_MEGAN
- 17 Mar 2010 H. Pye AEF\_SPARE must be a scalar local variable in GET\_EMMONOT\_MEGAN for parallelization.
- 20 Aug 2010 R. Yantosca Move CMN\_SIZE to top of module
- 20 Aug 2010 R. Yantosca Now set DAY\_DIM = 24 for MERRA, since the surface temperature is now an hourly field.
- 01 Sep 2010 R. Yantosca Bug fix in INIT\_MEGAN: now only read in NUM\_DAYS (instead of 15) days of sfc temp data
- 22 Nov 2011 R. Yantosca Do not use erroneous AEF's for nested grids
- 06 Dec 2011 E. Fischer Added Acetone emissions
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 01 Mar 2012 R. Yantosca Now reference new grid\_mod.F90

```
01 Mar 2012 - R. Yantosca - Use updated GET_LOCALTIME from time_mod.F
11 Apr 2012 - R. Yantosca - Replace lai_mod.F with modis_lai_mod.F90
13 Aug 2013 - M. Sulprizio- Modifications for updated SOA sim (H. Pye):
                             Add sesquiterpenes to MEGAN group;
                             Add plant functional types (PFT_xx);
                             Rename GET_EMMONOG_MEGAN to GET_EMTERP_MEGAN;
                             Add routines READ_PFT and GET_AEF_GEN
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
05 Oct 2013 - C. Keller
                          - Now a HEMCO extension
04 Aug 2014 - C. Keller
                          - Added 'manual' diagnostics for Acetone.
09 Oct 2014 - C. Keller
                          - Now use only GC_LAI (keep prev. LAI in memory)
22 Dec 2014 - C. Keller
                          - Now use flexible precision (hp) everywhere.
                            Option to read temperature/irradiation from
                            restart.
26 Jan 2015 - M. Sulprizio- Update from D. Millet (19 Jan 2013): Streamlined
                            computations into a single driver routine
                            and updated emissions according to MEGAN 2.1 as
                            described in:
                            Guenther et al., The Model of Emissions of Gases
                            and Aerosols from Nature version 2.1 (MEGAN2.1):
                            an extended and updated framework for modeling
                            biogenic emissions, GMD, 5, 1471-1492, 2012.
12 Feb 2015 - M. Sulprizio- Remove GET_AEF_GEN routine. We now calculate AEFs
                            for FARN, BCAR, and OSQT in CALC_AEF using
                            parameters from Guenther et al., 2012.
18 Feb 2015 - M. Sulprizio- Remove LPECCA logical flag since we use this
                            scheme exclusively now.
                            Restore emissions of individual MEGAN species to
                            diagnostics for consistency with pre-HEMCO code.
10 Jun 2015 - M. Sulprizio- Bug fix for SOA simulation: Now convert AEFs for
                            sesquiterpenes to kg/m2/s.
15 Sep 2015 - M. Sulprizio- Add CO2 inhibition effect on isoprene emissions
                            from Amos Tai (Jan 2013)
05 Nov 2015 - C. Keller
                          - Reorganize restart variables to running averages.
08 Dec 2015 - C. Keller
                          - Now treat previous' day LAI as running avg, too.
14 Oct 2016 - C. Keller
                          - Now use HCO_EvalFld instead of HCO_GetPtr.
```

# 2.13.1 HCOX\_Megan\_Run

Subroutine HCOX\_MEGAN\_Run is the driver routine for the MEGAN model within the new emissions structure. Note that all diagnostics are commented since those are still written as part of the old emission structure.

# **INTERFACE:**

SUBROUTINE HCOX\_Megan\_Run(am\_I\_Root, ExtState, HcoState, RC)

### **USES:**

```
USE HCO_FLUXARR_MOD, ONLY : HCO_EmisAdd

USE HCO_CLOCK_MOD, ONLY : HcoClock_First

USE HCO_CLOCK_MOD, ONLY : HcoClock_Rewind

USE HCO_CLOCK_MOD, ONLY : HcoClock_NewHour

USE HCO_CLOCK_MOD, ONLY : HcoClock_NewDay

USE HCO_Restart_Mod, ONLY : HCO_RestartWrite
```

# INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am\_I\_Root
TYPE(Ext\_State), POINTER :: ExtState
TYPE(HCO\_State), POINTER :: HcoState

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

### **REVISION HISTORY:**

```
05 Aug 2013 - C. Keller
                          - Initial version
08 Oct 2014 - C. Keller
                          - Now use HEMCO clock to get days between months
09 Oct 2014 - C. Keller
                          - Now use only GC_LAI. This makes days between months
                           obsolete
16 Oct 2014 - C. Keller
                         - Initialize flux arrays to avoid float invalid
 9 Mar 2015 - R. Yantosca - Bug fix: add EMIS_ALD2 to $OMP PRIVATE clause
08 May 2015 - C. Keller
                          - Now read/write restart variables from here to
                           accomodate replay runs in GEOS-5.
                          - Now add OCPI flux to BIOGENIC_OCPI diagnostics.
30 Sep 2015 - C. Keller
12 Dec 2015 - C. Keller
                          - Apply e-folding times to past conditions.
07 Jan 2016 - E. Lundgren - Update Avogadro's # to NIST 2014
01 Jun 2016 - R. Yantosca - Bug fix: Now use ExtNrMono in the call to
                           Hco_EmisAdd for the MONX (in order to make MONX
                            show up as nonzero in HEMCO diagnostics).
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

# 2.13.2 Get\_Megan\_Emissions

Subroutine Get\_Megan\_Emissions computes biogenic emissions in units of [kgC/m2/s] or [kg/m2/s] using the MEGAN inventory. (dbm, 12/2012)

### **INTERFACE:**

```
SUBROUTINE GET_MEGAN_EMISSIONS( am_I_Root, HcoState, ExtState, & Inst, I, J, CMPD, MEGAN_EMIS, RC )
```

## INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root
TYPE(HCO_STATE), POINTER :: HcoState
TYPE(Ext_State), POINTER :: ExtState
TYPE(MyInst), POINTER :: Inst
```

#### **OUTPUT PARAMETERS:**

```
REAL(hp), INTENT(OUT) :: MEGAN_EMIS ! VOC emission in kgC/m2/s ! or kg/m2/s, depending on ! units the compound is ! carried in
```

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

#### REMARKS:

References (see above for full citations):

\_\_\_\_\_\_

- (1) Guenther et al, 1995, 1999, 2000, 2004, 2006
- (2) Wang, et al, 1998
- (3) Guenther et al, 2007, MEGAN v2.1 User mannual
- (4 ) Guenther et al, 2012 GMD MEGANv2.1 description and associated code at http://acd.ucar.edu/~guenther/MEGAN/

# **REVISION HISTORY:**

- (1 ) Original code by Dorian Abbot (9/2003). Updated to the latest algorithm and modified for the standard code by May Fu (11/20/04)
- (2 ) All MEGAN biogenic emission are currently calculated using TS from DAO met field. TS is the surface air temperature, which should be carefully distinguished from TSKIN. (tmf, 11/20/04)
- (3) Restructing of function & implementation of activity factors (mpb,2009)
- 17 Dec 2009 R. Yantosca Added ProTeX headers
- 11 Apr 2012 R. Yantosca Now use data from modis\_lai\_mod.F90
- 11 Apr 2012 R. Yantosca Cosmetic changes
- 26 Jan 2015 M. Sulprizio- Update from D. Millet (21 Jun 2012): New driver routine for all MEGAN compounds
- 15 Sep 2015 M. Sulprizio- Add CO2 inhibition effect on isoprene emissions from Amos Tai (Jan 2013)

# 2.13.3 Get\_Megan\_Params

Subroutine Get\_Megan\_Params returns the emission parameters for each MEGAN compound needed to compute emissions. Called from GET\_MEGAN\_EMISSIONS.

#### **INTERFACE:**

```
SUBROUTINE GET_MEGAN_PARAMS( am_I_Root, HcoState, & CPD, BTA, LIDF, C_T1, C_EO, & A_NEW, A_GRO, A_MAT, A_OLD, BI_DIR, & RC )
```

# INPUT PARAMETERS:

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

TYPE(HCO_State), POINTER :: HcoState

CHARACTER(LEN=*), INTENT(IN) :: CPD ! Compound name
```

# INPUT/OUTPUT PARAMETERS:

```
REAL(hp), INTENT(INOUT) :: BTA
                                  ! Beta coefficient for temperature activity
                                  ! factor for light-independent fraction
REAL(hp), INTENT(INOUT) :: LIDF
                                  ! Light-dependent fraction of emissions
REAL(hp), INTENT(INOUT) :: C_T1
                                  ! CT1 parameter for temperature activity
                                  ! factor for light-dependent fraction
REAL(hp), INTENT(INOUT) :: C_EO
                                  ! Ceo parameter for temperature activity
                                  ! factor for light-dependent fraction
REAL(hp), INTENT(INOUT) :: A_NEW ! Relative emission factor (new leaves)
REAL(hp), INTENT(INOUT) :: A_GRO
                                  ! Relative emission factor (growing leaves)
REAL(hp), INTENT(INOUT) :: A_MAT ! Relative emission factor (mature leaves)
REAL(hp), INTENT(INOUT) :: A_OLD ! Relative emission factor (old leaves)
LOGICAL, INTENT(INOUT) :: BI_DIR ! Logical flag to indicate bidirectional exchange
INTEGER, INTENT(INOUT) :: RC
```

# **REMARKS:**

```
References (see above for full citations):
```

(1) Guenther et al, (GMD 2012) and associated MEGANv2.1 source code

#### REVISION HISTORY:

(1) Created by dbm 07/2012

# 2.13.4 Get\_Megan\_AEF

Function Get\_Megan\_AEF returns the appropriate AEF value for a given compound and grid square.

# **INTERFACE:**

SUBROUTINE GET\_MEGAN\_AEF(am\_I\_Root, HcoState, Inst, I, J, CPD, EMFAC, RC)

### INPUT PARAMETERS:

Source File: hcox\_megan\_mod.F, Date: Mon Dec 19 13:47:02 EST 2016 312 LOGICAL, INTENT(IN) :: am\_I\_Root ! Root CPU? TYPE(HCO\_State), POINTER :: HcoState :: Inst TYPE(MyInst), POINTER ! Lon & lat indices INTEGER, INTENT(IN) :: I, J CHARACTER(LEN=\*), INTENT(IN) :: CPD ! Compound name **OUTPUT PARAMETERS:** REAL(hp), INTENT(OUT) :: EMFAC ! MEGAN base emission factor ! (kgC/m2/s or kg/m2/s)! for grid cell (I,J) INPUT/OUTPUT PARAMETERS: INTENT(INOUT) :: RC INTEGER, ! Return code **REMARKS:** References (see above for full citations): \_\_\_\_\_\_ (1) Guenther et al, 2012, MEGANv2.1 source code **REVISION HISTORY:** (1) Created 11/2012 by dbm 2.13.5 Get\_Gamma\_PAR\_PCEEA Computes the PCEEA gamma activity factor with sensitivity to LIGHT. **INTERFACE:** FUNCTION GET\_GAMMA\_PAR\_PCEEA( am\_I\_Root, HcoState, ExtState,

```
FUNCTION GET_GAMMA_PAR_PCEEA( am_I_Root, HcoState, ExtState & Inst, I, J, Q_DIR_2, & Q_DIFF_2, PARDR_AVG_SIM, & PARDF_AVG_SIM) & RESULT( GAMMA_P_PCEEA )
```

### **USES:**

USE HCO\_CLOCK\_MOD, ONLY : HcoClock\_Get, HcoClock\_GetLocal

# INPUT PARAMETERS:

```
LOGICAL,
                 INTENT(IN) :: am_I_Root
TYPE(HCO_State), POINTER
                          :: HcoState
TYPE(Ext_State), POINTER
                            :: ExtState
TYPE(MyInst), POINTER
                           :: Inst
INTEGER,
                 INTENT(IN) :: I, J
                                                   ! Lon & lat indices
               INTENT(IN) :: PARDR_AVG_SIM
INTENT(IN) :: PARDF_AVG_SIM
INTENT(IN) :: Q_DIR_2
REAL(sp),
                                                   ! Avg direct PAR [W/m2]
                                                   ! Avg diffuse PAR [W/m2]
REAL(sp),
                                                   ! Direct PAR [umol/m2/s]
REAL(hp),
REAL(hp),
                INTENT(IN) :: Q_DIFF_2
                                                 ! Diffuse PAR [umol/m2/s]
```

# RETURN VALUE:

REAL(hp) :: GAMMA\_P\_PCEEA ! GAMMA factor for light

### **REMARKS:**

References (see above for full citations):

\_\_\_\_\_

- (1) Guenther et al, 2006
- (2) Guenther et al, 2007, MEGAN v2.1 user guide

### **REVISION HISTORY:**

- (1) Here PAR\*\_AVG\_SIM is the average light conditions over the simulation period. I've set this = 10 days to be consistent with temperature & as outlined in Guenther et al, 2006. (mpb, 2009)
- (2 ) Code was taken & adapted directly from the MEGAN v2.1 source code. (mpb,2009)
- 17 Dec 2009 R. Yantosca Added ProTeX headers
- 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

# 2.13.6 Solar\_Angle

Function SOLAR\_ANGLE computes the local solar angle for a given day of year, latitude and longitude (or local time). Called from routine Get\_Gamma\_P\_Pecca.

# **INTERFACE:**

```
FUNCTION SOLAR_ANGLE( HcoState, Inst, DOY, SHOUR, LAT )
& RESULT(SINbeta)
```

### INPUT PARAMETERS:

```
! Arguments
```

```
TYPE(HCO_State), POINTER :: HcoState
TYPE(MyInst), POINTER :: Inst
```

# RETURN VALUE:

```
REAL(hp) :: SINbeta ! Sin of the local solar angle
```

### **REMARKS:**

```
References (see above for full citations):
```

- (1) Guenther et al, 2006
- (2) Guenther et al, MEGAN v2.1 user mannual 2007-09

# **REVISION HISTORY:**

(1 ) This code was taken directly from the MEGAN v2.1 source code.(mpb,2009) 17 Dec 2009 - R. Yantosca - Added ProTeX headers

#### 2.13.7 Get\_Gamma\_T\_LI

Function Get\_Gamma\_T\_LI computes the temperature activity factor (GAMMA\_T\_LI) for the light-independent fraction of emissions

#### **INTERFACE:**

```
FUNCTION GET_GAMMA_T_LI( T, BETA ) RESULT( GAMMA_T_LI )
```

#### INPUT PARAMETERS:

```
! Current leaf temperature, the surface air temperature field (TS) ! is assumed equivalent to the leaf temperature over forests. 
 \mbox{REAL(hp), INTENT(IN)} :: \mbox{T}
```

```
! Temperature factor per species REAL(hp), INTENT(IN) :: BETA
```

# RETURN VALUE:

```
! Activity factor for the light-independent fraction of emissions \texttt{REAL}(\texttt{hp}) :: \texttt{GAMMA\_T\_LI}
```

# **REMARKS:**

References (see above for full citations):

\_\_\_\_\_\_

- (1) Guenther et al, 2006
- (2) Guenther et al, MEGAN user mannual 2007-08
- (3) Guenther et al., GMD 2012 and MEGANv2.1 source code.

```
(1 ) Original code by Michael Barkley (2009).
   Note: If T = Ts (i.e. standard conditions) then GAMMA_T = 1
17 Dec 2009 - R. Yantosca - Added ProTeX headers
(2 ) Modified to GAMMA_T_LI (dbm, 6/21/2012)
```

### 2.13.8 Get\_Gamma\_T\_LD

Function Get\_Gamma\_T\_LD computes the temperature sensitivity for the light-dependent fraction of emissions.

#### INTERFACE:

```
FUNCTION GET_GAMMA_T_LD( T, PT_15, PT_1, CT1, CE0 )
& RESULT( GAMMA_T_LD )
```

#### INPUT PARAMETERS:

```
! Current leaf temperature [K], the surface air temperature field (TS)
! is assumed equivalent to the leaf temperature over forests.
REAL(hp), INTENT(IN) :: T

! Average leaf temperature over the past 15 days
REAL(sp), INTENT(IN) :: PT_15

! Average leaf temperature over the past arbitray day(s).
! This is not used at present
REAL(sp), INTENT(IN) :: PT_1

! Compound-specific parameters for light-dependent temperature activity
! factor (dbm, 6/21/2012)
REAL(hp), INTENT(IN) :: CT1, CEO
```

## RETURN VALUE:

```
! Temperature activity factor for the light-dependent fraction of ! emissions  \mbox{REAL(hp)} \qquad :: \mbox{GAMMA\_T\_LD}
```

#### **REMARKS:**

References (see above for full citations):

- (1) Guenther et al, 1995
- (2) Guenther et al, 2006
- (3) Guenther et al, MEGAN v2.1 user mannual 2007-08
- (4) Guenther et al., GMD 2012 and MEGANv2.1 source code.

- (1 ) Includes the latest MEGAN v2.1 temperature algorithm (mpb, 2009). Note, this temp-dependence is the same for the PCEEA & hybrid models.
- 17 Dec 2009 R. Yantosca Added ProTeX headers
- (2) Modified to gamma\_t\_ld and to permit compound specific parameters CT1 and Ceo (dbm, 6/21/2012)
- 07 Jan 2016 Update ideal gas constant to NIST 2014 value

### 2.13.9 Get\_Gamma\_Lai

Function Get\_Gamma\_Lai computes the gamma exchange activity factor which is sensitive to leaf area (= GAMMA\_LAI).

#### **INTERFACE:**

```
FUNCTION GET_GAMMA_LAI( CMLAI, BIDIREXCH ) RESULT( GAMMA_LAI )
```

#### INPUT PARAMETERS:

### RETURN VALUE:

```
REAL(hp) :: GAMMA_LAI
```

#### **REMARKS:**

References (see above for full citations):

(1) Guenther et al, 2006

- (2) Guenther et al, MEGAN user mannual 2007-08
- (3) Guenther et al., GMD 2012 and MEGANv2.1 source code.

### REVISION HISTORY:

- (1 ) Original code by Dorian Abbot (9/2003). Modified for the standard code by May Fu (11/2004)
- (2 ) Update to publically released (as of 11/2004) MEGAN algorithm and modified for the standard code by May Fu (11/2004).
- (3) Algorithm is based on the latest MEGAN v2.1 User's Guide (mpb,2009)
- (4) Updated to treat bidirectional exchange compounds appropriately (dbm, 6/2012)
- 17 Dec 2009 R. Yantosca Added ProTeX headers

# 2.13.10 Get\_Gamma\_Age

Function Get\_Gamma\_Age computes the gamma exchange activity factor which is sensitive to leaf age (= Gamma\_Age).

### **INTERFACE:**

```
FUNCTION GET_GAMMA_AGE( CMLAI, PMLAI, DBTWN, TT, & AN, AG, AM, AO) & RESULT( GAMMA_AGE )
```

#### INPUT PARAMETERS:

```
REAL(hp), INTENT(IN) :: CMLAI ! Current month's LAI [cm2/cm2]
REAL(hp), INTENT(IN) :: PMLAI ! Previous months LAI [cm2/cm2]
REAL(hp), INTENT(IN) :: DBTWN ! Number of days between
REAL(sp), INTENT(IN) :: TT ! Daily average temperature [K]
REAL(hp), INTENT(IN) :: AN ! Relative emiss factor (new leaves)
REAL(hp), INTENT(IN) :: AG ! Relative emiss factor (growing leaves)
REAL(hp), INTENT(IN) :: AM ! Relative emiss factor (mature leaves)
REAL(hp), INTENT(IN) :: AO ! Relative emiss factor (old leaves)
```

### RETURN VALUE:

REAL(hp) :: GAMMA\_AGE ! Activity factor

### **REMARKS:**

References (see above for full citations):

\_\_\_\_\_\_

- (1) Guenther et al, 2006
- (2) Guenther et al, MEGAN user mannual 2007-08
- (3) Guenther et al., GMD 2012 and MEGANv2.1 source code

### **REVISION HISTORY:**

- (1) Original code by Dorian Abbot (9/2003). Modified for the standard code by May Fu (11/2004)
- (2) Update to publically released (as of 11/2004) MEGAN algorithm and modified for the standard code by May Fu (11/2004).
- (3) Algorithm is based on the latest User's Guide (tmf, 11/19/04)
- (4) Renamed & now includes specific relative emission activity factors for each BVOC based on MEGAN v2.1 algorithm (mpb,2008)
- (5 ) Now calculate TI (number of days after budbreak required to induce iso. em.) and TM (number of days after budbreak required to reach peak iso. em. rates) using the daily average temperature, instead of using fixed values (mpb,2008)
  NOTE: Can create 20% increases in tropics (Guenther et al 2006)
- (6 ) Implemented change for the calculation of FGRO if ( CMLAI > PMLAI ), i.e. if LAI has increased with time, and used new values for all foilage fractions if ( CMLAI = PMLAI ). Also removed TG variable as not now needed. (mpb,2000)
- (7) Updated to pass leaf age activity factors as arguments (dbm, 6/2012)
- 17 Dec 2009 R. Yantosca Added ProTeX headers
- 13 Aug 2013 M. Sulprizio- Updated for sesquiterpenes (H. Pye)

## 2.13.11 get\_gamma\_sm

Function GET\_GAMMA\_SM computes activity factor for soil moisture

#### INTERFACE:

```
FUNCTION GET_GAMMA_SM( ExtState, I, J, CMPD )
& RESULT( GAMMA_SM )
```

### **INPUT PARAMETERS:**

TYPE(Ext\_State), POINTER :: ExtState

INTEGER, INTENT(IN) :: I, J ! GEOS-Chem lon & lat indices CHARACTER(LEN=\*), INTENT(IN) :: CMPD ! Compound name (dbm, 6/21/2012)

#### RETURN VALUE:

REAL(hp) :: GAMMA\_SM ! Activity factor

# **REMARKS:**

References (see above for full citations):

\_\_\_\_\_\_

- (1) Guenther et al, ACP 2006
- (2) Guenther et al., GMD 2012 and MEGANv2.1 source code

#### **REVISION HISTORY:**

(1) Created by dbm (6/2012). We are not currently using a soil moisture effect for isoprene. For all compounds other than acetaldehyde and ethanol, gamma\_sm =1 presently.

16 Apr 2015 - C. Keller - Now restrict GWETROOT to values between 0.0 and 1.0. This only seems to be a problem within the GEOS-5 ESM, where GWETROOT values over the ocean become 1e+15 (= missing value).

12 Aug 2015 - R. Yantosca - Extend #ifdef for MERRA2 meteorology

\_\_\_\_\_

BOC

# LOCAL VARIABLES:

```
! By default gamma_sm is 1.0 GAMMA_SM = 1.0_hp
```

REAL(hp) :: GWETROOT

```
! GWETROOT is only defined for GEOS-5 #if defined( GEOS_5 ) || defined( GEOS_FP ) || defined( MERRA ) || defined( MERRA2 )
```

```
!GWETROOT = ExtState%GWETROOT%Arr%Val(I,J)
! Error trap: GWETROOT must be between 0.0 and 1.0 (ckeller, 4/16/15)
```

```
GWETROOT = MIN(MAX(ExtState%GWETROOT%Arr%Val(I, J), 0.0_hp), 1.0_hp)
      IF ( TRIM( CMPD ) == 'ALD2' .OR. TRIM ( CMPD ) == 'ETOH' ) THEN
         ! GWETROOT = degree of saturation or wetness in the root-zone
         ! (top meter of soil). This is defined as the ratio of the volumetric
         ! soil moisture to the porosity. We use a soil moisture activity factor
         ! for ALD2 to account for stimulation of emission by flooding.
         ! (Millet et al., ACP 2010)
         ! Constant value of 1.0 for GWETROOT = 0-0.9, increasing linearly to
         ! 3.0 at GWETROOT =1.
         GAMMA\_SM = MAX(20.0\_hp * GWETROOT - 17.0\_hp, 1.0\_hp)
      ENDIF
#endif
      ! return to calling program
      END FUNCTION GET_GAMMA_SM
 EOC
                 Harvard-NASA Emissions Component (HEMCO)
\mbox{}\hrulefill\
 \subsubsection [get\_gamma\_co2] {get\_gamma\_co2}
 Function GET\_GAMMA\_CO2 computes the CO2 activity factor
   associated with CO2 inhibition of isoprene emission. Called from
   GET\_MEGAN\_EMISSIONS only.
 //
 \\{\bf INTERFACE:}
                    FUNCTION GET_GAMMA_CO2( CO2a ) RESULT( GAMMA_CO2 )
\begin{verbatim}
INPUT PARAMETERS:
      REAL(hp), INTENT(IN) :: CO2a ! Atmospheric CO2 conc [ppmv]
RETURN VALUE:
      REAL(hp)
                 :: GAMMA_CO2 ! CO2 activity factor [unitless]
LOCAL VARIABLES:
      REAL(hp)
                 :: CO2i ! Intercellular CO2 conc [ppmv]
```

```
REAL(hp)
                    :: ISMAXi
                                 ! Asymptote for intercellular CO2
REAL(hp)
                    :: HEXPi
                                 ! Exponent for intercellular CO2
                   :: CSTARi
REAL(hp)
                                 ! Scaling coef for intercellular CO2
REAL(hp)
                                ! Asymptote for atmospheric CO2
                   :: ISMAXa
REAL(hp)
                                 ! Exponent for atmospheric CO2
                   :: HEXPa
REAL(hp)
                   :: CSTARa
                                ! Scaling coef for atmospheric CO2
LOGICAL
                   :: LPOSSELL ! Use Possell & Hewitt (2011)?
                    :: LWILKINSON ! Use Wilkinson et al. (2009)?
LOGICAL
```

### **REMARKS:**

#### References:

\_\_\_\_\_

- (1) Heald, C. L., Wilkinson, M. J., Monson, R. K., Alo, C. A., Wang, G. L., and Guenther, A.: Response of isoprene emission to ambient co(2) changes and implications for global budgets, Global Change Biology, 15, 1127-1140, 2009.
- (2) Wilkinson, M. J., Monson, R. K., Trahan, N., Lee, S., Brown, E., Jackson, R. B., Polley, H. W., Fay, P. A., and Fall, R.: Leaf isoprene emission rate as a function of atmospheric CO2 concentration, Global Change Biology, 15, 1189-1200, 2009.
- (3) Possell, M., and Hewitt, C. N.: Isoprene emissions from plants are mediated by atmospheric co2 concentrations, Global Change Biology, 17, 1595-1610, 2011.

#### **REVISION HISTORY:**

- (1 ) Implemented in the standard code by A. Tai (Jun 2012).
- 15 Sep 2015 M. Sulprizio- Implemented into hcox\_megan\_mod.F

#### 2.13.12 CALC NORM FAC

Function CALC\_NORM\_FAC calculates the normalization factor needed to compute emissions. Called from GET\_MEGAN\_EMISSIONS.

### **INTERFACE:**

SUBROUTINE CALC\_NORM\_FAC( am\_I\_Root, Inst, RC )

### INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am\_I\_Root TYPE(MyInst), POINTER :: Inst

!INPUT/OUTPUT PARAMETERS

INTEGER, INTENT(INOUT) :: RC

### **REMARKS:**

References (see above for full citations):

\_\_\_\_\_\_

(1) Guenther et al, (GMD 2012) and associated MEGANv2.1 source code

#### REVISION HISTORY:

(1) Created by dbm 11/2012. We calculate only 1 normalization factor for all compounds based on the isoprene gamma values. Formally there should be a different normalization factor for each compound, but we are following Alex Guenther's approach here and the MEGAN source code. "Hi Dylan, sorry for being so slow to get back to you. Since the change is only a few percent or less, I didn't bother to assign a different normalization factor to each compound. Since the MEGAN canopy environment model also has 8 different canopy types (tropical broadleaf tree, conifer tree, etc.) then to be correct we should have a different CCE for each canopy type for each compound class (which would be 160 slightly different values of CCE)." 07 Jan 2016 - E. Lundgren - Update ideal gas constant to NIST 2014 value

## 2.13.13 Fill\_Restart\_Vars

Subroutine FILL\_RESTART\_VARS fills the megan restart variables.

## **INTERFACE:**

```
SUBROUTINE FILL_RESTART_VARS( am_I_Root, HcoState,
                              ExtState, Inst, RC )
```

### **USES:**

#### INPUT PARAMETERS:

```
LOGICAL.
                INTENT(IN
                            ) :: am_I_Root
TYPE(HCO_State), POINTER
                              :: HcoState
TYPE(Ext_State), POINTER
                              :: ExtState
TYPE(MyInst), POINTER
                               :: Inst
```

# INPUT/OUTPUT PARAMETERS:

INTENT(INOUT) :: RC INTEGER,

```
19 Dec 2014 - C. Keller - Initial version
09 Mar 2015 - C. Keller - Now use HCO_RestartGet to fill restarts
```

# 2.13.14 **CALC\_AEF**

Subroutine CALC\_AEF reads Emission Factors for all biogenic VOC species from disk.

### **INTERFACE:**

SUBROUTINE CALC\_AEF( am\_I\_Root, HcoState, ExtState, Inst, RC )

### **USES:**

! References to F90 modules

USE HCO\_EMISLIST\_MOD, ONLY : HCO\_GetPtr
USE HCO\_CALC\_MOD, ONLY : HCO\_EvalFld

#### INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am\_I\_Root
TYPE(Ext\_State), POINTER :: ExtState
TYPE(HCO\_State), POINTER :: HcoState
TYPE(MyInst), POINTER :: Inst

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

#### **REMARKS:**

Reference: (5) Guenther et al, 2004

- (1 ) Original code by Dorian Abbot (9/2003). Modified for the standard code by May Fu (11/2004)
- (2 ) AEF detailed in the latest MEGAN User's Guide (tmf, 11/19/04)
- (3) Bug fix (tmf, 11/30/04)
- (4) Now reads 1x1 files and regrids to current resolution (bmy, 10/24/05)
- (5) Uses new v2.1 emission factors maps for isoprene, MBO and 7 monoterpene species, download in 2009. (mpb,2009)
- (6) Now use 2.1 emission factors for isoprene, MBO, and 7 monoterpenes. EFs for other compounds are computed by reading in the PFT fractions and multiplying the fractions by corresponding EF values. (dbm, 11/2012)
- (7) Also, now read in the EF values already gridded to model resolution. (dbm, 11/2012)
- 17 Dec 2009 R. Yantosca Added ProTeX headers
- 10 Jun 2015 M. Sulprizio- Bug fix: Now convert sesquiterpenes (FARN, BCAR, OSQT) from ug compound/m2/h to kg C/m2/s

# 2.13.15 HCOX\_Megan\_Init

Subroutine HCOX\_Megan\_Init allocates and initializes all module arrays.

### **INTERFACE:**

```
SUBROUTINE HCOX_Megan_Init( am_I_Root, HcoState, ExtName, & ExtState, RC )
```

### **USES:**

```
USE HCO_STATE_MOD, ONLY : Hco_GetHcoID

USE HCO_STATE_MOD, ONLY : HCO_GetExtHcoID

USE HCO_ExtList_Mod, ONLY : GetExtNr, GetExtOpt

USE HCO_Restart_Mod, ONLY : HCO_RestartDefine
```

## INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
TYPE(HCO_State), POINTER :: HcoState
CHARACTER(LEN=*), INTENT(IN ) :: ExtName
TYPE(Ext_State), POINTER :: ExtState
```

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

- (1) Change the logic in the #if block for G4AHEAD. (bmy, 12/6/05)
  (2) Bug fix: skip Feb 29th if GCAP (phs, 9/18/07)
  (3) Now call GET\_AEF\_05x0666 for GEOS-5 nested grids (yxw,dan,bmy, 11/6/08)
  17 Dec 2009 R. Yantosca Added ProTeX headers
- 26 Aug 2010 R. Yantosca Now reference merra\_a1\_mod.f
- 01 Sep 2010 R. Yantosca Now read in NUM\_DAYS of sfc temp data (this had been hardwired to 15 days previously)
- 07 Feb 2011 R. Yantosca Fix typos: make sure to zero out the proper  $PARDF_*$  and  $PARDR_*$  arrays after allocation
- 22 Nov 2011 R. Yantosca Do not use erroneous AEF's for nested grids
- 08 Feb 2012 R. Yantosca Now read surface temperature for GEOS-5.7.x
- 28 Feb 2012 R. Yantosca Removed support for GEOS-3
- 11 Apr 2012 R. Yantosca Now remove the call to INIT\_LAI; we shall initialize the LAI arrays from main.F
- 03 Aug 2012 R. Yantosca Move calls to findFreeLUN out of DEVEL block
- 11 Apr 2013 R. Yantosca Now pass directory info with Input\_Opt
- 18 Feb 2015 M. Sulprizio- Now allocate AEF arrays for species not read from file
- 26 Oct 2016 R. Yantosca Don't nullify local ptrs in declaration stmts

# 2.13.16 HCOX\_Megan\_Final

Subroutine HCOX\_Megan\_Final deallocates all allocated arrays at the end of a GEOS-Chem model run.

#### **INTERFACE:**

```
SUBROUTINE HCOX_MEGAN_FINAL ( am_I_Root, HcoState, ExtState, RC ) !USES
```

### INPUT PARAMETERS:

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

TYPE(HCO_State), POINTER :: HcoState ! HEMCO State obj

TYPE(Ext_State), POINTER :: ExtState ! Extension State obj
```

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

# **REVISION HISTORY:**

```
17 Dec 2009 - R. Yantosca - Added ProTeX headers
16 Aug 2013 - C. Keller - Now a HEMCO extension
18 Feb 2015 - M. Sulprizio - Added AEF arrays
09 Mar 2015 - C. Keller - Write variables to internal state in ESMF mode
```

## 2.13.17 InstGet

Subroutine InstGet returns a pointer to the desired instance.

#### **INTERFACE:**

```
SUBROUTINE InstGet (Instance, Inst, RC, PrevInst)
```

### INPUT PARAMETERS:

```
18 Feb 2016 - C. Keller - Initial version
```

#### 2.13.18 InstCreate

Subroutine InstCreate adds a new instance to the list of instances, assigns a unique instance number to this new instance, and archives this instance number to output argument Instance.

#### **INTERFACE:**

```
SUBROUTINE InstCreate (ExtNr, Instance, Inst, RC)
```

#### INPUT PARAMETERS:

### **OUTPUT PARAMETERS:**

INTEGER, INTENT( OUT) :: Instance TYPE(MyInst), POINTER :: Inst

### INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

### **REVISION HISTORY:**

```
18 Feb 2016 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

#### 2.13.19 InstRemove

Subroutine InstRemove removes an instance from the list of instances.

### INTERFACE:

```
SUBROUTINE InstRemove (Instance)
```

#### INPUT PARAMETERS:

INTEGER :: Instance

#### REVISION HISTORY:

18 Feb 2016 - C. Keller - Initial version

### 2.14 Fortran: Module Interface hcox\_paranox\_mod.F90

Module HCOX\_PARANOX\_MOD contains routines to compute ship emissions and associated concentrations of NO, NO2, HNO3 and O3 from NO ship emission data. This follows the implementation of the PARANOX ship plume model in GEOS-Chem.

This module calculates production rates of NO, NO2, HNO3, and O3, as well as loss rates of

O3 and HNO3. All fluxes are in kg species/m2/s. The O3 and HNO3 loss fluxes are not converted to a deposition velocity, but rather saved out as mass fluxes (kg/m2/s) into diagnostics 'PARANOX\_O3\_DEPOSITION\_FLUX' and 'PARANOX\_HNO3\_DEPOSITION\_FLUX' respectively. In order to use them, they must be imported explicitly via routine Diagn\_Get (from module hco\_diagn\_mod.F90). This approach avoids problems with uncrealistically high loss rates for loss ambient air concentrations of O3 or HNO3.

The PARANOx look-up-table can be provided in netCDF or ASCII (txt) format. The latter is particularly useful for running PARANOx in an ESMF environment, where 7-dimensional netCDF files are currently not supported. The input data format can be specified in the HEMCO configuration file (in the PARANOx extensions section). The txt-files can be generated from the previously read netCDF data using subroutine WRITE\_LUT\_TXTFILE.

#### References:

 Vinken, G. C. M., Boersma, K. F., Jacob, D. J., and Meijer, E. W.: Accounting for non-linear chemistry of ship plumes in the GEOS-Chem global chemistry transport model, Atmos. Chem. Phys., 11, 11707-11722, doi:10.5194/acp-11-11707-2011, 2011.

The initial look up tables (LUT) distributed with GEOS-Chem v9-01-03 used 7 input variables: Temperature, J(NO2), J(O1D), solar elevation angles at emission time and 5 hours later, and ambient concentrations of NOx and O3. This version was documented by Vinken et al. (2011). Subsequently, we added wind speed as an input variable. We also use J(OH) rather than J(O1D) to index the LUT (C. Holmes, 6 May 2013)

The LUTs contain 3 quantities: FracNOx: The fraction of NOx emitted from ships that remains as NOx after 5 hours of plume aging. mol/mol OPE: Ozone production efficiency, mol(O3)/mol(HNO3) The net production of O3 per mole of ship NOx oxidized over 5 hours of plume aging. Can be negative! Defined as OPE = [ P(O3) - L(O3) ] / P(HNO3), where each P and L term is an integral over 5 hours. Net O3 production in the plume is E(NOx) \* (1-FracNOx) \* OPE, where E(NOx) is the emission rate of NOx from the ship (e.g. units: mol/s). MOE: Methane oxidation efficiency, mol(CH4)/mol(NOx) The net oxidation of CH4 per mole of NOx emitted from ships over 5 hours of plume aging. Defined as MOE = E(EH4) / E(ENOx).

The solar elevation angles 5 hours ago are calculated using HEMCO subroutine HCO\_GetSUNCOS. This is the same routine that is used to calculate the solar zenith angles for the current time.

#### **INTERFACE:**

```
MODULE HCOX_ParaNOx_MOD
```

#### **USES:**

```
USE HCO_Error_MOD

USE HCO_Diagn_MOD

USE HCO_State_MOD, ONLY: HCO_State

USE HCOX_State_MOD, ONLY: Ext_State

IMPLICIT NONE

PRIVATE
```

### PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCOX\_ParaNOx\_Run
PUBLIC :: HCOX\_ParaNOx\_Init
PUBLIC :: HCOX\_ParaNOx\_Final

### PRIVATE MEMBER FUNCTIONS:

#### **REMARKS:**

Adapted from the code in GeosCore/paranox\_mod.F prior to GEOS-Chem v10-01.

#### **REVISION HISTORY:**

| 06  | Aug | 2013 | - | C. | Keller    | - | Initial version   |
|-----|-----|------|---|----|-----------|---|---|
| 03  | Jun | 2013 | _ | C. | Holmes    | - | Rewritten to include wind speed in the look-up            |
|     |     |      |   |    |           |   | table and to take input from netCDF                       |
| 15  | Oct | 2013 | _ | C. | Keller    | - | Now a HEMCO extension                                     |
| 06  | Jun | 2014 | - | R. | Yantosca  | - | Cosmetic changes in ProTeX headers                        |
| 06  | Jun | 2014 | - | R. | Yantosca  | - | Now indended with F90 free-format                         |
| 25  | Jun | 2014 | - | R. | Yantosca  | - | Now pass the look-up-table filenames                      |
| 15  | Jul | 2014 | - | C. | Holmes    | - | Make module variables allocatable, since they             |
|     |     |      |   |    |           |   | are used only in full chemistry simulations.              |
| 22  | Jul | 2014 | - | R. | Yantosca  | - | Added shadow copy of FAST-JX function FJXFUNC             |
| 28  | Jul | 2014 | - | C. | Keller    | - | Now pass J-Values through ExtState. This makes            |
|     |     |      |   |    |           |   | the FJXFUNC shadow copy obsolete                          |
| 13  | Aug | 2014 | - | C. | Keller    | - | Added manual diagnostics                                  |
| 16  | Oct | 2014 | - | C. | Keller    | - | Now store SUNCOSmid values internally over the            |
|     |     |      |   |    |           |   | past 5 hours and use these values for ${\tt SUNCOSmid5}.$ |
|     |     |      |   |    |           |   | This is required for standalone mode.                     |
| 05  | Feb | 2015 | - | C. | Keller    | - | Modified to bring in the updates from Chris               |
|     |     |      |   |    |           |   | Holmes (input data in netCDF format, include              |
|     |     |      |   |    |           |   | wind speed, calculated dry deposition freq.               |
|     |     |      |   |    |           |   | using whole troposheric column mass).                     |
| 23  | Feb | 2015 | - | C. | Keller    | - | Historic j-values can now be provided through             |
|     |     |      |   |    |           |   | HEMCO configuration file.                                 |
| 10  | Apr | 2015 | - | C. | Keller    | - | Now exchange deposition fluxes via diagnostics.           |
|     |     |      |   |    |           |   | Keep units of kg/m2/s for loss rates.                     |
| 20  | Apr | 2016 | - | Μ. | Sulprizio | - | Get J(OH) directly from FAST-JX and remove all            |
|     |     |      |   |    |           |   | references to J(O1D). In FlexChem, adjustment of          |
|     |     |      |   |    |           |   | photolysis rates are now done in routine                  |
| 4.0 | 0 . | 0046 |   | ~  | 77 7 7    |   | PHOTRATE_ADJ (found in GeosCore/fast_jx_mod.F).           |
| 14  | Uct | 2016 | - | C. | Keller    | _ | Now use HCO_EvalFld instead of HCO_GetPtr.                |

# 2.14.1 HCOX\_ParaNOx\_Run

Subroutine HCOX\_ParaNOx\_Run is the driver routine to calculate ship NOx emissions for the current time step. Emissions in [kg/m2/s] are added to the emissions array of the passed

#### **INTERFACE:**

```
SUBROUTINE HCOX_ParaNOx_Run( am_I_Root, ExtState, HcoState, RC )
```

### **USES:**

```
USE HCO_Calc_Mod, ONLY : HCO_CalcEmis
```

#### INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root ! Are we on the root CPU? TYPE(Ext_State), POINTER :: ExtState ! External data fields
```

### INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO State object INTEGER, INTENT(INOUT) :: RC ! Success or failure?
```

#### **REVISION HISTORY:**

```
06 Aug 2013 - C. Keller - Initial Version
06 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
06 Jun 2014 - R. Yantosca - Now indended with F90 free-format
28 Jul 2014 - C. Keller - Now call Hco_CalcEmis instead of Hco_Run.
```

### 2.14.2 Evolve\_Plume

Subroutine EVOLVE\_PLUME performs plume dilution and chemistry of ship NO emissions for every grid box and writes the resulting NO, HNO3 and O3 emission (production) rates into State\_Chm

#### **INTERFACE:**

```
SUBROUTINE Evolve_Plume( am_I_Root, ExtState, ShipNoEmis, HcoState, RC )
```

#### **USES:**

```
USE HCO_Types_Mod, ONLY : DiagnCont
USE HCO_FluxArr_mod, ONLY : HCO_EmisAdd
USE HCO_FluxArr_mod, ONLY : HCO_DepvAdd
USE HCO_Clock_Mod, ONLY : HcoClock_First
USE HCO_Restart_Mod, ONLY : HCO_RestartGet
USE HCO_Restart_Mod, ONLY : HCO_RestartWrite
USE HCO_Calc_Mod, ONLY : HCO_CheckDepv
USE HCO_GeoTools_Mod, ONLY : HCO_GetSUNCOS
```

### INPUT PARAMETERS:

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

TYPE(Ext_State), POINTER :: ExtState ! External data
```

### INPUT/OUTPUT PARAMETERS:

```
REAL(hp), INTENT(INOUT) :: ShipNoEmis(:,:,:) ! Emissions
TYPE(HCO_State), POINTER :: HcoState ! HEMCO State obj
INTEGER, INTENT(INOUT) :: RC ! Success or failure
```

#### **REVISION HISTORY:**

```
06 Aug 2013 - C. Keller - Initial Version
06 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
06 Jun 2014 - R. Yantosca - Now indended with F90 free-format
24 Jun 2014 - R. Yantosca - Now pass LUT_FILENAME to READ_PARANOX_LUT
22 Jul 2014 - R. Yantosca - Comment out debug print statements
28 Jul 2014 - C. Keller - Now get J-values through ExtState
12 Aug 2014 - R. Yantosca - READ_PARANOX_LUT is now called from Init phase
10 Nov 2014 - C. Keller - Added div-zero error trap for 03 deposition.
25 Nov 2014 - C. Keller - Now convert NO fluxes to HNO3 and O3 using
                           corresponding molecular weight ratios. Safe
                           division check for O3 deposition calculation.
                         - Now read/write restart variables from here to
08 May 2015 - C. Keller
                           accomodate replay runs in GEOS-5.
25 May 2015 - C. Keller
                         - Now calculate SC5 via HCO_GetSUNCOS
29 Mar 2016 - C. Keller - Bug fix: archive O3 deposition as positive flux.
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

#### 2.14.3 HCOX\_ParaNOx\_Init

Subroutine HcoX\_ParaNOx\_Init initializes the HEMCO PARANOX extension.

#### **INTERFACE:**

```
SUBROUTINE HCOX_ParaNOx_Init( am_I_Root, HcoState, ExtName, ExtState, RC )
```

### **USES:**

```
USE HCO_Chartools_Mod, ONLY : HCO_CharParse
USE HCO_State_MOD, ONLY : HCO_GetHcoID
USE HCO_State_MOD, ONLY : HCO_GetExtHcoID
USE HCO_ExtList_Mod, ONLY : GetExtNr
USE HCO_ExtList_Mod, ONLY : GetExtOpt
USE HCO_Restart_Mod, ONLY : HCO_RestartDefine
USE ParaNOx_Util_Mod, ONLY : Read_ParaNOx_LUT
```

#### INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
CHARACTER(LEN=*), INTENT(IN ) :: ExtName ! Extension name
TYPE(Ext_State), POINTER :: ExtState ! Module options
```

## INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! HEMCO state object INTEGER, INTENT(INOUT) :: RC ! Success or failure?
```

### **REVISION HISTORY:**

```
06 Aug 2013 - C. Keller - Initial Version
06 Jun 2014 - R. Yantosca - Cosmetic changes in ProTex Headers
06 Jun 2014 - R. Yantosca - Now indented using F90 free-format
13 Aug 2014 - R. Yantosca - Now read the PARANOX look-up tables here
14 Aug 2014 - R. Yantosca - Minor fix, read the PARANOX look-up tables
after displaying text about PARANOX extension
16 Oct 2014 - C. Keller - Added error check after READ_PARANOX_LUT
17 Oct 2014 - C. Keller - Now parse input files via HCO_CharParse
17 Apr 2015 - C. Keller - Now assign PARANOX_SUNCOS1 to SC5(:,:,1), etc.
25 May 2015 - C. Keller - Now calculate SC5 via HCO_GetSUNCOS
```

#### 2.14.4 HCOX\_ParaNOx\_Final

Subroutine HcoX\_ParaNox\_Final finalizes the HEMCO PARANOX extension.

### **INTERFACE:**

```
SUBROUTINE HCOX_ParaNOx_Final( am_I_Root, HcoState, RC )
```

#### **USES:**

#### INPUT PARAMETERS:

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

TYPE(HCO_State), POINTER :: HcoState ! HEMCO State obj
```

### INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

#### REVISION HISTORY:

```
06 Aug 2013 - C. Keller - Initial Version
06 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
06 Jun 2014 - R. Yantosca - Now indended with F90 free-format
```

# ${\bf 2.14.5} \quad {\bf read\_paranox\_lut\_nc}$

Subroutine READ\_PARANOX\_LUT\_NC reads look-up tables in netCDF format for use in the PARANOX ship plume model (G.C.M. Vinken)

### **INTERFACE:**

```
SUBROUTINE READ_PARANOX_LUT_NC ( am_I_Root, HcoState, RC )
```

#### **USES:**

```
!INPUT ARGUMENTS:
LOGICAL, INTENT(IN ) :: am_I_Root
```

TYPE(HCO\_State), POINTER :: HcoState ! HEMCO State object

!INPUT/OUTPUT ARGUMENTS: INTEGER, INTENT(INOUT) :: RC

#### **REVISION HISTORY:**

```
06 Feb 2012 - M. Payer - Initial version modified from code provided by G.C.M. Vinken

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

03 Jun 2013 - C. Holmes - Rewritten to include wind speed in the look-up table and to take input from netCDF
```

#### 2.14.6 read\_lut\_ncfile

Subroutine READ\_LUT\_NCFILE reads look up tables for use in the PARANOX ship plume model (C. Holmes)

### **INTERFACE:**

```
SUBROUTINE READ_LUT_NCFILE( am_I_Root, HcoState, FILENAME, FNOX, DNOx, OPE, MOE, & T, JNO2, O3, SEAO, SEA5, JRATIO, NOX)
```

#### **USES:**

```
! 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
TYPE(HCO_State), POINTER :: HcoState ! HEMCO State object
CHARACTER(LEN=*), INTENT(IN) :: FILENAME
```

#### **OUTPUT PARAMETERS:**

```
REAL*4, INTENT(OUT), DIMENSION(:,:,:,:,:) :: FNOX,OPE,MOE,DNOx REAL*4, INTENT(OUT), OPTIONAL :: T(:), JNO2(:), O3(:) REAL*4, INTENT(OUT), OPTIONAL :: SEAO(:), SEA5(:) REAL*4, INTENT(OUT), OPTIONAL :: JRATIO(:), NOX(:)
```

### **REVISION HISTORY:**

```
06 Feb 2012 - M. Payer - Initial version modified from code provided by G.C.M. Vinken

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

03 Jun 2013 - C. Holmes - Rewritten to include wind speed in the look-up table and to take input from netCDF
```

### 2.14.7 read\_paranox\_lut\_txt

Subroutine READ\_PARANOX\_LUT\_TXT reads look-up tables in txt format for use in the PARANOX ship plume model (G.C.M. Vinken)

### **INTERFACE:**

```
SUBROUTINE READ_PARANOX_LUT_TXT ( am_I_Root, HcoState, RC )
```

#### **USES:**

```
!INPUT ARGUMENTS:
```

```
LOGICAL, INTENT(IN ) :: am_I_Root
```

TYPE(HCO\_State), POINTER :: HcoState ! HEMCO State object

!INPUT/OUTPUT ARGUMENTS:
INTEGER, INTENT(INOUT) :: RC

#### **REVISION HISTORY:**

```
05 Feb 2015 - C. Keller - Initial version modified from code provided by G.C.M. Vinken and C. Holmes
```

### 2.14.8 read\_lut\_txtfile

Subroutine READ\_LUT\_TXTFILE reads look up tables for use in the PARANOX ship plume model (C. Holmes)

#### INTERFACE:

```
SUBROUTINE READ_LUT_TXTFILE( am_I_Root, HcoState, FILENAME, FNOX, DNOx, OPE, MOE, RC, & T, JNO2, O3, SEAO, SEA5, JRATIO, NOX )
```

### **USES:**

```
USE inquireMod, ONLY : findFreeLUN
```

### INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root
```

TYPE(HCO\_State), POINTER :: HcoState ! HEMCO State object

CHARACTER(LEN=\*),INTENT(IN) :: FILENAME

### INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

#### **OUTPUT PARAMETERS:**

```
REAL*4, INTENT(OUT), TARGET, DIMENSION(:,:,:,:,:):: FNOX,OPE,MOE,DNOx
REAL*4, INTENT(OUT), OPTIONAL:: T(:), JNO2(:), O3(:)
REAL*4, INTENT(OUT), OPTIONAL:: SEAO(:), SEA5(:)
REAL*4, INTENT(OUT), OPTIONAL:: JRATIO(:), NOX(:)
```

#### REVISION HISTORY:

05 Feb 2015 - C. Keller - Initial version modified from code provided by G.C.M. Vinken and C. Holmes

### 2.14.9 write\_lut\_txtfile

write\_lut\_txtfile

#### **INTERFACE:**

```
SUBROUTINE WRITE_LUT_TXTFILE( am_I_Root, HcoState, FILENAME, FNOX, DNOx, OPE, MOE, RC, & T, JNO2, O3, SEAO, SEA5, JRATIO, NOX)
```

#### **USES:**

USE inquireMod, ONLY : findFreeLUN

#### **INPUT PARAMETERS:**

```
LOGICAL, INTENT(IN) :: am_I_Root

TYPE(HCO_State), INTENT(INOUT) :: HcoState ! HEMCO state obj

CHARACTER(LEN=*), INTENT(IN) :: FILENAME
```

### INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

### **OUTPUT PARAMETERS:**

```
REAL*4, INTENT(IN), TARGET, DIMENSION(:,:,:,:,:) :: FNOX,OPE,MOE,DNOx REAL*4, INTENT(IN), OPTIONAL :: T(:), JNO2(:), O3(:) REAL*4, INTENT(IN), OPTIONAL :: SEAO(:), SEA5(:) REAL*4, INTENT(IN), OPTIONAL :: JRATIO(:), NOX(:)
```

```
05 Feb 2015 - C. Keller - Initial version modified from code provided by G.C.M. Vinken and C. Holmes
```

### 2.14.10 INTERPOL\_LINWEIGHTS

Subroutine INTERPOL\_LINWEIGHTS finds the array elements and weights for piecewise 1-D linear interpolation. The input array of NODES must be in monotonic ascending order. (C. Holmes 3/27/2014)

If Y is an array containing values of a function evaluated at the points given in NODES, then its interpolated value at the point VALUESIN will be Y(VALUEIN) = Y(INDICES(1))\* WEIGHTS(1) + Y(INDICES(2)) \* WEIGHTS(2)

This subroutine finds indices of consecutive nodes that bracket VALUEIN and weights such that VALUEIN = NODES(INDICES(1)) \* WEIGHTS(1) + NODES(INDICES(1)+1) \* (1-WEIGHTS(1))

For convenience, the returned values of INDICES and WEIGHTS are 2-element arrays, where INDICES(2) = INDICES(1)+1 and WEIGHTS(2) = 1 - WEIGHTS(1)

#### **INTERFACE:**

```
SUBROUTINE INTERPOL_LINWEIGHTS( NODES, VALUEIN, INDICES, WEIGHTS)

USES:
```

### INPUT PARAMETERS:

```
REAL*4, INTENT(IN) :: NODES(:), VALUEIN
```

#### **OUTPUT PARAMETERS:**

```
! These arrays are always 2 elements each, but declaring ! as deferred shape avoids array temporaries INTEGER,INTENT(OUT) :: INDICES(:) REAL*4, INTENT(OUT) :: WEIGHTS(:)
```

#### **REVISION HISTORY:**

```
03 Jun 2013 - C. Holmes - Initial version
```

#### 2.14.11 paranox\_lut

Subroutine PARANOX.LUT returns fractional remainder of ship NOx (FNOx), fraction of NOx that dry deposits as NOy species (DNOx), ozone production efficiency (OPE), and methane oxidation efficiency (MOE) after 5-hrs of plume aging. Values are taken taken from a lookup table using piecewise linear interpolation. The look-up table is derived from the PARANOx gaussian plume model (Vinken et al. 2011; Holmes et al. 2014) (G.C.M. Vinken, KNMI, June 2010; C. Holmes June 2013)

The lookup table uses 8 input variables: TEMP : model temperature, K JNO2 : J(NO2) value, 1/s O3 : concentration O3 in ambient air, ppb SEA0 : solar elevation angle at emission time 5 hours ago, degree SEA5 : solar elevation angle at this time, degree JRatio : ratio J(OH)/J(NO2), unitless NOx : concentration NOx in ambient air, ppt WS : wind speed, m/s

In GEOS-Chem v9-01-03 through v9-02, the effects of wind speed on FNOx and OPE were not included (wind speed set at 6 m/s). The JRatio also used J(O1D) rather than J(OH); this has only a small effect on interpolated values. To reproduce the behavior of these earlier versions, modify code below marked with \*\*\*\*\*\*\* and call READ\_PARANOX\_LUT\_v913 in emissions\_mod.F

#### **INTERFACE:**

```
SUBROUTINE PARANOX_LUT( am_I_Root, ExtState, HcoState, & I, J, RC, FNOX, DNOx, OPE, MOE_OUT)
```

#### **USES:**

USE HCO\_STATE\_MOD, ONLY : HCO\_State
USE HCOX\_STATE\_MOD, ONLY : Ext\_State

#### INPUT PARAMETERS:

LOGICAL, INTENT(IN) :: am\_I\_Root
TYPE(Ext\_State), POINTER :: ExtState
TYPE(HCO\_State), POINTER :: HcoState

INTEGER, INTENT(IN) :: I, J ! Grid indices

#### **OUTPUT PARAMETERS:**

```
REAL*8, INTENT(OUT) :: FNOX ! fraction of NOx remaining, mol/mol REAL*8, INTENT(OUT) :: DNOX ! fraction of NOx deposited, mol/mol REAL*8, INTENT(OUT) :: OPE ! net OPE, mol(net P(O3))/mol(P(HNO3)) REAL*8, INTENT(OUT), OPTIONAL :: MOE_OUT ! net MOE, mol(L(CH4))/mol(E(NOx))
```

### INPUT/OUTPUT PARAMETERS:

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

```
Jun 2010 - G.C.M. Vinken - Initial version
03 Jun 2013 - C. Holmes
                            - Heavily modified and simplified from previous
                              LUT interpolation code by G.C.M. Vinken and
                              M. Payer. LUT now includes wind speed.
04 Feb 2015 - C. Keller
                            - Updated for use in HEMCO.
24 Sep 2015 - E. Lundgren
                            - ExtState vars 03, NO2, and NO now in
                              kg/kg dry air (previously kg)
07 Jan 2016 - E. Lundgren
                            - Update H2O molec wt to match GC value
20 Apr 2016 - M. Sulprizio
                            - Remove calculation of J(OH). We now get J(OH),
                              the effective rate for O3+hv(+H2O)->OH+OH,
                              directly from FAST-JX. In FlexChem, adjustment
                              of the photolysis rates are done in routine
                              PHOTRATE_ADJ (found in GeosCore/fast_jx_mod.F).
                            - Replace non-standard ASIND function with ASIN,
20 Sep 2016 - R. Yantosca
                              and convert to degrees (divide by PI/180)
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

### 2.15 Fortran: Module Interface hcox\_seaflux\_mod.F90

Module HCOX\_SeaFlux\_Mod contains routines to calculate the oceanic emissions of a number of defined species. The oceanic flux is parameterized according to Liss and Slater, 1974: F = Kg \* (Cair - H Cwater) where F is the net flux, Kg is the exchange velocity, Cair and Cwater are the air and aqueous concentrations, respectively, and H is the dimensionless air over water Henry constant.

This module calculates the source and sink terms separately. The source is given as flux, the sink as deposition rate: source = Kg \* H \* Cwater [kg m-2 s-1] sink = Kg / DEPHEIGHT [s-1]

The deposition rate is obtained by dividing the exchange velocity Kg by the deposition height DEPHEIGHT, e.g. the height over which deposition occurs. This can be either the first grid box only, or the entire planetary boundary layer. The HEMCO option 'PBL\_DRYDEP' determines which option is being used.

Kg is calculated following Johnson, 2010, which is largely based on the work of Nightingale et al., 2000a/b. The salinity and seawater pH are currently set to constant global values of 35 ppt and 8.0, respectively. Since Kg is only little sensitive to these variables, this should not introduce a notable error.

This is a HEMCO extension module that uses many of the HEMCO core utilities.

Air-sea exchange is calculated for all species defined during extension initialization. For each species, the following parameter must be specified: species name, model species ID (i.e. ID of this species in the external model), parameterization type of Schmidt number in water, liquid molar volume of species, and the name of the field containing species seawater concentrations. See initialization routine for more details. To add new species to this module, the abovementioned arrays have to be extended accordingly.

#### References:

- Johnson, M.: A numerical scheme to calculate temperature and salinity dependent air-water transfer velocities for any gas, Ocean Science, 6, 2010.
- Liss and Slater: Flux of gases across the air-sea interface, Nature, 247, 1974.
- Nightingale et al.: In situ evaluation of air-sea gas exchange parameterizations using novel conservative and volatile tracers, Global Biogeochemical Cycles, 14, 2000a.
- Nightingale et al.: Measurements of air-sea gas transfer during an open ocean algal bloom, Geophys. Res. Lett., 27, 2000b.
- Saltzman et al.: Experimental determination of the diffusion coefficient of dimethylsulfide in water, J. Geophys. Res., 98, 1993.

#### **INTERFACE:**

MODULE HCOX\_SeaFlux\_Mod

### **USES:**

```
USE HCO_Error_MOD
USE HCO_Diagn_MOD
USE HCO_State_MOD, ONLY: HCO_State
USE HCOX_State_MOD, ONLY: Ext_State
IMPLICIT NONE
PRIVATE
```

#### PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCOX\_SeaFlux\_Init
PUBLIC :: HCOX\_SeaFlux\_Run
PUBLIC :: HCOX\_SeaFlux\_Final

#### PRIVATE MEMBER FUNCTIONS:

PRIVATE :: Calc\_SeaFlux

#### REVISION HISTORY:

```
16 Apr 2013 - C. Keller - Initial version

01 Oct 2013 - C. Keller - Now a HEMCO extension module

11 Dec 2013 - C. Keller - Now define container name during initialization

01 Jul 2014 - R. Yantosca - Now use F90 free-format indentation

01 Jul 2014 - R. Yantosca - Cosmetic changes in ProTeX headers

06 Nov 2015 - C. Keller - Now use land type definitions instead of FRCLND

14 Oct 2016 - C. Keller - Now use HCO_EvalFld instead of HCO_GetPtr.
```

### 2.15.1 HCOX\_SeaFlux\_Run

Subroutine  $HcoX_SeaFlux_Run$  is the run routine to calculate oceanic emissions for the current time step.

#### **INTERFACE:**

```
SUBROUTINE HCOX_SeaFlux_Run( am_I_Root, ExtState, HcoState, RC )
```

### **USES:**

```
USE HCO_FLUXARR_MOD, ONLY : HCO_EmisAdd
USE HCO_FLUXARR_MOD, ONLY : HCO_DepvAdd
USE HCO_CALC_MOD, ONLY : HCO_EvalFld
USE HCO_EMISLIST_MOD, ONLY : HCO_GetPtr
```

#### INPUT PARAMETERS:

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

TYPE(HCO_State), POINTER :: HcoState ! Output obj

TYPE(Ext_State), POINTER :: ExtState ! Module options
```

# INPUT/OUTPUT PARAMETERS:

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

#### **REVISION HISTORY:**

```
16 Apr 2013 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

### 2.15.2 Calc SeaFlux

Subroutine CALC\_SEAFLUX calculates oceanic emissions of the specified tracer using the parameterization described in Johnson, 2010.

The net emission flux is given by F = -Kg (  $Cg - Caq^*H$  ). Here, we calculate the source term ( Kg \* H \* Caq ) in units of kg/m2/s as well as the deposition velocity Kg in m/s.

### **INTERFACE:**

```
SUBROUTINE Calc_SeaFlux( am_I_Root, HcoState, ExtState, & SOURCE, SINK, SeaConc, & OcID, HcoID, RC )
```

#### USES:

```
USE Ocean_ToolBox_Mod, ONLY : CALC_KG
USE Henry_Mod, ONLY : CALC_KH, CALC_HEFF
USE HCO_CALC_MOD, ONLY : HCO_CheckDepv
USE HCO_GeoTools_Mod, ONLY : HCO_LANDTYPE
```

### INPUT PARAMETERS:

```
) :: am_I_Root
                                                ! root CPU?
LOGICAL,
               INTENT(IN
                                                ! ocean species ID
INTEGER,
               INTENT(IN
                          ) :: OcID
INTEGER,
                                                ! HEMCO species ID
              INTENT(IN ) :: HcoID
TYPE(HCO_State), POINTER
                          :: HcoState
                                                ! Output obj
TYPE(Ext_State), POINTER
                         :: ExtState
```

#### **OUTPUT PARAMETERS:**

```
REAL(hp), INTENT( OUT) :: SOURCE(HcoState%NX,HcoState%NY) REAL(hp), INTENT( OUT) :: SINK (HcoState%NX,HcoState%NY)
```

### INPUT/OUTPUT PARAMETERS:

```
REAL(hp), INTENT(INOUT) :: SeaConc(HcoState%NX,HcoState%NY)
INTEGER, INTENT(INOUT) :: RC ! Error stat
```

### **REMARKS:**

For now, the salinity and pH of seawater are prescribed to 35ppt and 8.0, respectively. The oceanic flux is not expected to be sensitive to these parameters (which have only little variations anyway), but we may use climatologies for these parameter at some point nevertheless!

#### **REVISION HISTORY:**

```
16 Apr 2013 - C. Keller
                          - Initial version
15 Aug 2014 - C. Keller
                          - Now restrict calculations to temperatures above
                            10 deg C.
03 Oct 2014 - C. Keller
                          - Added surface temperature limit of 45 degrees C
                            to avoid negative Schmidt numbers.
                          - Now use skin temperature instead of air temperature
07 Oct 2014 - C. Keller
06 Mar 2015 - C. Keller
                          - Now calculate deposition rate over entire PBL.
14 Oct 2015 - R. Yantosca - Pulled variables MW, VB, SCW out of the parallel
                            loop.
                          - Now use HCO_LANDTYPE instead of FRCLND
06 Nov 2015 - C. Keller
```

#### 2.15.3 HCOX\_SeaFlux\_Init

Subroutine HCOX\_SeaFlux\_Init initializes all module variables, including all species - specific parameter such as the liquid molar volume (Vb), the parameterization type for the Schmidt number in water (SCWPAR) and the name of the field containing oceanic concentrations.

LiqVol is the liquid molar volume [cm3/mol]. If not stated otherwise, it is calculated using the Schroeder additive method as described in Johnson, 2010. Note that experimental values for LiqVol should be used if available!

Table 3 of Johnson, 2010: Schroeder additive method for calculating Vb. For all atoms/structural items a molecule contains, the sum of the incre- ments will give the molar volume. e.g. CH2=CH2 contains 2 car- bon atoms, 4 hydrogen atoms and 1 double bond so the Schroeder Vb is 2x7 + 4x7 + 7 = 49cm3mol-1. \* applies to all kinds of cyclic features and is applied only once to ring-containing compounds irrespective of the number of rings present.

- Atom/feature Increment/cm3mole-1
- Carbon 7.0
- Hydrogen 7.0
- Oxygen 7.0
- Nitrogen 7.0
- Bromine 31.5
- Chlorine 24.5
- Fluorine 10.5
- Iodine 38.5
- Sulfur 21.0
- Ring\* -7.0

- Double bond 7.0
- Triple bond 14.0

SCWPAR denotes which parameterization will be used to calculate the Schmidt number in water (in ocean\_toolbox\_mod). The following parameterizations are currently supported:

- 1. Parameterization as in Johnson, 2010 (default).
- 2. Parameterization for DMS according to Saltzman et al., 1993.
- 3. Parameterization for Acetone as in former acetone\_mod.F in GC.

The oceanic surface concentrations of all species are obtained from external fields. These field names are specified in array OcDataName. For now, we obtain these concentrations from netCDF-files through the HEMCO core module, i.e. for each species there need to be a corresponding seawater concentration data file specified in the HEMCO configuration file. Once we use a coupled (ESMF) system, these names may be used to refer to the names of the concentration fields imported from the ocean model component.

#### **INTERFACE:**

```
SUBROUTINE HCOX_SeaFlux_Init( am_I_Root, HcoState, ExtName, ExtState, RC )
USES:
```

```
USE HCO_ExtList_Mod, ONLY : GetExtNr
USE HCO_STATE_MOD, ONLY : HCO_GetExtHcoID
```

#### **INPUT PARAMETERS:**

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

TYPE(HCO_State), POINTER :: HcoState ! Hemco State obj.

CHARACTER(LEN=*), INTENT(IN ) :: ExtName ! Extension name

TYPE(Ext_State), POINTER :: ExtState ! Ext. obj.
```

#### INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC ! Return status
```

### **REVISION HISTORY:**

```
16 Apr 2013 - C. Keller - Initial version
```

#### 2.15.4 HCOX\_SeaFlux\_Final

Subroutine HCOX\_SeaFlux\_Final deallocates all module arrays.

#### **INTERFACE:**

```
SUBROUTINE HCOX_SeaFlux_Final()
```

```
16 Apr 2013 - C. Keller - Initial version
```

#### 2.16 Fortran: Module Interface hcox\_seasalt\_mod.F90

Module HCOX\_SeaSalt\_Mod contains routines to calculate sea salt aerosol emissions, following the implementation in GEOS-Chem. Emission number densities of the fine and coarse mode sea salt aerosols are written into diagnostic containers 'SEASALT\_DENS\_FINE' and 'SEASALT\_DENS\_COARSE', respectively.

This is a HEMCO extension module that uses many of the HEMCO core utilities.

#### **INTERFACE:**

```
MODULE HCOX_SeaSalt_Mod
```

#### **USES:**

```
USE HCO_Error_Mod
USE HCO_Diagn_Mod
USE HCO_State_Mod, ONLY : HCO_State
USE HCOX_State_Mod, ONLY : Ext_State
IMPLICIT NONE
PRIVATE
```

#### PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: HCOX_SeaSalt_Init
PUBLIC :: HCOX_SeaSalt_Run
PUBLIC :: HCOX_SeaSalt_Final
```

### PRIVATE MEMBER FUNCTIONS:

```
PRIVATE :: EMIT_SSABr2
```

#### **REVISION HISTORY:**

```
15 Dec 2013 - C. Keller - Now a HEMCO extension module
09 Jul 2014 - R. Yantosca - Now use F90 free-format indentation
09 Jul 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
09 Jul 2015 - E. Lundgren - Add marine organoc aerosols (B.Gantt, M.Johnson)
```

#### 2.16.1 HCOX\_SeaSalt\_Run

Subroutine HcoX\_SeaSalt\_Run is the driver run routine to calculate SeaSalt emissions in HEMCO.

### **INTERFACE:**

```
SUBROUTINE HCOX_SeaSalt_Run( am_I_Root, ExtState, HcoState, RC )
```

### **USES:**

USE HCO\_FluxArr\_Mod, ONLY : HCO\_EmisAdd
USE HCO\_GeoTools\_Mod, ONLY : HCO\_LANDTYPE

#### INPUT PARAMETERS:

LOGICAL, INTENT(IN ) :: am\_I\_Root ! root CPU?

TYPE(HCO\_State), POINTER :: HcoState ! Output obj

TYPE(Ext\_State), POINTER :: ExtState ! Module options

### INPUT/OUTPUT PARAMETERS:

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

#### **REMARKS:**

#### 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.
- (3) Gong, S. L., "A parameterization of sea-salt aerosol source function for sub- and super-micron particles", Global Biogeochem. Cy., 17(4), 1097, doi:10.1029/2003GB002079, 2003.
- (4) Jaegle, L., P.K. Quinn, T.S. Bates, B. Alexander, J.-T. Lin, "Global distribution of sea salt aerosols: New constraints from in situ and remote sensing observations", Atmos. Chem. Phys., 11, 3137-3157, doi:10.5194/acp-11-3137-2011.

- (1 ) Now references SALA\_RREDGE\_um and SALC\_RREDGE\_um from "tracer\_mod.f" (bmy, 7/20/04)
- (2) Now references GET\_FRAC\_OF\_PBL and GET\_PBL\_TOP\_L from "pbl\_mix\_mod.f".

  Removed reference to header file CMN. Removed reference to

  "pressure\_mod.f". (bmy, 2/22/05)
- (3 ) Now also compute alkalinity and number density of SeaSalt emissions. (bec, bmy, 4/13/05)
- (4) Now references XNUMOL & XNUMOLAIR from "tracer\_mod.f" (bmy, 10/25/05)
- (5) The source function is for wet aerosol radius (RH=80%, with a radius twice the size of dry aerosols) so BETHA should be set to 2 instead of 1. Also now use LOG10 instead of LOG in the expressions for the SeaSalt base source, since we need the logarithm to the base 10. (jaegle, bec, bmy, 11/23/09)
- (6) Update to use the Gong (2003) source function (jaegle 5/11/11)
- (7) Apply an empirical sea surface temperature dependence to Gong (2003) (jaegle 5/11/11)
- 22 Dec 2011 M. Payer 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
15 Dec 2013 - C. Keller - Now a HEMCO extension
09 Jul 2015 - E. Lundgren - Add marine organic aerosols (B.Gantt, M.Johnson)
19 Oct 2015 - C. Keller - Now pass I and J index to EMIT_SSABr2 to support
curvilinear grids.
22 Oct 2015 - E. Lundgren - Bug fix: include CHLR in OMP PRIVATE statement
```

#### 2.16.2 HCOX\_SeaSalt\_Init

Subroutine HcoX\_SeaSalt\_Init initializes all extension variables.

#### INTERFACE:

```
SUBROUTINE HCOX_SeaSalt_Init( am_I_Root, HcoState, ExtName, ExtState, RC )
```

# **USES:**

```
USE HCO_State_Mod, ONLY : HCO_GetHcoID

USE HCO_STATE_MOD, ONLY : HCO_GetExtHcoID

USE HCO_ExtList Mod ONLY : GetExtNr
```

USE HCO\_ExtList\_Mod, ONLY : GetExtNr USE HCO\_ExtList\_Mod, ONLY : GetExtOpt

#### INPUT PARAMETERS:

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

TYPE(HCO\_State), POINTER :: HcoState ! HEMCO state object CHARACTER(LEN=\*), INTENT(IN ) :: ExtName ! Extension name TYPE(Ext\_State), POINTER :: ExtState ! Options object

### INPUT/OUTPUT PARAMETERS:

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

### **REVISION HISTORY:**

#### 2.16.3 HCOX\_SeaSalt\_Final

Subroutine HcoX\_SeaSalt\_Final deallocates all module arrays.

#### INTERFACE:

SUBROUTINE HCOX\_SeaSalt\_Final

#### **REVISION HISTORY:**

15 Dec 2013 - C. Keller - Initial version

### 2.16.4 Emit\_SsaBr2

Subroutine Emit\_SsaBr2 calculates aerosol emissions of Br2.

#### **INTERFACE:**

```
SUBROUTINE Emit_SsaBr2( am_I_Root, ExtState, HcoState, ilon, & ilat, rmid, p_kgsalt, br2_emiss_kg, RC )
!USE:
USE HCO_Clock_Mod, ONLY: HcoClock_Get
```

#### INPUT PARAMETERS:

```
INTENT(IN
                            ) :: am_I_Root ! root CPU?
LOGICAL.
TYPE(Ext_State), POINTER
                               :: ExtState ! Module options
TYPE(HCO_State), POINTER
                               :: HcoState ! Output obj
INTEGER,
                INTENT(IN)
                               :: ilon
                                          ! Grid longitude index
INTEGER,
                INTENT(IN)
                               :: ilat
                                           ! Grid latitude index
                                          ! Dry radius of aerosol
REAL*8,
                INTENT(IN)
                              :: rmid
                              :: p_kgsalt ! SeaSalt aerosol production [kgNaCl]
REAL*8,
                INTENT(IN)
```

### **OUTPUT PARAMETERS:**

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

REAL*8, INTENT(OUT) :: br2_emiss_kg ! Br2 emissions [kg NaCl]
```

### **REMARKS:**

#### References:

\_\_\_\_\_\_

- (1) Parrella, J. P., Jacob, D. J., Liang, Q., Zhang, Y., Mickley, L. J., Miller, B., Evans, M. J., Yang, X., Pyle, J. A., Theys, N., and Van Roozendael, M.: Tropospheric bromine chemistry: implications for present and pre-industrial ozone and mercury, Atmos. Chem. Phys., 12, 6723-6740, doi:10.5194/acp-12-6723-2012, 2012.
- (2) Yang, X., Cox, R. A., Warwick, N. J., Pyle, J. A., Carver, G. D., O'Connor, F. M., and Savage, N. H.: Tropospheric bromine chemistry and its impacts on ozone: A model study, J. Geophys. Res., 110, D23311, doi:10.1029/2005JD006244, 2005.
- (2) Yang, X., Pyle, J. A., and Cox, R. A.: Sea salt aerosol production and bromine release: Role of snow on sea ice, Geophys. Res. Lett., 35, L16815, doi:10.1029/2008GL034536, 2008.

```
02 Mar 2010 - J. Parrella - Initial version

22 May 2012 - M. Payer - Added ProTeX headers

08 Aug 2012 - M. Payer - Modified for size-dependent depletion factors from Yang et al. (2008)

07 Aug 2013 - C. Keller - Moved to SeaSalt_mod.F

15 Dec 2013 - C. Keller - Now a HEMCO extension

19 Oct 2015 - C. Keller - Now use lon and lat index to work on curvilinear grids.
```

#### 2.17 Fortran: Module Interface hcox\_soilnox\_mod.F90

Module HCOX\_SoilNOx\_Mod contains routines to compute soil NOx emissions. We follow the implementation in GEOS-Chem by Hudman et al 2012.

#### **INTERFACE:**

MODULE HCOX\_SoilNOx\_Mod

#### **USES:**

```
USE HCO_ERROR_Mod
USE HCO_CHARTOOLS_MOD
USE HCO_DIAGN_Mod
USE HCOX_TOOLS_MOD
USE HCOX_State_Mod, ONLY : Ext_State
USE HCO_STATE_Mod, ONLY : HCO_State

IMPLICIT NONE
PRIVATE
```

### PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCOX\_SoilNOx\_Run
PUBLIC :: HCOX\_SoilNOx\_Init
PUBLIC :: HCOX\_SoilNOx\_Final

#### **REMARKS:**

This is a HEMCO extension module that uses many of the HEMCO core utilities.

```
Original codes from:

HARVARD ATMOSPHERIC CHEMISTRY MODELING GROUP

MODULE FOR SOIL NOX EMISSIONS

by Yuhang Wang, Gerry Gardner, and Prof. Daniel Jacob

Updated model code:

by Rynda Hudman, Neil Moore, Randall Martin, and Bram Maasakkers
```

The soil NOx code has been updated from the original implementation

of Yienger & Levy [1995] from Wang et al., [1998] as summarized below.

01d:

ENOx = f( T, biome, w/d) x Pulse(precip) x canopy uptake + FERT

New:

ENOx = f( T, biome, WFPS, Fert) x Pulse(dryspell) x canopy uptake

- 1 Update moisture treatment: soil moisture as a continuous variable using WFPS rather than discrete wet/dry states and purely exponential T impact (impact = -1. Tg N/yr)
- 2 Update to Fertilizer: new fertilizer maps including chemical and manure fertilizer from Potter et al., [2010] distributed using MODIS EVI seasonality, online-N deposition as a fertilizer source, and N-fertilizer source subject to T, WFPS, and pulsing like other N (impact = +1.3 Tg N/yr)
- 3- Update Pulsing Scheme: Yan et al., [2005] (shorter, stronger pulses) (impact = +1. Tg N/yr). Also added restart file containing dry spell information to properly account for dry spell length in continuing runs.

### References:

-----

- (1 ) Wang, Y., D.J. Jacob, and J.A. Logan, Global simulation of tropospheric O3-NOx-hydrocarbon chemistry, 1. Model formulation, J. Geophys. Res., 103/D9, 10, 713-10,726, 1998.
- (2) Yienger, J.J, and H. Levy, Empirical model of global soil-biogenic NOx emissions, J. Geophys. Res., 100, D6, 11,447-11464, June 20, 1995.
- (3) Yan, X., T. Ohara, and H. Akimoto, Statistical modeling of global soil NOx emissions, Global Biogeochem. Cycles, 19, GB3019, doi:10.1029/2004GB002276, 2005.
- (4) Potter, P., Ramankutty, N., Bennett, E., and Donner, S.: Characterizing the Spatial Patterns of Global Fertilizer Application and Manure Production, Earth Interactions, 14, 1-22, 10.1175/2009EI288.1, 2010.
- (5) Moore, N.E., Improving global bottom-up biogenic soil NOx inventories, Master's Thesis, Dalhousie University, 2007.
- (6) Hudman, R.C., N.E. Moore, A.K. Mebust, R.V. Martin, A.R. Russell, L.C. Valin, and R.C Cohen, Steps toward a mechanistic model of global soil nitric oxide emissions: implementation and space based-constraints, Atmos. Chem. Phys., 12, 7779-7795, doi:10.5194/acp-12-7779-2012, 2012.

- 17 Aug 2009 R. Yantosca Columnized and cleaned up
- 17 Aug 2009 R. Yantosca Added ProTeX headers
- 31 Jan 2011 R. Hudman Added new code12259.perceus-ucb0
- 31 Jan 2011 R. Hudman Updated headers

```
29 Aug 2012 - J.D. Maasakkers - Implemented Jacob and Bakwin CRF
29 Aug 2012 - J.D. Maasakkers - Adapted code to work with new (online
                                regridded) landfraction, climate and
                                fertilizer data
29 Aug 2012 - J.D. Maasakkers - Removed all unused Wang et al. code
                                (comments)
04 Nov 2013 - C. Keller
                              - Moved all soil NOx routines into one
                                module. Now a HEMCO extension.
28 Jul 2014 - C. Keller
                              - Now allow DRYCOEFF to be read through
                                configuration file (as setting)
11 Dec 2014 - M. Yannetti
                              - Changed REAL*8 to REAL(hp)
14 Oct 2016 - C. Keller
                              - Now use HCO_EvalFld instead of HCO_GetPtr.
```

#### 2.17.1 HCOX\_SoilNOx\_Run

Subroutine HcoX\_SoilNox\_Run is the driver routine to calculate ship NOx emissions for the current time step. Emissions in [kg/m2/s] are added to the emissions array of the passed

#### **INTERFACE:**

```
SUBROUTINE HCOX_SoilNOx_Run( am_I_Root, ExtState, HcoState, RC ) USES:
```

```
USE HCO_Types_Mod,
                        ONLY : DiagnCont
USE HCO_CLOCK_MOD,
                        ONLY : HcoClock_First
USE HCO_CLOCK_MOD,
                        ONLY : HcoClock_Rewind
USE HCO_FLuxArr_Mod,
                        ONLY : HCO_EmisAdd
USE HCO_EmisList_Mod,
                        ONLY : HCO_GetPtr
USE HCO_Calc_Mod,
                        ONLY : HCO_EvalFld
USE HCO_ExtList_Mod,
                        ONLY : GetExtOpt
USE HCO_ExtList_Mod,
                        ONLY : HCO_GetOpt
USE HCO_Restart_Mod,
                        ONLY : HCO_RestartGet
                        ONLY : HCO_RestartWrite
USE HCO_Restart_Mod,
```

### INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
```

TYPE(Ext\_State), POINTER :: ExtState ! Module options

### INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! Output obj
```

# INTEGER, INTENT(INOUT) :: RC

### **REVISION HISTORY:**

```
05 Nov 2013 - C. Keller - Initial Version
08 May 2015 - C. Keller - Now read/write restart variables from here to accomodate replay runs in GEOS-5.
```

26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts

### 2.17.2 HCOX\_SoilNOx\_Init

Subroutine HcoX\_SoilNox\_Init initializes the HEMCO SOILNOX extension.

#### **INTERFACE:**

```
SUBROUTINE HCOX_SoilNOx_Init( am_I_Root, HcoState, ExtName, & ExtState, RC
```

### USES:

```
USE HCO_ExtList_Mod, ONLY : GetExtNr, GetExtOpt
USE HCO_ExtList_Mod, ONLY : GetExtSpcVal
USE HCO_STATE_MOD, ONLY : HCO_GetExtHcoID
USE HCO_Restart_Mod, ONLY : HCO_RestartDefine
```

#### ARGUMENTS:

```
LOGICAL, INTENT(IN ) :: am_I_Root

TYPE(HCO_State), POINTER :: HcoState ! Output obj

CHARACTER(LEN=*), INTENT(IN ) :: ExtName ! Extension name

TYPE(Ext_State), POINTER :: ExtState ! Module options

INTEGER, INTENT(INOUT) :: RC
```

#### **REMARKS:**

### **REVISION HISTORY:**

```
05 Nov 2013 - C. Keller - Initial Version
12 May 2015 - R. Yantosca - Cosmetic changes
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

#### 2.17.3 HCOX\_SoilNOx\_Final

Subroutine HcoX\_SoilNOx\_Final finalizes the HEMCO SOILNOX extension.

### **INTERFACE:**

```
SUBROUTINE HCOX_SoilNOx_Final( am_I_Root, HcoState, ExtState, RC )
!USES
```

### INPUT PARAMETERS:

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

TYPE(HCO_State), POINTER :: HcoState ! HEMCO State obj

TYPE(Ext_State), POINTER :: ExtState ! Extension state
```

### INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

```
05 Nov 2013 - C. Keller - Initial Version !NOTES:
```

-----

### 2.17.4 HCOX\_SoilNOx\_GetFertScale

Function HCOX\_SoilNOx\_GETFERTSCALE returns the scale factor applied to fertilizer NOx emissions.

```
INTERFACE:
```

```
FUNCTION HCOX_SoilNOx_GetFertScale() RESULT ( FERT_SCALE )
```

#### **ARGUMENTS:**

```
REAL(hp) :: FERT_SCALE
```

#### **REMARKS:**

#### REVISION HISTORY:

### LOCAL VARIABLES:

```
! Scale factor so that fertilizer emission = 1.8 Tg N/yr
! (Stehfest and Bouwman, 2006)
! before canopy reduction
FERT_SCALE = 0.0068
! Value calculated by running the 2x2.5 model
! For now, use this value for all resolutions since regular soil NOx
! emissions change with resolution as well (J.D. Maasakkers)

END FUNCTION HCOX_SoilNOx_GetFertScale
EOC

Harvard-NASA Emissions Component (HEMCO)
```

```
\mbox{}\hrulefill\
```

```
\subsubsection [Soil\_NOx\_Emission] {Soil\_NOx\_Emission}

Subroutine Soil\_NOx\_Emission computes the emission of soil and fertilizer NOx for the GEOS-Chem model.

\\{\bf INTERFACE:}
```

#### INPUT PARAMETERS:

### **OUTPUT PARAMETERS:**

```
REAL(hp), INTENT(OUT) :: SOILNOX ! Soil NOx emissions [kg/m2/s] REAL(sp), INTENT(OUT) :: GWET_PREV ! Soil Moisture Prev timestep REAL(sp), INTENT(OUT) :: DRYPERIOD ! Dry period length in hours REAL(sp), INTENT(OUT) :: PFACTOR ! Pulsing Factor REAL(hp), INTENT(OUT) :: FERTDIAG ! Fert emissions [kg/m2/s]
```

#### **REMARKS:**

R\_CANOPY is computed in routine GET\_CANOPY\_NOX of "canopy\_nox\_mod.f". This was originally in the GEOS-Chem dry deposition code, but was split off in order to avoid an ugly code dependency between the dry deposition and soil NOx codes.

As of v9-02, this module uses the MODIS/Koppen biome types instead of the Olson land type / biome type, making it different from the original dry deposition code  $(J.D.\ Maasakkers)$ 

```
17 Aug 2009 - R. Yantosca - Columnized and cleaned up
17 Aug 2009 - R. Yantosca - Added ProTeX headers
31 Jan 2011 - R. Hudman - New Model added
23 Oct 2012 - M. Payer - Now reference Headers/gigc_errcode_mod.F90
12 May 2015 - R. Yantosca - Cosmetic changes
```

### 2.17.5 Get\_Canopy\_NOx

Subroutine Get\_Canopy\_NOx computes the bulk surface resistance of the canopy to NOx. This computation was originally done within legacy routine DEPVEL (in "drydep\_mod.f"). Moving this computation to Get\_Canopy\_NOx now allows for a totally clean separation between dry deposition routines and emissions routines in GEOS-Chem.

#### **INTERFACE:**

```
SUBROUTINE Get_Canopy_NOx( am_I_Root, HcoState, ExtState, Inst, RC )
```

### **USES:**

```
USE Drydep_Toolbox_Mod, ONLY : BIOFIT
```

#### ARGUMENTS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
TYPE(HCO_State), POINTER :: HcoState
TYPE(Ext_State), POINTER :: ExtState
TYPE(MyInst), POINTER :: Inst
INTEGER, INTENT(INOUT) :: RC
```

#### REMARKS:

For backwards compatibility, the bulk surface resistance is stored in common block array CANOPYNOX in "commsoil.h". Leave it like this for the time being...we'll clean it up when we fix all of the soil NOx routines.

### REVISION HISTORY:

```
22 Jun 2009 - R. Yantosca - Split off from "drydep_mod.f"

14 Jun 2012 - J.D. Maasakkers - Rewritten as a function of the

MODIS/Koppen biometype

09 Nov 2012 - M. Payer - Replaced all met field arrays with State_Met

derived type object

13 Dec 2012 - R. Yantosca - Removed ref to obsolete CMN_DEP_mod.F

28 Jul 2014 - C. Keller - Added error trap for DRYCOEFF

11 Dec 2014 - M. Yannetti - Added BIO_RESULT

12 May 2015 - R. Yantosca - Cosmetic changes
```

### 2.17.6 DiffG

Function 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].

### INTERFACE:

```
FUNCTION DiffG( TK, PRESS, XM ) RESULT( DIFF_G )
```

#### INPUT PARAMETERS:

```
REAL(hp), INTENT(IN) :: TK   ! Temperature [K]
REAL(hp), INTENT(IN) :: PRESS  ! Pressure [hPa]
```

REAL(hp), INTENT(IN) :: XM ! Molecular weight of gas [kg]

#### RETURN VALUE:

```
REAL(hp)
             :: DIFF_G ! Molecular diffusivity [m2/s]
```

#### **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:**

```
22 Jun 2009 - R. Yantosca - Copied from "drydep_mod.f"
07 Jan 2016 - E. Lundgren - Update Avogadro's # to NIST 2014 value
```

# $2.17.7 \text{ Get\_Dep\_N}$

Subroutine GET\_DEP\_N sums dry and wet deposition since prev. timestep and calculates contribution to fertilizer N source. Output is in kg NO/m2.

#### **INTERFACE:**

```
SUBROUTINE Get_Dep_N( I, J, ExtState, HcoState, Inst, DEP_FERT )
```

### INPUT PARAMETERS:

```
:: I
INTEGER, INTENT(IN)
```

INTEGER, INTENT(IN) :: J

TYPE(Ext\_State), POINTER :: ExtState TYPE(HCO\_State), POINTER :: HcoState TYPE(MyInst), POINTER :: Inst

### INPUT/OUTPUT PARAMETERS:

```
! Dep emitted as Fert [kgNO/m2]
REAL(hp) , INTENT(INOUT) :: DEP_FERT
```

```
23 Oct 2012 - M. Payer - Added ProTeX headers
```

### 2.17.8 Source\_DryN

Subroutine SOURCE\_DRYN gets dry deposited Nitrogen since last emission time step, converts to kg NO/m2/s.

#### **INTERFACE:**

```
FUNCTION Source_Dryn( I, J, ExtState, HcoState, Inst ) RESULT( DRYN )
```

#### INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I INTEGER, INTENT(IN) :: J
```

TYPE(Ext\_State), POINTER :: ExtState ! Module options
TYPE(HCO\_State), POINTER :: HcoState ! Output obj
TYPE(MyInst), POINTER :: Inst

# RETURN VALUE:

```
REAL(hp) :: DRYN ! Dry dep. N since prev timestep
```

### REVISION HISTORY:

```
23 Oct 2012 - M. Payer - Added ProTeX headers
```

### 2.17.9 Source\_WetN

Subroutine Source\_WetN gets wet deposited Nitrogen since last emission time step, converts to kg NO/m2/s.

#### **INTERFACE:**

```
FUNCTION Source_WetN( I, J, ExtState, HcoState ) RESULT(WETN )
```

### INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: I INTEGER, INTENT(IN) :: J
```

TYPE(Ext\_State), POINTER :: ExtState ! Module options
TYPE(HCO\_State), POINTER :: HcoState ! Output obj

# RETURN VALUE:

```
REAL(hp) :: WETN ! Dry dep. N since prev timestep
```

```
23 Oct 2012 - M. Payer - Added ProTeX headers
```

### 2.17.10 SoilTemp

Function SoilTemp computes the temperature-dependent term of the soil NOx emissions in ng  $\rm N/m2/s$  and converts to molec/cm2/s

#### **INTERFACE:**

```
FUNCTION SoilTemp( NN, TC, GWET ) RESULT( SOIL_TEMP )
```

#### INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: NN     ! Soil biome type
```

REAL(hp), INTENT(IN) :: GWET ! Top soil moisture

#### RETURN VALUE:

```
REAL(hp) :: SOIL_TEMP ! Temperature-dependent term of ! soil NOx emissions [unitless]
```

#### **REMARKS:**

Based on Ormeci et al., [1999] and Otter et al., [1999] there exists and entirely exponential relationship between temperature and soil NOx emissions at constant soil moisture Therefore we use the following relationship based on Yienger and Levy et al., [1995] for temperatures 0-30C:

```
f(T) = \exp(0.103 + /-0.04 * T)
in ng N/m2/s
```

where T is the temperature in degrees Celsius....Below 0 C, we assume emissions are zero because they are insignificant for the purposes of this global source. ...

### References:

\_\_\_\_\_\_

- (1) Ormeci, B., S. L. Sanin, and J. J. Pierce, Laboratory study of NO flux from agricultural soil: Effects of soil moisture, pH, and temperature, J. Geophys. Res., 104,16211629, 1999.
- (2) Otter, L. B., W. X. Yang, M. C. Scholes, and F. X. Meixner, Nitric oxide emissions from a southern African savanna, J. Geophys. Res., 105, 20,69720,706, 1999.
- (3) Yienger, J.J, and H. Levy, Empirical model of global soil-biogenic NOx emissions, J. Geophys. Res., 100, D6, 11,447-11464, June 20, 1995.

```
17 Aug 2009 - R. Yantosca - Initial Version
17 Aug 2009 - R. Yantosca - Added ProTeX headers
```

```
31 Jan 2011 - R. Hudman - Added new soil T dependance
31 Jan 2011 - R. Hudman - Updated headers
12 May 2015 - R. Yantosca - Cosmetic changes
```

2.17.11 SoilWet

Function SoilWet returns the soil moisture scaling of soil NOx emissions (values from 0-1).

#### **INTERFACE:**

```
FUNCTION SoilWet( GWET, ARID, NONARID ) RESULT( WETSCALE )
```

#### INPUT PARAMETERS:

```
! Top soil wetness [unitless]
REAL(hp), INTENT(IN) :: GWET

! Fraction of arid & non-arid soil in the gridbox
REAL(hp), INTENT(IN) :: ARID
REAL(hp), INTENT(IN) :: NONARID
!RETURN_VALUE:

! A scaling term between 0-1 based on soil moisture
REAL(hp) :: WETSCALE
```

#### **REMARKS:**

Soil moisture and temperature and now decoupled, the temperature term is scaled with a value from 0-1 based on water filled pore space WFPS in top-soil.

### From N.E. Moore thesis:

The response of SNOx is not monotonic to WFPS. SNOx are low for the extreme values of WFPS (0 and 1). For low values, emissions are substrate-limited. For high values, emissions are trapped and cannot diffuse to the surface [Yan et al., 2005]. SNOx dependence on soil moisture is best described as a Poisson function [Parsons et al., 1996; Otter et al., 1999; Pierce and Aneja, 2000; Kirkman et al., 2001; van Dijk and Meixner, 2001; van Dijk et al., 2002]:

```
scaling = a*x*exp(-b*x^2)
```

where the values of a and b are chosen such that the maximum value (unity) occurs for WFPS=0.3, which laboratory and field measurements have found to be the optimal value for emissions in most soils. The typical range of values are 0.2 (arid) up to 0.45 (floodplain) [Yang and Meixner, 1997; Ormeci et al., 1999].

Rice paddies no longer have to be scaled as in the Yienger & Levy model.

#### References:

\_\_\_\_\_\_

- (1) Galbally, I. E., and R. Roy, Loss of fixed nitrogen from soils by nitric oxide exhalation, Nature, 275, 734735, 1978.
- (2) Kirkman, G. A., W. X. Yang, and F. X. Meixner, Biogenic nitric oxide emissions upscaling: An approach for Zimbabwe, Global Biogeochemical Cycles, 15, 1005 1020, 2001.
- (3) Ormeci, B., S. L. Sanin, and J. J. Pierce, Laboratory study of NO flux from agricultural soil: Effects of soil moisture, pH, and temperature, J. Geophys. Res., 104, 16211629, 1999.
- (4) Otter, L. B., W. X. Yang, M. C. Scholes, and F. X. Meixner, Nitric oxide emissions from a southern African savanna, J. Geophys. Res., 105, 20,69720,706, 1999.
- (5) Parsons, D. A., M. C. Scholes, R. J. Scholes, and J. S. Levine, Biogenic NO emissions from savanna soils as a function of fire regime, soil type, soil nitrogen, and water status, J. Geophys. Res., 101, 23,68323,688, 1996.
- (6) Pierce, J. J., and V. P. Aneja, Nitric oxide emissions from engineered soil systems, Journal of Environmental Engineering, pp. 225232, 2000.
- (7) van Dijk, S. M., and J. H. Duyzer, Nitric oxide emissions from forest soils, J. Geophys. Res., 104, 15,95515,961, 1999.
- (8) van Dijk, S. M., and F. X. Meixner, Production and consumption of NO in forest and pasture soils from the Amazon basin, Water, Air, and Soil Pollution: Focus 1, pp. 119130, 2001.
- (9) Yang, W. X., and F. X. Meixner, Gaseous Nitrogen Emissions from Grasslands, CAB Int., Wallingford, UK, 1997, 67-71.

#### **REVISION HISTORY:**

- 17 Aug 2009 R. Yantosca Columnized and cleaned up
- 17 Aug 2009 R. Yantosca Added ProTeX headers
- 31 Jan 2011 R. Hudman Rewrote scaling scheme
- 31 Jan 2011 R.Hudman Updated ProTeX headers

#### 2.17.12 SoilCrf

Computes the canopy reduction factor for the soil NOx emissions according to Jacob % Bakwin [1991] (and as used in Wang et al [1998]).

#### **INTERFACE:**

FUNCTION SoilCrf( K, LAI, CPYNOX, WINDSQR, SUNCOS ) RESULT( SOIL\_CRF )

#### INPUT PARAMETERS:

```
INTEGER, INTENT(IN) :: K     ! Soil biome type
REAL(hp), INTENT(IN) :: LAI     ! Leaf area index [cm2/cm2]
REAL(hp), INTENT(IN) :: CPYNOX     ! Bulk sfc resistance to NOx [1/s]
REAL(hp), INTENT(IN) :: WINDSQR     ! Square of sfc wind speed [m2/s2]
REAL(hp), INTENT(IN) :: SUNCOS     ! Cosine of solar zenith angle
!RETURN_VALUE:
```

REAL(hp) :: SOIL\_CRF ! Canopy reduction factor (see below)

#### **REMARKS:**

Also note, CANOPYNOX (the bulk surface resistance to NOx) is computed in routine GET\_CANOPY\_NOx (in "canopy\_nox\_mod.f") and is passed here as an argument.

#### REVISION HISTORY:

17 Aug 2009 - R. Yantosca - Initial Version

#### 2.17.13 FertAdd

Function FertAdd computes fertilizer emissions

#### **INTERFACE:**

FUNCTION FertAdd( SOILFRT, DEPN ) RESULT( FERT\_ADD )

### INPUT PARAMETERS:

```
REAL(hp), INTENT(IN) :: DEPN ! N emissions from deposition
REAL(hp), INTENT(IN) :: SOILFRT ! N emissions from fertilizers
! read in from disk and passed
! here as an argument [ng N/m2/s]
!RETURN_VALUE:
```

REAL(hp) :: FERT\_ADD ! Total Fert emissions

#### **REMARKS:**

We use a new spatially explicit data set of chemical and manure fert (native resolution  $0.5\B0x0.5\B0$ ) from Potter et al., [2010] distributed using MODIS EVI seasonality as described in N.E. Moore thesis, and Hudman et al., in prep.

In previous model, fertilizer emissions were emitted instantaneously as 2.5% of applied fertilizer, independent of soil moisture/soil temperature, so that they were constant over the growing season.

Similar to the YL parameterization, we now treat fertilizer emissions as part of the  ${\tt Aw}$ . If we treat the wet biome coefficient as a measure of

available N multiplied by a mean emission rate, we can treat fertilizer N in the same manner.

AW = SOILAW(BinewsoilAWS\_08112011\_emissonlyome) + N available in soil x mean emission rate

Instead of choosing an emission rate for each box equivalent to 2.5% of applied N yearly as done in the YL scheme, we chose the mean emission rate so that the total global above canopy SNOx due to fertilizer matches observed estimates of fertilizer emissions of 1.8 Tg N yr-1 from Stehfest and Bouman [2006]. This treatment allows for interannual and daily variability in the strength of response to temperature and precipitation. Note: this scaling must be set for each resolution.

#### References:

\_\_\_\_\_\_

- (1) Potter, P., Ramankutty, N., Bennett, E., and Donner, S.: Characterizing the Spatial Patterns of Global Fertilizer Application and Manure Production, Earth Interactions, in press, 2010.
- (2) Stehfest, E. and L. Bouwman, N2O and NO emission from agricultural fields and soils under natural vegetation: summarizing available measurement data and modeling of global annual emissions, Nutrient Cycling in Agroecosystems (2006), 74:207-228 DOI 10.1007/s10705-006-9000-7.

#### REVISION HISTORY:

```
17 Aug 2009 - R. Yantosca - Columnized and cleaned up
17 Aug 2009 - R. Yantosca - Added ProTeX headers
31 Jan 2011 - R. Hudman - Rewrote pulsing scheme
31 Jan 2011 - R. Hudman - Updated ProTex headers
```

### 2.17.14 Pulsing

Function Pulsing calculates the increase (or "pulse") of soil NOx emission that happens after precipitation falls on dry soil. According to Yan et al., [2005], this pulsing process is thought to be due to a release of inorganic nitrogen trapped on top of the dry soil and a subsequent reactivation of water-stressed bacteria, which then metabolize the excess nitrogen. This can happen in seasonally dry grasslands and savannahs or over freshly fertilized fields.

### **INTERFACE:**

```
FUNCTION Pulsing( GWET, TS_EMIS, & GWET_PREV, PFACTOR, DRYPERIOD ) & RESULT( THE_PULSING )
```

#### INPUT PARAMETERS:

```
REAL(hp), INTENT(IN)
                  :: GWET
                                ! Soil Moisture
```

REAL\*4, INTENT(IN) :: TS\_EMIS ! Emissions timestep [s]

### INPUT/OUTPUT PARAMETERS:

```
REAL(sp), INTENT(INOUT) :: GWET_PREV
REAL(sp), INTENT(INOUT) :: PFACTOR
                                                          ! Soil Moisture Prev timestep
```

! Pulsing Factor

REAL(sp), INTENT(INOUT) :: DRYPERIOD ! Dry period length in hours

#### RETURN VALUE:

```
REAL(hp)
              :: THE_PULSING ! Factor to multiply baseline
                                   ! emissions by to account for
```

! soil pulsing of all types

#### **REMARKS:**

Soil NOx emissions consist of baseline emissions plus discrete "pulsing" episodes. We follow thw Yan et al., [2005] algorithm, where the pulse (relative to the flux prewetting) is determined by the antecedent dry period, with a simple logarithmic relationship,

```
PFACTOR = 13.01 ln ( DRYPERIOD ) - 53.6
```

where PFACTOR is the magnitude of peak flux relative to prewetting flux, and DRYPERIOD is the length of the antecedent dry period in hours.

The pulse decays with

```
PFACTOR = PFACTOR * EXP( -0.068e+0_hp * DTSRCE )
```

#### References:

\_\_\_\_\_\_

(1) Yan, X., T. Ohara, and H. Akimoto (2005), Statistical modeling of global soil NOx emissions, Global Biogeochem. Cycles, 19, GB3019, doi:10.1029/2004GB002276.Section 2.3.3

```
17 Aug 2009 - R. Yantosca - Columnized and cleaned up
```

- 31 Jan 2011 R. Hudman Updated ProTex header
- 29 May 2013 R. Yantosca Bug fix: prevent log(0) from happening
- 21 Oct 2014 C. Keller Limit PFACTOR to 1.
- 12 May 2015 R. Yantosca Cosmetic changes

<sup>17</sup> Aug 2009 - R. Yantosca - Added ProTeX headers

<sup>31</sup> Jan 2011 - R. Hudman - Rewrote pulsing scheme

#### 2.17.15 InstGet

Subroutine InstGet returns a pointer to the desired instance.

#### **INTERFACE:**

```
SUBROUTINE InstGet (Instance, Inst, RC, PrevInst)
```

#### INPUT PARAMETERS:

#### **REVISION HISTORY:**

```
18 Feb 2016 - C. Keller - Initial version
```

#### 2.17.16 InstCreate

Subroutine InstCreate adds a new instance to the list of instances, assigns a unique instance number to this new instance, and archives this instance number to output argument Instance.

### **INTERFACE:**

```
SUBROUTINE InstCreate (ExtNr, Instance, Inst, RC)
```

## **INPUT PARAMETERS:**

INTEGER, INTENT(IN) :: ExtNr

#### **OUTPUT PARAMETERS:**

INTEGER, INTENT( OUT) :: Instance TYPE(MyInst), POINTER :: Inst

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

```
18 Feb 2016 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

#### 2.17.17 InstRemove

Subroutine InstRemove removes an instance from the list of instances.

### **INTERFACE:**

```
SUBROUTINE InstRemove (ExtState)
```

### **INPUT PARAMETERS:**

```
TYPE(Ext_State), POINTER :: ExtState ! Extension state
```

#### REVISION HISTORY:

```
18 Feb 2016 - C. Keller - Initial version
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

### 2.18 Fortran: Module Interface hcox\_state\_mod.F90

Module HCOX\_State\_Mod contains routines and variables to organize the extensions state type ExtState. ExtState contains the logical switches for each extension (denoting whether or not it is enabled) as well as pointers to all met fields used by the extensions. ExtState is passed to all extension modules, and the met fields defined in here are thus available to all extensions. Additional met fields (and extension switches) can be added as required. This module contains the routines to initialize and finalize the ExtState object, but doesn't link the met field pointers to the corresponding fields. This is done in the HEMCO-model interface routines (e.g. hcoi\_standalone\_mod.F90, hcoi\_gc\_main\_mod.F90). Newly added met fields will only work if the corresponding pointer assignments are added to these interface routines!

#### **INTERFACE:**

```
MODULE HCOX_STATE_MOD
```

### **USES:**

```
USE HCO_ERROR_MOD
USE HCO_ARR_MOD

IMPLICIT NONE
PRIVATE
```

#### PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: ExtStateInit
PUBLIC :: ExtStateFinal
PUBLIC :: ExtDat_Set
!DERIVED TYPES:
```

```
! ExtDat_*: Derived types containing pointers to the met field arrays ! (Arr) and a logical flag whether or not the field is used by any of
```

```
! the extensions (DoUse). Arrays can be 3D reals or 2D reals or integer
! All real values are of default precision! (df), as specified in
! HCO\_ERROR\_MOD. You can add more types if necessary.
! 2D real, default precision
TYPE, PUBLIC :: ExtDat_2R
  TYPE(Arr2D_HP), POINTER :: Arr
  LOGICAL
                        :: DoUse
  LOGICAL
                        :: FromList
END TYPE ExtDat_2R
! 2D real, single precision
TYPE, PUBLIC :: ExtDat_2S
  TYPE(Arr2D_SP), POINTER :: Arr
  LOGICAL
                       :: DoUse
  LOGICAL
                        :: FromList
END TYPE ExtDat_2S
! 2D integer
TYPE, PUBLIC :: ExtDat_2I
  TYPE(Arr2D_I), POINTER :: Arr
  LOGICAL
                        :: DoUse
  LOGICAL
                        :: FromList
END TYPE ExtDat_2I
! 3D real, default precision
TYPE, PUBLIC :: ExtDat_3R
  TYPE(Arr3D_HP), POINTER :: Arr
  LOGICAL
                       :: DoUse
  LOGICAL
                        :: FromList
END TYPE ExtDat_3R
! 3D real, single precision
TYPE, PUBLIC :: ExtDat_3S
  TYPE(Arr3D_SP), POINTER :: Arr
  LOGICAL
                        :: DoUse
  LOGICAL
                        :: FromList
END TYPE ExtDat_3S
!-----
! Ext_State: Derived type declaration for the State object containing
! pointers to all met fields and related quantities used by the HEMCO
! extensions. An 'Ext_State' type called ExtState is defined at the
! beginning of a HEMCO run and populated according to the specifications
! set in the configuration file. You can add more fields if necessary.
TYPE, PUBLIC :: Ext_State
```

```
l-----
! Extension switches (enabled?)
! NOTE: When adding a new extension, don't forget to initialize this
! switch in subroutine ExtStateInit below!
                      :: Custom ! Customizable ext.
:: DustDead ! DEAD dust model
:: DustGinoux ! Ginoux dust emissions
LOGICAL
INTEGER
LOGICAL
                      :: DustAlk
                                      ! Dust alkalinity
LOGICAL
                                    ! Lightning NOx
! PARANOX ship emissions
INTEGER
                      :: LightNOx
LOGICAL
                      :: ParaNOx
                      :: SoilNOx
                                     ! Soil NOx emissions
INTEGER
INTEGER
                       :: Megan
                                       ! MEGAN biogenic emissions
                      :: SeaFlux ! air-sea exchange
:: SeaSalt ! Seasalt emissions
:: MarinePOA ! Marine organic aerosols
LOGICAL
LOGICAL
LOGICAL
                      :: GFED
                                      ! GFED biomass burning
LOGICAL
                      :: FINN ! FINN biomass burning
:: GC_RnPbBe ! GEOS-Chem Rn-Pb-Be simulation
:: GC_POPs ! GEOS-Chem POPs simulation
LOGICAL
LOGICAL
LOGICAL
                      :: Wetland_CH4 ! Methane emiss from wetlands
INTEGER
                       :: TOMAS_Jeagle ! TOMAS Jeagle sea salt
LOGICAL
INTEGER
                       :: TOMAS_DustDead ! TOMAS sectional Dead Dust
                       :: AeroCom ! AeroCom volcano
INTEGER
!-----
! Data directory
I-----
CHARACTER(LEN=255) :: DATA_DIR ! Directory for data
!-----
! Met fields
!-----
TYPE(ExtDat_2R), POINTER :: U10M
                                    ! E/W 10m wind speed [m/s]
                                  ! E/w rom wring.
! N/S 10m wind speed [m/s]
TYPE(ExtDat_2R), POINTER :: V10M
TYPE(ExtDat_2R), POINTER :: ALBD
                                    ! Surface albedo [-]
                                    ! O=water, 1=land, 2=ice
TYPE(ExtDat_2R), POINTER :: WLI
TYPE(ExtDat_2R), POINTER :: T2M
                                     ! 2m Sfce temperature [K]
                                     ! Surface skin temperature [K]
TYPE(ExtDat_2R), POINTER :: TSKIN
TYPE(ExtDat_2R), POINTER :: GWETROOT
                                     ! Root soil wetness [1]
TYPE(ExtDat_2R), POINTER :: GWETTOP
                                     ! Top soil moisture [-]
                                     ! Snow height [mm H20 = kg H20/m2]
TYPE(ExtDat_2R), POINTER :: SNOWHGT
TYPE(ExtDat_2R), POINTER :: SNODP
                                     ! Snow depth [m ]
TYPE(ExtDat_2R), POINTER :: SNICE
                                     ! Fraction of snow/ice [1]
TYPE(ExtDat_2R), POINTER :: USTAR
                                     ! Friction velocity [m/s]
                                     ! Sfc roughness height [m]
TYPE(ExtDat_2R), POINTER :: ZO
TYPE(ExtDat_2R), POINTER :: TROPP
                                     ! Tropopause pressure [Pa]
TYPE(ExtDat_2R), POINTER :: SUNCOS
                                    ! COS (SZA)
```

```
TYPE(ExtDat_2R), POINTER :: SZAFACT
                                      ! current SZA/total daily SZA
TYPE(ExtDat_2R), POINTER :: PARDR
                                      ! direct photsyn radiation [W/m2]
TYPE(ExtDat_2R), POINTER :: PARDF
                                     ! diffuse photsyn radiation [W/m2]
                                     ! Interpolated sfc pressure [hPa]
TYPE(ExtDat_2R), POINTER :: PSC2_WET
TYPE(ExtDat_2R), POINTER :: RADSWG
                                     ! surface radiation [W/m2]
TYPE(ExtDat_2R), POINTER :: FRCLND
                                     ! Olson land fraction [-]
TYPE(ExtDat_2R), POINTER :: FRLAND
                                     ! land fraction [-]
TYPE(ExtDat_2R), POINTER :: FROCEAN
                                     ! ocean fraction [-]
TYPE(ExtDat_2R), POINTER :: FRLAKE
                                     ! lake fraction [-]
TYPE(ExtDat_2R), POINTER :: FRLANDIC
                                     ! land ice fraction [-]
TYPE(ExtDat_2R), POINTER :: CLDFRC
                                     ! cloud fraction [-]
TYPE(ExtDat_2R), POINTER :: JNO2
                                     ! J-Value for NO2 [1/s]
TYPE(ExtDat_2R), POINTER :: JOH
                                     ! J-Value for 03->OH [1/s]
TYPE(ExtDat_2R), POINTER :: LAI
                                     ! daily leaf area index [cm2/cm2]
TYPE(ExtDat_2R), POINTER :: CHLR
                                     ! daily chlorophyll-a [mg/m3]
                                     ! Max height of PBL [level]
                POINTER :: PBL_MAX
INTEGER,
                                     ! Convective cloud mass flux [kg/m2/s]
TYPE(ExtDat_3R), POINTER :: CNV_MFC
TYPE(ExtDat_3R), POINTER :: FRAC_OF_PBL ! Fraction of grid box in PBL
TYPE(ExtDat_3R), POINTER :: SPHU
                                     ! Spec. humidity [kg H2O/kg total air]
TYPE(ExtDat_3R), POINTER :: TK
                                     ! Air temperature [K]
                                     ! Dry air mass [kg]
TYPE(ExtDat_3R), POINTER :: AIR
TYPE(ExtDat_3R), POINTER :: AIRVOL
                                     ! Air volume [m3]
TYPE(ExtDat_3R), POINTER :: AIRDEN
                                     ! Dry air density [kg/m3]
TYPE(ExtDat_3R), POINTER :: 03
                                     ! 03 mass [kg/kg dry air]
TYPE(ExtDat_3R), POINTER :: NO
                                     ! NO mass [kg/kg dry air]
                                     ! NO2 mass [kg/kg dry air]
TYPE(ExtDat_3R), POINTER :: NO2
TYPE(ExtDat_3R), POINTER :: HNO3
                                     ! HNO3 mass [kg/kg dry air]
TYPE(ExtDat_3R), POINTER :: POPG
                                    ! POPG mass [kg/kg dry air]
1-----
! Deposition parameter
! DRY_TOTN and WET_TOTN are the total (dry/wet) deposited N since the
! last emission timestep. Even though these numbers are per second,
! they may represent accumulated deposition velocities if chemistry
! and/or dynamic timestep are not equal to the emission timestep.
! These values are used by the soil NOx module. Note that it is assumed
! that DRY_TOTN and WET_TOTN are summed over chemistry and transport
! timesteps, respectively!
TYPE(ExtDat_2R), POINTER :: DRY_TOTN
                                     ! Dry deposited N
                                                        [molec/cm2/s]
TYPE(ExtDat_2R), POINTER :: WET_TOTN
                                    ! Wet deposited N
                                                        [kg N/s]
                POINTER :: DRYCOEFF(:) ! Baldocci drydep coeff.
REAL(hp),
!-----
! Constants for POPs emissions module
!-----
REAL(dp)
                       :: POP_DEL_H ! Delta H [J/mol]
REAL(dp)
                      :: POP_DEL_Hw ! Delta Hw [J/mol]
```

```
:: POP_HSTAR
REAL(dp)
                                 ! Henry's law constant [atm/M/L]
                    :: POP_KOA
REAL(dp)
                                ! POP octanol-water partition coef
REAL(dp)
                    :: POP_KBC
                                ! POP BC-air partition coeff.
                    :: POP_XMW
REAL(dp)
                                ! POP molecular weight [kg/mol]
1-----
! Fields used in ESMF environment only. These arrays won't be used
! in a classic environment. They become filled in HCO_SetExtState_ESMF
! in hcoi_esmf_mod.F90 (called from within hcoi_gc_main_mod.F90).
I-----
TYPE(ExtDat_3S), POINTER :: BYNCY
                                ! Buoyancy
TYPE(ExtDat_2R), POINTER :: CNV_FRC
                               ! convective fraction (filled
                                ! from State_Met)
```

END TYPE Ext\_State

#### PRIVATE MEMBER FUNCTIONS:

#### **REVISION HISTORY:**

```
02 Oct 2013 - C. Keller - Initial version
23 Jun 2014 - R. Yantosca - Now add DATA_DIR to Ext_State declaration
23 Jun 2014 - R. Yantosca - Now use F90 freeform indentation
23 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
27 Jun 2014 - C. Keller - Added FINN biomass burning extension
07 Jul 2014 - R. Yantosca - Modified for GEOS-Chem Rn-Pb-Be simulation
28 Jul 2014 - C. Keller - Added J-Values for NO2 and O3 to state obj.
20 Aug 2014 - M. Sulprizio- Modified for GEOS-Chem POPs emissions module
01 Oct 2014 - R. Yantosca - Modified for TOMAS sea salt emissions module
11 Dec 2014 - M. Yannetti - Updated DRYCOEFF to REAL(hp)
10 Mar 2015 - C. Keller - Fields can now be in HEMCO precision or single
                           precision. Single precision is useful for
                           fields used in ESMF setting.
03 Apr 2015 - C. Keller - Added ExtDat_Set.
21 Feb 2016 - C. Keller
                         - Update to HEMCO v2.0
03 Mar 2016 - C. Keller
                         - Added CNV_FRC
20 Apr 2016 - M. Sulprizio- Change JOID pointer to JOH to reflect that it now
                           points to the effective O3 + hv -> 20H rates
01 Nov 2016 - M. Sulprizio- Rename TOMAS sea salt to TOMAS Jeagle (J. Kodros)
```

### 2.18.1 ExtStateInit

Initializes all fields of the ExtState object.

```
SUBROUTINE ExtStateInit( ExtState, RC )
```

# INPUT/OUTPUT PARAMETERS:

### **REMARKS:**

You can add more initialization statements as is necessary.

### **REVISION HISTORY:**

```
15 Dec 2013 - C. Keller - Initial version
23 Jun 2014 - R. Yantosca - Now use F90 freeform indentation
23 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
```

### 2.18.2 ExtStateFinal

Finalizes the ExtState object. This removes all defined pointer links (i.e. nullifies ExtDat%Arr), but does not deallocate the target array!

#### **INTERFACE:**

```
SUBROUTINE ExtStateFinal( ExtState )
```

#### INPUT PARAMETERS:

```
TYPE(Ext_State), POINTER :: ExtState
```

### REVISION HISTORY:

```
03 Oct 2013 - C. Keller - Initial version
23 Jun 2014 - R. Yantosca - Now use F90 freeform indentation
23 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
09 Jul 2015 - E. Lundgren - Add chlorophyll-a (CHLR)
```

### 2.18.3 ExtDat\_Init\_2R

Subroutine ExtDat\_Init\_2R initializes the given ExtDat type.

### **INTERFACE:**

```
SUBROUTINE ExtDat_Init_2R ( ExtDat, RC )
```

### **INPUT PARAMETERS:**

```
20 Apr 2013 - C. Keller - Initial version
23 Jun 2014 - R. Yantosca - Now use F90 freeform indentation
23 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers
```

### 2.18.4 ExtDat\_Init\_2S

Subroutine ExtDat\_Init\_2S initializes the given ExtDat type.

#### **INTERFACE:**

```
SUBROUTINE ExtDat_Init_2S ( ExtDat, RC )
```

### INPUT PARAMETERS:

```
TYPE(ExtDat_2S), POINTER :: ExtDat
```

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

#### REVISION HISTORY:

```
20 Apr 2013 - C. Keller - Initial version
```

- 23 Jun 2014 R. Yantosca Now use F90 freeform indentation
- 23 Jun 2014 R. Yantosca Cosmetic changes in ProTeX headers

### 2.18.5 ExtDat\_Init\_2I

Subroutine ExtDat\_Init\_2I initializes the given ExtDat type.

#### **INTERFACE:**

```
SUBROUTINE ExtDat_Init_2I ( ExtDat, RC )
```

### INPUT PARAMETERS:

```
TYPE(ExtDat_2I), POINTER :: ExtDat
```

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

# **REVISION HISTORY:**

```
20 Apr 2013 - C. Keller - Initial version
```

- 23 Jun 2014 R. Yantosca Now use F90 freeform indentation
- 23 Jun 2014 R. Yantosca Cosmetic changes in ProTeX headers

### 2.18.6 ExtDat\_Init\_3R

Subroutine ExtDat\_Init\_3R initializes the given ExtDat type.

#### **INTERFACE:**

```
SUBROUTINE ExtDat_Init_3R ( ExtDat, RC )
```

### INPUT PARAMETERS:

```
TYPE(ExtDat_3R), POINTER :: ExtDat
```

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

```
20 Apr 2013 - C. Keller - Initial version
```

- 23 Jun 2014 R. Yantosca Now use F90 freeform indentation
- 23 Jun 2014 R. Yantosca Cosmetic changes in ProTeX headers

### 2.18.7 ExtDat\_Init\_3S

Subroutine ExtDat\_Init\_3S initializes the given ExtDat type.

### **INTERFACE:**

```
SUBROUTINE ExtDat_Init_3S ( ExtDat, RC )
```

### INPUT PARAMETERS:

```
TYPE(ExtDat_3S), POINTER :: ExtDat
```

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

#### **REVISION HISTORY:**

```
20 Apr 2013 - C. Keller - Initial version
```

- 23 Jun 2014 R. Yantosca Now use F90 freeform indentation
- 23 Jun 2014 R. Yantosca Cosmetic changes in ProTeX headers

### 2.18.8 ExtDat\_Cleanup\_2R

Subroutine ExtDat\_Cleanup\_2R removes the given ExtDat type.

### **INTERFACE:**

```
SUBROUTINE ExtDat_Cleanup_2R ( ExtDat )
```

### INPUT PARAMETERS:

```
TYPE(ExtDat_2R), POINTER :: ExtDat
```

### **REVISION HISTORY:**

```
20 Apr 2013 - C. Keller - Initial version
```

23 Jun 2014 - R. Yantosca - Now use F90 freeform indentation

23 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers

# 2.18.9 ExtDat\_Cleanup\_2S

Subroutine ExtDat\_Cleanup\_2S removes the given ExtDat type.

### **INTERFACE:**

```
SUBROUTINE ExtDat_Cleanup_2S ( ExtDat )
```

### INPUT PARAMETERS:

```
TYPE(ExtDat_2S), POINTER :: ExtDat
```

```
20 Apr 2013 - C. Keller - Initial version
```

- 23 Jun 2014 R. Yantosca Now use F90 freeform indentation
- 23 Jun 2014 R. Yantosca Cosmetic changes in ProTeX headers

### 2.18.10 ExtDat\_Cleanup\_2I

Subroutine ExtDat\_Cleanup\_2I removes the given ExtDat type.

### **INTERFACE:**

```
SUBROUTINE ExtDat_Cleanup_2I ( ExtDat )
```

#### INPUT PARAMETERS:

```
TYPE(ExtDat_2I), POINTER :: ExtDat
```

### REVISION HISTORY:

```
20 Apr 2013 - C. Keller - Initial version
```

23 Jun 2014 - R. Yantosca - Now use F90 freeform indentation

23 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers

# 2.18.11 ExtDat\_Cleanup\_3R

Subroutine ExtDat\_Cleanup\_3R removes the given ExtDat type.

### **INTERFACE:**

```
SUBROUTINE ExtDat_Cleanup_3R( ExtDat )
```

### INPUT PARAMETERS:

```
TYPE(ExtDat_3R), POINTER :: ExtDat
```

### **REVISION HISTORY:**

```
20 Apr 2013 - C. Keller - Initial version
```

23 Jun 2014 - R. Yantosca - Now use F90 freeform indentation

23 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers

### 2.18.12 ExtDat\_Cleanup\_3S

Subroutine ExtDat\_Cleanup\_3S removes the given ExtDat type.

#### **INTERFACE:**

```
SUBROUTINE ExtDat_Cleanup_3S( ExtDat )
```

### INPUT PARAMETERS:

```
TYPE(ExtDat_3S), POINTER :: ExtDat
```

### **REVISION HISTORY:**

```
20 Apr 2013 - C. Keller - Initial version
```

23 Jun 2014 - R. Yantosca - Now use F90 freeform indentation

23 Jun 2014 - R. Yantosca - Cosmetic changes in ProTeX headers

### 2.18.13 ExtDat\_Set\_2R

Subroutine ExtDat\_Set\_2R sets/updates the data array of an ExtDat object.

### **INTERFACE:**

```
SUBROUTINE ExtDat_Set_2R ( am_I_Root, HcoState, ExtDat, & FldName, RC, First, & Trgt, Filled, NotFillOk)
```

### **USES:**

```
USE HCO_ARR_MOD, ONLY : HCO_ArrAssert
USE HCO_STATE_MOD, ONLY : HCO_State
USE HCO_CALC_MOD, ONLY : HCO_EvalFld
```

### INPUT PARAMETERS:

```
INTENT(IN
                                                  :: am_I_Root
LOGICAL,
                              )
TYPE(HCO_State), POINTER
                                                   :: HcoState
TYPE(ExtDat_2R), POINTER
                                                  :: ExtDat
                                                  :: FldName
CHARACTER(LEN=*), INTENT(IN
                              )
INTEGER,
                                                  :: RC
                 INTENT(INOUT)
LOGICAL,
                 INTENT(IN
                              ), OPTIONAL
                                                  :: First
                               , OPTIONAL
                                                  :: Trgt(:,:)
REAL(hp),
                  POINTER
                                                  :: Filled
                  INTENT( OUT), OPTIONAL
LOGICAL,
                              ), OPTIONAL
LOGICAL,
                  INTENT(IN
                                                  :: NotFillOk
```

### **REVISION HISTORY:**

```
03 Apr 2015 - C. Keller - Initial version
11 May 2015 - C. Keller - Now use HCO_EvalFld instead of HCO_GetPtr. This allows the application of scale factors to

ExtState fields read through the HEMCO interface.
```

### 2.18.14 ExtDat\_Set\_2S

Subroutine ExtDat\_Set\_2S sets/updates the data array of an ExtDat object.

### **INTERFACE:**

```
SUBROUTINE ExtDat_Set_2S ( am_I_Root, HcoState, ExtDat, & FldName, RC, First, & Trgt, Filled, NotFillOk)
```

#### USES:

```
USE HCO_ARR_MOD, ONLY : HCO_ArrAssert
USE HCO_STATE_MOD, ONLY : HCO_State
USE HCO_CALC_MOD, ONLY : HCO_EvalFld
```

#### INPUT PARAMETERS:

```
)
                                                :: am_I_Root
LOGICAL,
                 INTENT(IN
TYPE(HCO_State), POINTER
                                                :: HcoState
TYPE(ExtDat_2S), POINTER
                                                :: ExtDat
CHARACTER(LEN=*), INTENT(IN )
                                               :: FldName
INTEGER,
                INTENT (INOUT)
                                               :: RC
LOGICAL,
                 INTENT(IN
                                               :: First
                            ), OPTIONAL
                            , OPTIONAL
REAL(sp),
               POINTER
                                               :: Trgt(:,:)
LOGICAL,
                 INTENT( OUT), OPTIONAL
                                              :: Filled
LOGICAL,
                 INTENT(IN ), OPTIONAL
                                              :: NotFillOk
```

### **REVISION HISTORY:**

```
03 Apr 2015 - C. Keller - Initial version
11 May 2015 - C. Keller - Now use HCO_EvalFld instead of HCO_GetPtr. This allows the application of scale factors to

ExtState fields read through the HEMCO interface.
```

### 2.18.15 ExtDat\_Set\_2I

Subroutine ExtDat\_Set\_2I sets/updates the data array of an ExtDat object.

#### **INTERFACE:**

```
SUBROUTINE ExtDat_Set_2I ( am_I_Root, HcoState, ExtDat, & FldName, RC, First, & Trgt, Filled, NotFillOk)
```

### **USES:**

```
USE HCO_ARR_MOD, ONLY: HCO_ArrAssert
USE HCO_STATE_MOD, ONLY: HCO_State
USE HCO_CALC_MOD, ONLY: HCO_EvalFld
```

### INPUT PARAMETERS:

```
LOGICAL,
                 INTENT(IN
                             )
                                                :: am_I_Root
TYPE(HCO_State), POINTER
                                                :: HcoState
TYPE(ExtDat_2I), POINTER
                                                :: ExtDat
CHARACTER(LEN=*), INTENT(IN )
                                               :: FldName
INTEGER,
                 INTENT(INOUT)
                                                :: RC
LOGICAL,
                INTENT(IN
                           ), OPTIONAL
                                               :: First
INTEGER,
                 POINTER,
                               OPTIONAL
                                               :: Trgt(:,:)
                                                :: Filled
LOGICAL,
                 INTENT( OUT), OPTIONAL
LOGICAL,
                 INTENT(IN ), OPTIONAL
                                                :: NotFillOk
```

```
03 Apr 2015 - C. Keller - Initial version
11 May 2015 - C. Keller - Now use HCO_EvalFld instead of HCO_GetPtr. This allows the application of scale factors to

ExtState fields read through the HEMCO interface.
```

### 2.18.16 ExtDat\_Set\_3R

Subroutine ExtDat\_Set\_3R sets/updates the data array of an ExtDat object.

### **INTERFACE:**

```
SUBROUTINE ExtDat_Set_3R (am_I_Root, HcoState, ExtDat, FldName, & RC, First, Trgt, OnLevEdge, & Filled, NotFillOk
```

### **USES:**

```
USE HCO_ARR_MOD, ONLY: HCO_ArrAssert
USE HCO_STATE_MOD, ONLY: HCO_State
USE HCO_CALC_MOD, ONLY: HCO_EvalFld
```

### INPUT PARAMETERS:

```
LOGICAL,
                  INTENT(IN
                              )
                                                   :: am_I_Root
TYPE(HCO_State), POINTER
                                                   :: HcoState
TYPE(ExtDat_3R), POINTER
                                                   :: ExtDat
CHARACTER(LEN=*), INTENT(IN
                              )
                                                   :: FldName
                                                   :: RC
INTEGER,
                  INTENT(INOUT)
LOGICAL,
                  INTENT(IN
                              ), OPTIONAL
                                                   :: First
                               , OPTIONAL
REAL(hp),
                  POINTER
                                                   :: Trgt(:,:,:)
                  INTENT(IN
                              ), OPTIONAL
                                                   :: OnLevEdge
LOGICAL,
LOGICAL,
                  INTENT( OUT), OPTIONAL
                                                   :: Filled
                  INTENT(IN
                              ), OPTIONAL
                                                   :: NotFillOk
LOGICAL,
```

### **REVISION HISTORY:**

```
03 Apr 2015 - C. Keller - Initial version
11 May 2015 - C. Keller - Now use HCO_EvalFld instead of HCO_GetPtr. This allows the application of scale factors to ExtState fields read through the HEMCO interface.
```

### 2.18.17 ExtDat\_Set\_3S

Subroutine ExtDat\_Set\_3S sets/updates the data array of an ExtDat object.

### INTERFACE:

```
SUBROUTINE ExtDat_Set_3S ( am_I_Root, HcoState, ExtDat, FldName, & RC, First, Trgt, OnLevEdge, & Filled, NotFillOk
```

### **USES:**

```
USE HCO_ARR_MOD, ONLY : HCO_ArrAssert
USE HCO_STATE_MOD, ONLY : HCO_State
USE HCO_CALC_MOD, ONLY : HCO_EvalFld
```

### INPUT PARAMETERS:

```
LOGICAL,
                  INTENT(IN
                              )
                                                   :: am_I_Root
TYPE(HCO_State), POINTER
                                                   :: HcoState
                                                   :: ExtDat
TYPE(ExtDat_3S), POINTER
CHARACTER(LEN=*), INTENT(IN
                              )
                                                   :: FldName
INTEGER,
                                                   :: RC
                  INTENT(INOUT)
LOGICAL,
                  INTENT(IN
                                                   :: First
                              ), OPTIONAL
REAL(sp),
                  POINTER
                               , OPTIONAL
                                                   :: Trgt(:,:,:)
                                                   :: OnLevEdge
                              ), OPTIONAL
LOGICAL,
                  INTENT(IN
                  INTENT( OUT), OPTIONAL
                                                   :: Filled
LOGICAL,
                              ), OPTIONAL
                                                   :: NotFillOk
LOGICAL,
                  INTENT(IN
```

### **REVISION HISTORY:**

```
03 Apr 2015 - C. Keller - Initial version
11 May 2015 - C. Keller - Now use HCO_EvalFld instead of HCO_GetPtr. This allows the application of scale factors to ExtState fields read through the HEMCO interface.
```

# 2.19 Fortran: Module Interface hcox\_template\_mod.F90

Module hcox\_template\_mod.F90 is a HEMCO extension template. It serves as a starting point for a new emission extension within HEMCO. Specifically, it provides the framework to use multiple 'instances' of the extension at the same time.

### **INTERFACE:**

```
MODULE HCOX_<yourname>_mod

USES:

USE HCO_Error_MOD

USE HCO_Diagn_MOD

USE HCOX_TOOLS_MOD

USE HCOX_State_MOD, ONLY : Ext_State

USE HCO_State_MOD, ONLY : HCO_State

IMPLICIT NONE

PRIVATE
```

### PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: HCOX_<yourname>_Run
PUBLIC :: HCOX_<yourname>_Init
PUBLIC :: HCOX_<yourname>_Final
```

#### PRIVATE MEMBER FUNCTIONS:

```
19 Feb 2016 - C. Keller - Initial version
```

# 2.19.1 HCOX\_iyourname;\_Run

Write a description here

### **INTERFACE:**

```
SUBROUTINE HCOX_<yourname>_Run( am_I_Root, ExtState, HcoState, RC )
```

#### **USES:**

```
USE HCO_FluxArr_Mod, ONLY : HCO_EmisAdd
```

# INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root ! Are we on the root CPU? TYPE(Ext_State), POINTER :: ExtState ! Module options
```

### INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! Hemco state INTEGER, INTENT(INOUT) :: RC ! Success or failure
```

### REMARKS:

### **REVISION HISTORY:**

```
19 Feb 2016 - C. Keller - Initial version
```

# 2.19.2 HCOX\_iyourname;\_Init

Write a description here

### INTERFACE:

```
SUBROUTINE HCOX_<yourname>_Init( am_I_Root, HcoState, ExtName, & ExtState, RC )
```

### **USES:**

```
USE HCO_ExtList_Mod, ONLY : GetExtNr
USE HCO_ExtList_Mod, ONLY : GetExtOpt
USE HCO_ExtList_Mod, ONLY : GetExtSpcVal
USE HCO_STATE_MOD, ONLY : HCO_GetExtHcoID
```

### INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
CHARACTER(LEN=*), INTENT(IN ) :: ExtName ! Extension name
TYPE(Ext_State), POINTER :: ExtState ! Module options
```

# INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_State), POINTER :: HcoState ! Hemco state
INTEGER, INTENT(INOUT) :: RC
```

### REVISION HISTORY:

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

# 2.19.3 HCOX\_iyourname;\_Final

Write a description here

### **INTERFACE:**

```
SUBROUTINE HCOX_AeroCom_Final ( ExtState )
```

### INPUT PARAMETERS:

```
TYPE(Ext_State), POINTER :: ExtState ! Module options
```

### **REVISION HISTORY:**

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

#### 2.19.4 InstGet

Subroutine InstGet returns a pointer to the desired instance.

#### **INTERFACE:**

```
SUBROUTINE InstGet (Instance, Inst, RC, PrevInst)
```

### INPUT PARAMETERS:

# **REVISION HISTORY:**

```
18 Feb 2016 - C. Keller - Initial version
```

#### 2.19.5 InstCreate

Subroutine InstCreate adds a new instance to the list of instances, assigns a unique instance number to this new instance, and archives this instance number to output argument Instance.

SUBROUTINE InstCreate (ExtNr, Instance, Inst, RC)

### INPUT PARAMETERS:

INTEGER, INTENT(IN) :: ExtNr

# **OUTPUT PARAMETERS:**

INTEGER, INTENT( OUT) :: Instance
TYPE(MyInst), POINTER :: Inst

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

### **REVISION HISTORY:**

18 Feb 2016 - C. Keller - Initial version

#### 2.19.6 InstRemove

Subroutine InstRemove removes an instance from the list of instances.

### **INTERFACE:**

SUBROUTINE InstRemove (Instance)

### INPUT PARAMETERS:

INTEGER :: Instance

#### **REVISION HISTORY:**

18 Feb 2016 - C. Keller - Initial version

#### 2.20 Fortran: Module Interface hcox\_dust\_dead\_mod.F

Module hcox\_dust\_dead\_mod.F contains routines and variables from Charlie Zender's DEAD dust mobilization model. Most routines are from Charlie Zender, but have been modified and/or cleaned up for inclusion into GEOS-Chem.

This is a HEMCO extension module that uses many of the HEMCO core utilities.

NOTE: The current (dust) code was validated at 2 x 2.5 resolution. We have found that running at 4x5 we get much lower (50emissions than at 2x2.5. Recommend we either find a way to scale the U\* computed in the dust module, or run a 1x1 and store the the dust emissions, with which to drive lower resolution runs. – Duncan Fairlie, 1/25/07

(We'll) implement the [dust] code in the standard [GEOS-Chem] model and put a warning about expected low bias when the simulation is run at 4x5. Whoever is interested in running dust at 4x5 in the future can deal with making the fix. – Daniel Jacob, 1/25/07

#### !REFERENCES:

• Zender, C. S., Bian, H., and Newman, D.: Mineral Dust Entrainment and Deposition (DEAD) model: Description and 1990s dust climatology, Journal of Geophysical Research: Atmospheres, 108, 2003.

#### **INTERFACE:**

MODULE HCOX\_TOMAS\_DustDead\_Mod

#### **USES:**

USE HCO\_ERROR\_MOD

USE HCO\_DIAGN\_MOD

USE HCOX\_State\_MOD, ONLY : Ext\_State

USE HCO\_STATE\_MOD, ONLY : HCO\_State

IMPLICIT NONE

PRIVATE

### PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCOX\_TOMAS\_DustDead\_Run

PUBLIC :: HCOX\_TOMAS\_DustDead\_Init

PUBLIC :: HCOX\_TOMAS\_DustDead\_Final

PUBLIC :: HCOX\_TOMAS\_DustDead\_GetFluxTun

#### REVISION HISTORY:

- (1) Added parallel DO loop in GET\_ORO (bmy, 4/14/04)
- (2) Now references "directory\_mod.f" (bmy, 7/20/04)
- (3) Fixed typo in ORO\_IS\_LND for PGI compiler (bmy, 3/1/05)
- (4) Modified for GEOS-5 and GCAP met fields (swu, bmy, 8/16/05)
- (5 ) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (6) Now uses GOCART source function (tdf, bmy, 1/25/07)
- (7) Modifications for  $0.5 \times 0.667$  grid (yxw, dan, bmy, 11/6/08)
- (8) Updates for nested grids (amv, bmy, 12/18/09)
- 01 Mar 2012 R. Yantosca Now reference new grid\_mod.F90
- 25 Nov 2013 C. Keller Now a HEMCO extension
- 06 Oct 2014 C. Keller Allow mass flux tuning factor be set in configuration file.
- 07 Jan 2016 E. Lundgren Change dry air gas constant and molec wt to match GC values and update acc due to gravity and universal gas constant to NIST 2014 values
- 14 Oct 2016 C. Keller Now use HCO\_EvalFld instead of HCO\_GetPtr.

### 2.20.1 HCOX\_TOMAS\_DustDead\_Run

Subroutine HcoX\_DustDead\_Run is the driver routine for the HEMCO DEAD dust extension.

SUBROUTINE HCOX\_TOMAS\_DustDead\_Run( am\_I\_Root, ExtState, HcoState
& , RC )

#### **USES:**

USE HCO\_CALC\_MOD, ONLY : HCO\_EvalFld
USE HCO\_FLUXARR\_MOD, ONLY : HCO\_EmisAdd
USE HCO\_CLOCK\_MOD, ONLY : HcoClock\_Get
USE HCO\_CLOCK\_MOD, ONLY : HcoClock\_First
USE HCO\_State\_Mod, ONLY : HCO\_GetHcoID

#### INPUT PARAMETERS:

LOGICAL, INTENT(IN ) :: am\_I\_Root

TYPE(Ext\_State), POINTER :: ExtState ! Module options TYPE(HCO\_State), POINTER :: HcoState ! Hemco state

# INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

### **REVISION HISTORY:**

- 08 Apr 2004 T. D. Fairlie Initial version
- (1) Added OpenMP parallelization, added comments (bmy, 4/8/04)
- (2) Bug fix: DSRC needs to be held PRIVATE (bmy, 4/14/04)
- (3 ) Now references DATA\_DIR from "directory\_mod.f" (bmy, 7/20/04)
- (4) Now make sure all USE statements are USE, ONLY (bmy, 10/3/05)
- (5 ) Bug fix: It should be SNOW/1d3 not SNOW\*1d3 (tdf, bmy, 11/18/05)
- (6) Updated output statement (bmy, 1/23/07)
- (7) Use SNOMAS (m H2O) for GEOS-5 (bmy, 1/24/07)
- 25 Aug 2010 R. Yantosca Treat MERRA in the same way as for GEOS-5
- 25 Aug 2010 R. Yantosca Added ProTeX headers
- 03 Sep 2010 R. Yantosca Bug fix, SNOMAS was mislabled in GEOS-5 and has units of mm H2O instead of m H2O so we need to convert to m H2O.
- 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\_R(I,J,L) from grid\_mod.F90
- 09 Nov 2012 M. Payer Replaced all met field arrays with State\_Met derived type object
- 25 Nov 2013 C. Keller Now a HEMCO extension
- 06 Oct 2014 C. Keller Now calculate pressure center from edges.
- 26 Oct 2016 R. Yantosca Don't nullify local ptrs in declaration stmts

#### 2.20.2 HCOX\_TOMAS\_DustDead\_Init

Subroutine HcoX\_DustDead\_Init initializes the HEMCO DUST\_DEAD extension.

### **USES:**

```
USE HCO_ExtList_Mod, ONLY : GetExtNr, GetExtOpt
USE HCO_STATE_MOD, ONLY : HCO_GetExtHcoID
```

### INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
```

TYPE(HCO\_State), POINTER :: HcoState ! Hemco state
CHARACTER(LEN=\*), INTENT(IN ) :: ExtName ! Extension name
TYPE(Ext\_State), POINTER :: ExtState ! Module options

# INPUT/OUTPUT PARAMETERS:

```
INTEGER, INTENT(INOUT) :: RC
```

### **REVISION HISTORY:**

```
25 Nov 2013 - C. Keller - Now a HEMCO extension
14 Aug 2014 - R. Yantosca - Now always print out extension info
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

### 2.20.3 HCOX\_TOMAS\_DustDead\_Final

Subroutine HcoX\_DustDead\_Final finalizes the HEMCO DUST\_DEAD extension.

# **INTERFACE:**

```
SUBROUTINE HCOX_TOMAS_DustDead_Final( ExtState )
```

### INPUT PARAMETERS:

```
TYPE(Ext_State), POINTER :: ExtState ! Module options
```

### **REVISION HISTORY:**

```
25 Nov 2013 - C. Keller - Now a HEMCO extension !NOTES:
```

### 2.20.4 InstGet

Subroutine InstGet returns a pointer to the desired instance.

```
SUBROUTINE InstGet (Instance, Inst, RC, PrevInst)
```

### INPUT PARAMETERS:

INTEGER :: Instance TYPE(MyInst), POINTER :: Inst INTEGER :: RC

TYPE(MyInst), POINTER, OPTIONAL :: PrevInst

### REVISION HISTORY:

18 Feb 2016 - C. Keller - Initial version

### 2.20.5 InstCreate

Subroutine InstCreate creates a new instance.

### **INTERFACE:**

SUBROUTINE InstCreate (ExtNr, Instance, Inst, RC)

#### INPUT PARAMETERS:

INTEGER, INTENT(IN) :: ExtNr

### **OUTPUT PARAMETERS:**

### INPUT/OUTPUT PARAMETERS:

INTEGER, INTENT(INOUT) :: RC

### **REVISION HISTORY:**

18 Feb 2016 - C. Keller - Initial version

26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts

# 2.20.6 InstRemove

Subroutine InstRemove creates a new instance.

### **INTERFACE:**

SUBROUTINE InstRemove (Instance)

### INPUT PARAMETERS:

INTEGER :: Instance

# **REVISION HISTORY:**

18 Feb 2016 - C. Keller - Initial version

26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts

## 2.21 Fortran: Module Interface hcox\_tomas\_jeagle\_mod.F90

Module HCOX\_TOMAS\_JEAGLE\_Mod contains routines to calculate sea salt aerosol emissions for the TOMAS aerosol microphysics package. JKODROS - This is an update of hcox\_tomas\_seasalt\_mod.F90 to use Jeagle emissions. Should bring TOMAS emissions in line with bulk sea salt.

This is a HEMCO extension module that uses many of the HEMCO core utilities.

### References:

• Clarke, A.D., Owens, S., Zhou, J. An ultrafine sea-salt flux from breaking waves: Implications for CCN in the remote marine atmosphere, J. Geophys. Res., 2006.

### **INTERFACE:**

```
MODULE HCOX_TOMAS_Jeagle_Mod
```

#### **USES:**

```
USE HCO_Error_Mod
USE HCO_Diagn_Mod
USE HCO_State_Mod, ONLY : HCO_State
USE HCOX_State_Mod, ONLY : Ext_State
IMPLICIT NONE
PRIVATE
```

### PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: HCOX_TOMAS_Jeagle_Init
PUBLIC :: HCOX_TOMAS_Jeagle_Run
PUBLIC :: HCOX_TOMAS_Jeagle_Final
```

### **REVISION HISTORY:**

```
01 Oct 2014 - R. Yantosca - Initial version, based on TOMAS code

20 May 2015 - J. Kodros - Added fixes to integrate TOMAS with HEMCO

02 JUL 2015 - J. Kodros - Updating to use scale factors from Jeagle

et al. (2011)
```

# ${\bf 2.21.1 \quad HCOX\_TOMAS\_Jeagle\_Run}$

Subroutine HCOX\_TOMAS\_Jeagle\_Run emits sea-salt into the TOMAS sectional sea-salt mass and aerosol number arrays. Sea-salt emission parameterization of Jeagle et al. (2011).

```
SUBROUTINE HCOX_TOMAS_Jeagle_Run( am_I_Root, ExtState, HcoState, RC )
USES:
```

```
USE HCO_GeoTools_Mod, ONLY : HCO_LandType
USE HCO_FluxArr_mod, ONLY : HCO_EmisAdd
USE HCO_State_Mod, ONLY : HCO_GetHcoID
```

#### INPUT PARAMETERS:

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

TYPE(Ext\_State), POINTER :: ExtState ! Extension Options object

TYPE(HCO\_State), POINTER :: HcoState ! HEMCO state object

### INPUT/OUTPUT PARAMETERS:

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

### **REMARKS:**

#### REVISION HISTORY:

```
01 Oct 2014 - R. Yantosca - Initial version, based on TOMAS SRCSALT30 code 20 May 2015 - J. Kodros - Add seasalt number & mass to HEMCO state
```

20 May 2015 - R. Yantosca - Pass am\_I\_Root to HCO\_EMISADD routine

22 May 2015 - R. Yantosca - Extend up to 40 size bins

10 Jul 2015 - R. Yantosca - Fixed minor issues in the ProTeX headers

26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts

### 2.21.2 HCOX\_TOMAS\_Jeagle\_Init

Subroutine HcoX\_TOMAS\_Jeagle\_Init initializes all extension variables.

### **INTERFACE:**

#### **USES:**

```
USE HCO_State_Mod, ONLY : HCO_GetHcoID
USE HCO_STATE_MOD, ONLY : HCO_GetExtHcoID
USE HCO_ExtList_Mod, ONLY : GetExtNr
```

INPUT PARAMETERS:

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

TYPE(HCO\_State), POINTER :: HcoState ! HEMCO state object CHARACTER(LEN=\*), INTENT(IN ) :: ExtName ! Extension name

TYPE(Ext\_State), POINTER :: ExtState ! Extension options object

# INPUT/OUTPUT PARAMETERS:

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

### REVISION HISTORY:

```
15 Dec 2013 - C. Keller - Initial version
10 Jul 2015 - R. Yantosca - Fixed minor issues in ProTeX header
```

### 2.21.3 HCOX\_TOMAS\_Jeagle\_Final

Subroutine HcoX\_TOMAS\_Jeagle\_Final deallocates all module arrays.

#### **INTERFACE:**

```
SUBROUTINE HCOX_TOMAS_Jeagle_Final
```

### **REVISION HISTORY:**

```
15 Dec 2013 - C. Keller - Initial version
20 May 2015 - J. Kodros - Deallocate HcoIDs, TC1, TC2 arrays
```

### 2.22 Fortran: Module Interface hcox\_tools\_mod.F90

Module HCOX\_Tools\_Mod contains a collection of helper routines for the HEMCO extensions.

### **INTERFACE:**

```
MODULE HCOX_TOOLS_MOD
```

### **USES:**

```
USE HCO_ERROR_MOD
```

IMPLICIT NONE PRIVATE

### PUBLIC MEMBER FUNCTIONS:

```
PUBLIC :: HCOX_SCALE
!MODULE VARIABLES:
```

CHARACTER(LEN=31), PARAMETER, PUBLIC :: HCOX\_NOSCALE = 'none'

# PRIVATE MEMBER FUNCTIONS:

```
11 Jun 2015 - C. Keller - Initial version
```

### 2.22.1 HCOX\_SCALE\_sp2D

Applies mask 'SCALENAME' to the passed 2D sp field.

### **INTERFACE:**

```
SUBROUTINE HCOX_SCALE_sp2D( am_I_Root, HcoState, Arr, SCALENAME, RC )
USES:
```

```
USE HCO_CALC_MOD, ONLY : HCO_EvalFld USE HCO_STATE_MOD, ONLY : HCO_State
```

### INPUT PARAMETERS:

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

TYPE(HCO_STATE), POINTER :: HcoState ! HcoState obj

CHARACTER(LEN=*), INTENT(IN ) :: SCALENAME ! SCALE to be used
```

# INPUT/OUTPUT PARAMETERS:

```
REAL(sp), INTENT(INOUT) :: Arr(:,:) ! Array to be scaled INTEGER, INTENT(INOUT) :: RC ! Success or failure?
```

# **REVISION HISTORY:**

```
11 Jun 2013 - C. Keller - Initial version
```

# 2.22.2 HCOX\_SCALE\_sp3D

Applies mask 'SCALENAME' to the passed 3D sp field.

### INTERFACE:

```
SUBROUTINE HCOX_SCALE_sp3D( am_I_Root, HcoState, Arr, SCALENAME, RC )
USES:
```

```
USE HCO_CALC_MOD, ONLY : HCO_EvalFld USE HCO_STATE_MOD, ONLY : HCO_State
```

### INPUT PARAMETERS:

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

TYPE(HCO_STATE), POINTER :: HcoState ! HcoState obj

CHARACTER(LEN=*), INTENT(IN ) :: SCALENAME ! SCALE to be used
```

### INPUT/OUTPUT PARAMETERS:

```
REAL(sp), INTENT(INOUT) :: Arr(:,:,:) ! Array to be scaled INTEGER, INTENT(INOUT) :: RC ! Success or failure?
```

```
11 Jun 2013 - C. Keller - Initial version
```

### 2.22.3 HCOX\_SCALE\_dp2D

Applies mask 'SCALENAME' to the passed 2D dp field.

### **INTERFACE:**

```
SUBROUTINE HCOX_SCALE_dp2D( am_I_Root, HcoState, Arr, SCALENAME, RC )
USES:
```

```
USE HCO_CALC_MOD, ONLY : HCO_EvalFld USE HCO_STATE_MOD, ONLY : HCO_State
```

### INPUT PARAMETERS:

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

TYPE(HCO_STATE), POINTER :: HcoState ! HcoState obj

CHARACTER(LEN=*), INTENT(IN ) :: SCALENAME ! SCALE to be used
```

# INPUT/OUTPUT PARAMETERS:

```
REAL(dp), INTENT(INOUT) :: Arr(:,:) ! Array to be scaled INTEGER, INTENT(INOUT) :: RC ! Success or failure?
```

# **REVISION HISTORY:**

```
11 Jun 2013 - C. Keller - Initial version
```

### 2.22.4 HCOX\_SCALE\_dp3D

Applies mask 'SCALENAME' to the passed 3D dp field.

### INTERFACE:

```
SUBROUTINE HCOX_SCALE_dp3D( am_I_Root, HcoState, Arr, SCALENAME, RC )
USES:
```

```
USE HCO_CALC_MOD, ONLY : HCO_EvalFld USE HCO_STATE_MOD, ONLY : HCO_State
```

### INPUT PARAMETERS:

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

TYPE(HCO_STATE), POINTER :: HcoState ! HcoState obj

CHARACTER(LEN=*), INTENT(IN ) :: SCALENAME ! SCALE to be used
```

### INPUT/OUTPUT PARAMETERS:

```
REAL(dp), INTENT(INOUT) :: Arr(:,:,:) ! Array to be scaled INTEGER, INTENT(INOUT) :: RC ! Success or failure?
```

```
11 Jun 2013 - C. Keller - Initial version
```

#### 2.23 Fortran: Module Interface ocean\_toolbox\_mod.F90

Module Ocean\_ToolBox\_Mod contains functions and routines to calculate the ocean exchange velocity for any gas, according to Johnson, 2010. References:

- M.T. Johnson: "A numerical scheme to calculate temperature and salinity dependent air-water transfer velocities for any gas", Ocean Sci. 6, 913-932, 2010.
- Liss and Slater: Flux of gases across the air-sea interface, Nature, 247, 1974.
- Laliberte, M: "Model for calculating the viscosity of aqueous solutions", Journal of Chemical & Engineering Data, 52, 2007.
- Millero and Poisson: "International one-atmosphere equation of state of seawater", Deep Sea Res. Pt A, 28, 1981.
- Wilke and Chang: "Correlation of diffusion coefficients in dilute solutions", AIChE Journal, 1, 1955.
- Hayduk and Minhas, "Correlations for prediction of molecular diffusivities in liquids, Can. J. Chem. Eng., 60, 1982,
- E. Fuller et al.: "New method for prediction of binary gas-phase diffusion coefficients", Industrial & Engineering Chemistry, 58, 1966.

#### **INTERFACE:**

MODULE Ocean\_ToolBox\_Mod

### **USES:**

IMPLICIT NONE PRIVATE

### PUBLIC MEMBER FUNCTIONS:

PUBLIC :: Calc\_Kg

### PRIVATE MEMBER FUNCTIONS:

PRIVATE :: Calc\_Ka PRIVATE :: Calc\_Kl PRIVATE :: N\_SW PRIVATE :: P\_SW PRIVATE :: V\_SW PRIVATE :: D\_WC PRIVATE :: D\_HM PRIVATE :: Schmidt\_W

PRIVATE :: Schmidt\_Saltzmann

PRIVATE :: Schmidt\_Acet

PRIVATE :: N\_Air PRIVATE :: P\_Air PRIVATE :: V\_Air PRIVATE :: D\_Air
PRIVATE :: Schmidt\_G

! PARAMETER

INTEGER, PARAMETER :: OC\_SUCCESS = 0
INTEGER, PARAMETER :: OC\_FAIL = -999

### REVISION HISTORY:

```
11 Apr 2013 - C. Keller: Adapted from F. Paulot
03 Oct 2-14 - C. Keller: Added error trap for negative Schmidt numbers
```

## 2.23.1 Calc\_Kg

Subroutine Calc\_Kg is the wrapper routine to calculate the exchange velocity Kg used for calculating the ocean-air flux (cf. Liss & Slater 1974) as:

$$F = Kg (Cg - H * Cl)$$

where Cg and Cl are the bulk gas and liquid concentrations and H is the Henry constant (H= Cgs/Cls).

$$1/\text{Kg} = 1/\text{ka} + \text{H/Kl} = \text{Ra} + \text{Rl}.$$

Note that Kg is returned in m/s and not cm h-1, as is usually reported for exchange velocities!

#### **INTERFACE:**

```
SUBROUTINE Calc_Kg( T, P, V, SALT, H, VB, MW, SCW, KG, RC, RA_OVER_RL, VERBOSE )
```

#### INPUT PARAMETERS:

```
REAL*8, INTENT(IN
                              ! Surface temperature
                                                       [C]
                   ) :: T
REAL*8, INTENT(IN ) :: P
                              ! Surface pressure
                                                       [Pa]
REAL*8, INTENT(IN ) :: V ! Surface wind speed
                                                       [m/s]
REAL*8, INTENT(IN ) :: SALT ! Salinity
                                                       [PSU]
                              ! Henry constant
                  ) :: H
                                                       [-]
REAL*8, INTENT(IN
                             ! Liquid mol. volume
                                                       [cm3/mol]
REAL*8, INTENT(IN
                   ) :: VB
                      :: MW ! Molecular weight
REAL*8, INTENT(IN
                   )
                                                       [g/mol]
INTEGER, INTENT(IN
                      :: SCW ! Parameterization type
                              ! for Schmidt number in water
LOGICAL, INTENT(IN
                   ), OPTIONAL :: VERBOSE
                                           ! turn on verbose output
```

# **OUTPUT PARAMETERS:**

```
REAL*8, INTENT( OUT) :: KG ! Exchange velocity [ms-1]
INTEGER, INTENT( OUT) :: RC ! Error code
REAL*8, INTENT( OUT), OPTIONAL :: RA_OVER_RL ! Ra/Rl [-]
```

```
11 Apr 2013 - C. Keller: Adapted from F. Paulot
```

21 May 2013 - C. Keller: SCW added to argument list

15 Aug 2014 - C. Keller: Now limit temperature to -40 degC to avoid overflow

error. Also added error trap for temperatures

between -10.7 and -10.9 degrees that cause a div-zero

error in subroutine N\_SW.

### 2.23.2 Calc\_Ka

Calc\_Ka returns the air exchange velocity KA.

### **INTERFACE:**

FUNCTION Calc\_Ka(T,P,V,MW,VB,VERB) RESULT(KA)

### INPUT PARAMETERS:

```
REAL*8, INTENT(IN) :: T,P,V, MW, VB!T in C, P in Pa {}^{\circ}
```

LOGICAL, INTENT(IN) :: VERB

### RETURN VALUE:

REAL\*8 :: KA

### REVISION HISTORY:

```
11 Apr 2013 - C. Keller: Adapted from F. Paulot
```

### 2.23.3 Calc\_Kl

Calc\_Kl calculates the water exchange velocity Kl following Nightingale et al., Geophysical Research Letters, 2000.

#### **INTERFACE:**

```
FUNCTION Calc_Kl(T,V,S,VB,SCW,VERB) RESULT(K)
```

# INPUT PARAMETERS:

```
REAL*8, INTENT(IN) :: T,S,V,VB
INTEGER, INTENT(IN) :: SCW
LOGICAL, INTENT(IN) :: VERB
```

### RETURN VALUE:

REAL\*8 :: K

```
11 Apr 2013 - C. Keller: Adapted from F. Paulot
```

### 2.23.4 N<sub>-</sub>SW

N\_SW returns the dynamic seawater viscosity following Laliberte, 2007.

### **INTERFACE:**

FUNCTION N\_SW(T,S) RESULT(N)

### INPUT PARAMETERS:

REAL\*8, INTENT(IN) :: T,S !temperature (C) and salinity

### RETURN VALUE:

REAL\*8 :: N ! Dynamic viscosity

#### REVISION HISTORY:

```
11 Apr 2013 - C. Keller - Adapted from F. Paulot
```

1 Jul 2014 - R. Yantosca - Bug fix: Don't take LOG(NI) if NI is zero

#### 2.23.5 P\_SW

P\_SW returns the seawater density following Millero and Poisson, 1981.

### **INTERFACE:**

FUNCTION P\_SW(T,S) RESULT(P)

### INPUT PARAMETERS:

REAL\*8, INTENT(IN) :: T,S

### RETURN VALUE:

REAL\*8 :: P

# **REVISION HISTORY:**

11 Apr 2013 - C. Keller: Adapted from F. Paulot

### $2.23.6 V_SW$

V\_SW returns the ???

### **INTERFACE:**

FUNCTION V\_SW(T,S) RESULT(V)

### INPUT PARAMETERS:

REAL\*8, INTENT(IN) :: T,S

# RETURN VALUE:

REAL\*8 :: V

### **REVISION HISTORY:**

11 Apr 2013 - C. Keller: Adapted from F. Paulot

### 2.23.7 D<sub>-</sub>WC

D\_WC returns the (water) diffusion coefficient following Wilke and Chang, 1955.

### **INTERFACE:**

FUNCTION D\_WC(T,S,VB) RESULT(D)

### INPUT PARAMETERS:

REAL\*8, INTENT(IN) :: T,S,VB

### RETURN VALUE:

REAL\*8 :: D

# **REVISION HISTORY:**

11 Apr 2013 - C. Keller: Adapted from F. Paulot

### 2.23.8 D\_HM

D\_HM returns the (water) diffusivity following Hayduk and Minhas, 1982.

### INTERFACE:

FUNCTION D\_HM(T,S,VB) RESULT(D)

# INPUT PARAMETERS:

REAL\*8, INTENT(IN) :: T,S,VB

### RETURN VALUE:

REAL\*8 :: D

### **REVISION HISTORY:**

11 Apr 2013 - C. Keller: Adapted from F. Paulot

### 2.23.9 Schmidt\_W

Schmidt\_W returns the Schmidt number of the gas in the water following Johnson, 2010.

#### **INTERFACE:**

FUNCTION Schmidt\_W(T,S,VB) RESULT(SC)

### INPUT PARAMETERS:

REAL\*8, INTENT(IN) :: T,S,VB

# RETURN VALUE:

REAL\*8 :: SC

### **REVISION HISTORY:**

11 Apr 2013 - C. Keller: Adapted from F. Paulot

### 2.23.10 Schmidt\_Saltzmann

Schmidt\_Saltzmann returns the Schmidt number of the gas in the water calculated according to Saltzmann et al., 1993.

#### INTERFACE:

FUNCTION Schmidt\_Saltzmann(T) RESULT(SC)

# INPUT PARAMETERS:

REAL\*8, INTENT(IN) :: T ! Temperature in C

#### RETURN VALUE:

REAL\*8 :: SC

### **REVISION HISTORY:**

11 Apr 2013 - C. Keller: Adapted from F. Paulot

#### 2.23.11 Schmidt\_Acet

Schmidt\_Acet returns the Schmidt number of acetone.

### **INTERFACE:**

FUNCTION Schmidt\_Acet(T) RESULT(SC)

### INPUT PARAMETERS:

REAL\*8, INTENT(IN) :: T ! Temperature in C

# RETURN VALUE:

REAL\*8 :: SC

### **REVISION HISTORY:**

11 Aug 2013 - C. Keller: Initial version

### 2.23.12 N\_Air

N\_Air returns the dynamic air viscosity.

### **INTERFACE:**

FUNCTION N\_Air(T) RESULT(N)

### INPUT PARAMETERS:

REAL\*8, INTENT(IN) :: T

# RETURN VALUE:

REAL\*8 :: N

### **REVISION HISTORY:**

11 Apr 2013 - C. Keller: Adapted from F. Paulot

### 2.23.13 P\_Air

P\_Air returns the kinematic air viscosity.

### **INTERFACE:**

FUNCTION P\_Air(T) RESULT(P)

### INPUT PARAMETERS:

REAL\*8, INTENT(IN) :: T

### RETURN VALUE:

REAL\*8 :: P

### **REVISION HISTORY:**

11 Apr 2013 - C. Keller: Adapted from F. Paulot

### 2.23.14 V\_Air

V\_Air returns the kinematic air viscosity (m2/s).

### INTERFACE:

FUNCTION V\_Air(T) RESULT(V)

### INPUT PARAMETERS:

REAL\*8, INTENT(IN) :: T

### RETURN VALUE:

REAL\*8 :: V

# **REVISION HISTORY:**

11 Apr 2013 - C. Keller: Adapted from F. Paulot

# 2.23.15 D\_Air

D\_Air returns the gas phase diffusion coefficient according to Fuller et al., 1966.

#### **INTERFACE:**

FUNCTION D\_Air(T,P,MW,VB) RESULT(D)

# INPUT PARAMETERS:

REAL\*8, INTENT(IN) :: T !T in C
REAL\*8, INTENT(IN) :: P !P in Pa
REAL\*8, INTENT(IN) :: MW !MW in g/mol

REAL\*8, INTENT(IN) :: VB !Liq. molar volume (cm3/mol)

### **RETURN VALUE:**

REAL\*8 :: D

### **REVISION HISTORY:**

11 Apr 2013 - C. Keller: Adapted from F. Paulot

#### 2.23.16 Schmidt\_G

Schmidt\_G returns the schmidt number of the gas in the air.

### **INTERFACE:**

FUNCTION Schmidt\_G(T,P,MW,VB) RESULT(SC)

### INPUT PARAMETERS:

REAL\*8, INTENT(IN) :: T, P, MW, VB

### RETURN VALUE:

REAL\*8 :: SC

### **REVISION HISTORY:**

11 Apr 2013 - C. Keller: Adapted from F. Paulot

# 3 HEMCO "Interfaces" modules

These modules contain routines that are used to connect HEMCO to other models, or to use HEMCO in standalone mode.

## 3.1 Fortran: Module Interface hcoi\_esmf\_mod

Module HCOI\_ESMF\_MOD is the HEMCO-ESMF interface module.

#### **INTERFACE:**

MODULE HCOI\_ESMF\_MOD

### **USES:**

USE HCO\_ERROR\_MOD USE HCO\_Types\_Mod

#if defined (ESMF\_)

#include "MAPL\_Generic.h"
USE ESMF

USE MAPL\_Mod

IMPLICIT NONE

PRIVATE

### PUBLIC MEMBER FUNCTIONS:

! ESMF environment only: PUBLIC :: HCO\_SetServices PUBLIC :: HCO\_SetExtState\_ESMF

PUBLIC :: HCO\_Imp2Ext

### PRIVATE MEMBER FUNCTIONS:

PRIVATE :: Diagn2Exp
PRIVATE :: HCO\_Imp2Ext2R
PRIVATE :: HCO\_Imp2Ext2S
PRIVATE :: HCO\_Imp2Ext2I
PRIVATE :: HCO\_Imp2Ext3R
PRIVATE :: HCO\_Imp2Ext3S

### REVISION HISTORY:

10 Oct 2014 - C. Keller - Initial version

#### 3.1.1 HCO SetServices

Subroutine HCO\_SetServices registers all required HEMCO data so that it can be imported through the ESMF import state. This routine determines all required HEMCO input fields from the HEMCO configuration file. Note that each file needs an equivalent ESMF-style entry in the registry file (typically ExtData.rc). Otherwise, ESMF won't read these files and HEMCO will fail when attempting to get pointers to these data arrays.

The field names provided in ExtData.rc must match the names in the HEMCO configuration file! Also, all time settings (average and update interval) and data units need to be properly specified in ExtData.rc. For now, ExtData.rc and HEMCO configuration file need to be synchronized manually. The pyHEMCO interface will automate this process!

This routine also prepares an emissions export field for every species found in the HEMCO configuration file. These export fields will only be filled if specified so in the MAPL History registry. The corresponding HEMCO diagnostics must be created separately via Diagn\_Create (e.g. in hcoi\_gc\_diagn\_mod.F90).

#### **INTERFACE:**

```
SUBROUTINE HCO_SetServices( am_I_Root, GC, HcoConfig, & ConfigFile, RC)
```

### **USES:**

USE HCO\_TYPES\_MOD, ONLY : ListCont

USE HCO\_DATACONT\_MOD, ONLY : ListCont\_NextCont
USE HCO\_CONFIG\_MOD, ONLY : Config\_ReadFile

USE HCO\_EXTLIST\_MOD, ONLY : GetExtOpt

```
USE HCO_CONFIG_MOD, ONLY : Config_GetnSpecies
USE HCO_CONFIG_MOD, ONLY : Config_GetSpecNames
USE HCO_DIAGN_MOD, ONLY : DiagnFileOpen
USE HCO_DIAGN_MOD, ONLY : DiagnFileGetNext
USE HCO_DIAGN_MOD, ONLY : DiagnFileClose
```

### ARGUMENTS:

```
LOGICAL, INTENT(IN) :: am_I_Root
TYPE(ESMF_GridComp), INTENT(INOUT) :: GC
TYPE(ConfigObj), POINTER :: HcoConfig
CHARACTER(LEN=*), INTENT(IN) :: ConfigFile
INTEGER, INTENT(OUT) :: RC
```

### **REVISION HISTORY:**

```
29 Aug 2013 - C. Keller - Initial version.

10 Sep 2015 - C. Keller - Added RESTART=MAPL_RestartSkip.

21 Feb 2016 - C. Keller - Update to v2.0, added default diagnostics (optional)

26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

### 3.1.2 Diagn2Exp

Subroutine Diagn2Exp is a helper routine to add a potential HEMCO diagnostics to the Export state.

#### **INTERFACE:**

```
SUBROUTINE Diagn2Exp( GC, SNAME, LNAME, UNITS, NDIM, RC )
```

### **USES:**

### **ARGUMENTS:**

```
TYPE(ESMF_GridComp), INTENT(INOUT) :: GC
CHARACTER(LEN=*), INTENT(IN ) :: SNAME
CHARACTER(LEN=*), INTENT(IN ) :: LNAME
CHARACTER(LEN=*), INTENT(IN ) :: UNITS
INTEGER, INTENT(IN ) :: NDIM
INTEGER, INTENT(OUT) :: RC
```

```
05 Jan 2015 - C. Keller - Initial version
```

### 3.1.3 HCO\_SetExtState\_ESMF

Subroutine HCO\_SetExtState\_ESMF tries to populate some fields of the ExtState object from the ESMF import state.

#### **INTERFACE:**

```
SUBROUTINE HCO_SetExtState_ESMF( am_I_Root, HcoState, ExtState, RC )
```

### **USES:**

```
USE HCO_STATE_MOD, ONLY : Hco_State USE HCOX_STATE_MOD, ONLY : Ext_State
```

### **ARGUMENTS:**

```
LOGICAL, INTENT(IN ) :: am_I_Root
TYPE(HCO_State), POINTER :: HcoState
TYPE(Ext_State), POINTER :: ExtState
INTEGER, INTENT(INOUT) :: RC
```

### REVISION HISTORY:

```
06 Mar 2015 - C. Keller - Initial version
```

# 3.1.4 HCO\_Imp2Ext2S

Subroutine HCO\_Imp2Ext copies fields from the import state to the HEMCO ExtState object.

### INTERFACE:

```
SUBROUTINE HCO_Imp2Ext2S( am_I_Root, HcoState, ExtDat, FldName, RC )
```

### **USES:**

```
USE HCO_ARR_MOD, ONLY : HCO_ArrAssert
USE HCO_STATE_MOD, ONLY : Hco_State
USE HCOX_STATE_MOD, ONLY : ExtDat_2S
```

### **ARGUMENTS:**

```
LOGICAL,
                                      :: am_I_Root
                      INTENT(IN
                                  )
CHARACTER(LEN=*),
                      INTENT(IN
                                  )
                                      :: FldName
TYPE(HCO_State),
                                      :: HcoState
                     POINTER
TYPE(ExtDat_2S),
                                      :: ExtDat
                     POINTER
INTEGER,
                      INTENT(INOUT)
                                      :: RC
```

```
08 Feb 2016 - C. Keller - Initial version
```

## 3.1.5 HCO\_Imp2Ext3S

Subroutine HCO\_Imp2Ext copies fields from the import state to the HEMCO ExtState object.

#### **INTERFACE:**

```
SUBROUTINE HCO_Imp2Ext3S( am_I_Root, HcoState, ExtDat, FldName, RC )
```

## **USES:**

```
USE HCO_ARR_MOD, ONLY : HCO_ArrAssert
USE HCO_STATE_MOD, ONLY : Hco_State
USE HCOX_STATE_MOD, ONLY : ExtDat_3S
```

#### **ARGUMENTS:**

```
LOGICAL,
                     INTENT(IN
                                  )
                                      :: am_I_Root
CHARACTER(LEN=*),
                                  )
                                      :: FldName
                     INTENT(IN
TYPE(HCO_State),
                                      :: HcoState
                     POINTER
TYPE(ExtDat_3S),
                     POINTER
                                      :: ExtDat
                     INTENT(INOUT)
                                      :: RC
INTEGER,
```

#### **REVISION HISTORY:**

```
08 Feb 2016 - C. Keller - Initial version
```

## 3.1.6 HCO\_Imp2Ext2R

Subroutine HCO\_Imp2Ext copies fields from the import state to the HEMCO ExtState object.

#### **INTERFACE:**

```
SUBROUTINE HCO_Imp2Ext2R( am_I_Root, HcoState, ExtDat, FldName, RC )
```

### **USES:**

```
USE HCO_STATE_MOD, ONLY : Hco_State
USE HCOX_STATE_MOD, ONLY : ExtDat_2R
USE HCO_ARR_MOD, ONLY : HCO_ArrAssert
```

## **ARGUMENTS:**

```
:: am_I_Root
LOGICAL,
                     INTENT(IN
                                 )
                                     :: FldName
CHARACTER(LEN=*),
                                 )
                     INTENT(IN
TYPE(HCO_State),
                     POINTER
                                     :: HcoState
TYPE(ExtDat_2R),
                     POINTER
                                     :: ExtDat
INTEGER,
                     INTENT(INOUT)
                                     :: RC
```

```
08 Feb 2016 - C. Keller - Initial version
```

## 3.1.7 HCO\_Imp2Ext3R

Subroutine HCO\_Imp2Ext copies fields from the import state to the HEMCO ExtState object.

#### **INTERFACE:**

```
SUBROUTINE HCO_Imp2Ext3R( am_I_Root, HcoState, ExtDat, FldName, RC )
```

## **USES:**

```
USE HCO_STATE_MOD, ONLY : Hco_State
USE HCOX_STATE_MOD, ONLY : ExtDat_3R
USE HCO_ARR_MOD, ONLY : HCO_ArrAssert
```

#### **ARGUMENTS:**

```
LOGICAL,
                     INTENT(IN
                                  )
                                      :: am_I_Root
CHARACTER(LEN=*),
                                  )
                                      :: FldName
                     INTENT(IN
TYPE(HCO_State),
                                      :: HcoState
                     POINTER
TYPE(ExtDat_3R),
                     POINTER
                                      :: ExtDat
                     INTENT(INOUT)
INTEGER,
                                      :: RC
```

### **REVISION HISTORY:**

```
08 Feb 2016 - C. Keller - Initial version
```

## 3.1.8 HCO\_Imp2Ext2I

Subroutine HCO\_Imp2Ext copies fields from the import state to the HEMCO ExtState object.

## **INTERFACE:**

```
SUBROUTINE HCO_Imp2Ext2I( am_I_Root, HcoState, ExtDat, FldName, RC )
```

### **USES:**

```
USE HCO_STATE_MOD, ONLY : Hco_State
USE HCOX_STATE_MOD, ONLY : ExtDat_2I
USE HCO_ARR_MOD, ONLY : HCO_ArrAssert
```

### **ARGUMENTS:**

```
:: am_I_Root
LOGICAL,
                     INTENT(IN
                                 )
                                      :: FldName
CHARACTER(LEN=*),
                                 )
                     INTENT(IN
TYPE(HCO_State),
                     POINTER
                                      :: HcoState
TYPE(ExtDat_2I),
                     POINTER
                                      :: ExtDat
INTEGER,
                     INTENT (INOUT)
                                     :: RC
```

```
08 Feb 2016 - C. Keller - Initial version
```

## 3.2 Fortran: Module Interface hcoi\_standalone\_mod.F90

Module HCOI\_StandAlone\_Mod contains all wrapper routines to run HEMCO in standalone mode, i.e. without any external model connected to it. All HEMCO input variables (grid, species, times) are read from disk. All meteorological variables needed by the (enabled) HEMCO extensions must be provided through the HEMCO configuration file (see ExtOpt\_SetPointers).

Subroutine HCOLStandAlone\_Run will execute the standalone version of HEMCO. The following input files are needed for a standalone run:

- HEMCO\_sa\_Config: the HEMCO configuration file. Must be passed as argument to HCO\_StandAlone\_Run.
- HEMCO\_sa\_Spec: contains the HEMCO species definitions. The first row must contain the total number of species. For each species, the following parameter need to be specified (separated by at least one space character): species ID, name, molecular weight [g/mol], emitted molecular weight [g/mol], the molecule emission ratio, the liq. over gas Henry constant [M/atm], the temperature dependency of the Henry constant (K0, in [K]), and the pKa (for correction of the Henry constant).
- HEMCO\_sa\_Grid: contains the definition of the emission grid. Must contain the grid dimensions (NX, NY, NZ) in the first three rows (e.g. NX: 72), followed by the horizontal grid spaces (DX and DY) in rows four and five, respectively. DX and DY can be only one value (applied to all grid boxes), or a vector of length NX or NY, respectively. For now, no vertical regridding is supported, e.g. all emissions input file need to be either 2D fields or already remapped onto the correct model levels.
- HEMCO\_sa\_Time: contains the time definitions. The first two rows must contain the start and end date of the simulation, in format Start/End: YYYY-MM-DD HH:MM:SS (e.g. 2013-07-01 00:00:00). The third row must contain the emission time step (e.g. TS\_EMIS: 3600.0).

The file names of the species, grid, and time input files can be provided in the settings section of the HEMCO configuration file. For instance, to set the species file to 'mySpecFile', add the following line to the con-figuration file: 'SpecFile: mySpecFile'. The same applies to grid and time definitions (GridFile and TimeFile, respectively). If no file names are provided in the configuration file, the default file names (HEMCO\_sa\_Spec, HEMCO\_sa\_Grid, HEMCO\_sa\_Time) will be used. **INTERFACE:** 

MODULE HCOI\_StandAlone\_Mod

```
USE HCO_Error_Mod
USE HCO_Diagn_Mod
USE HCO_CharTools_Mod
USE HCO_Types_Mod
USE HCOX_State_Mod, ONLY : Ext_State
USE HCO_State_Mod, ONLY : HCO_State

IMPLICIT NONE
PRIVATE
```

## PUBLIC MEMBER FUNCTIONS:

PUBLIC :: HCOI\_StandAlone\_Run

PUBLIC :: HCOI\_SA\_Init
PUBLIC :: HCOI\_SA\_Run
PUBLIC :: HCOI\_SA\_Final

PUBLIC :: HCOI\_SA\_InitCleanup

PUBLIC :: Get\_nnMatch
PUBLIC :: Register\_Species

PUBLIC :: Define\_Diagnostics

### PRIVATE MEMBER FUNCTIONS:

PRIVATE :: Model\_GetSpecies

PRIVATE :: Set\_Grid
PRIVATE :: Read\_Time

PRIVATE :: ExtState\_SetFields
PRIVATE :: ExtState\_UpdateFields

## **REVISION HISTORY:**

20 Aug 2013 - C. Keller - Initial version.

14 Jul 2014 - R. Yantosca - Now use F90 free-format indentation 14 Jul 2014 - R. Yantosca - Cosmetic changes in ProTeX headers

09 Apr 2015 - C. Keller - Now accept comments and empty lines in

all input files.

15 Feb 2015 - C. Keller - Update to v2.0

## 3.2.1 HCOI\_StandAlone\_Run

Subroutine HCOI\_StandAlone\_Run runs the standalone version of HEMCO. All input variables are taken from input files.

### **INTERFACE:**

```
SUBROUTINE HCOI_StandAlone_Run( ConfigFile )
```

### INPUT PARAMETERS:

```
CHARACTER(LEN=*), INTENT(IN) :: ConfigFile
```

#### **REVISION HISTORY:**

```
12 Sep 2013 - C. Keller - Initial version
```

#### 3.2.2 HCOI\_SA\_Init

Subroutine HCOLSA\_Init initializes the HEMCO derived types and arrays.

#### **INTERFACE:**

SUBROUTINE HCOI\_SA\_Init( am\_I\_Root, ConfigFile, RC )

#### **USES:**

USE HCO\_Config\_Mod, ONLY : Config\_ReadFile
USE HCO\_State\_Mod, ONLY : HcoState\_Init
USE HCO\_Driver\_Mod, ONLY : HCO\_Init
USE HCOX\_Driver\_Mod, ONLY : HCOX\_Init

USE HCO\_EXTLIST\_Mod, ONLY : GetExtOpt, CoreNr

#### INPUT PARAMETERS:

LOGICAL, INTENT(IN ) :: am\_I\_Root ! root CPU?

CHARACTER(LEN=\*), INTENT(IN ) :: ConfigFile ! Configuration file

## INPUT/OUTPUT PARAMETERS:

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

#### REVISION HISTORY:

12 Sep 2013 - C. Keller - Initial version

### 3.2.3 HCOI\_SA\_Run

Subroutine HCOLSA\_RUN runs HCO from GEOS-Chem.

#### **INTERFACE:**

SUBROUTINE HCOI\_SA\_RUN( am\_I\_Root, RC )

### **USES:**

USE HCO\_FluxArr\_Mod, ONLY : HCO\_FluxarrReset
USE HCO\_Clock\_Mod, ONLY : HcoClock\_Set
USE HCO\_Clock\_Mod, ONLY : HcoClock\_Get

USE HCO\_Clock\_Mod, ONLY : HcoClock\_Increase

USE HCO\_Driver\_Mod, ONLY : HCO\_RUN
USE HCOX\_Driver\_Mod, ONLY : HCOX\_RUN

### INPUT PARAMETERS:

LOGICAL, INTENT(IN ) :: am\_I\_Root ! root CPU?

## INPUT/OUTPUT PARAMETERS:

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

#### **REVISION HISTORY:**

12 Sep 2013 - C. Keller - Initial version

## 3.2.4 HCOI\_SA\_Final

Subroutine HCOI\_SA\_Final cleans up HEMCO.

#### **INTERFACE:**

```
SUBROUTINE HCOI_SA_Final( am_I_Root )
```

#### **USES:**

```
USE HCO_Driver_Mod, ONLY : HCO_Final
USE HCOX_Driver_Mod, ONLY : HCOX_Final
USE HCO_State_Mod, ONLY : HcoState_Final
```

#### INPUT PARAMETERS:

```
LOGICAL, INTENT(IN) :: am_I_Root
```

## **REVISION HISTORY:**

```
12 Sep 2013 - C. Keller - Initial version
```

## 3.2.5 Model\_GetSpecies

SUBROUTINE Model\_GetSpecies returns 'model' species information from the HEMCO standalone input file.

#### **INTERFACE:**

```
SUBROUTINE Model_GetSpecies( am_I_Root, HcoConfig, & nModelSpec, ModelSpecNames, & ModelSpecIDs, ModelSpecMW, & ModelSpecEmMW, ModelSpecMolecRatio,& ModelSpecKO, ModelSpecCR, & ModelSpecPKA, RC )
```

## **USES:**

```
USE inquireMod, ONLY : findfreeLUN
USE HCO_EXTLIST_Mod, ONLY : GetExtOpt, CoreNr
```

#### **OUTPUT PARAMETERS:**

```
LOGICAL,
                   INTENT(IN ) :: am_I_Root
TYPE(ConfigObj),
                   POINTER
                              :: HcoConfig
                   INTENT(OUT) :: nModelSpec
INTEGER,
                              :: ModelSpecNames(:)
CHARACTER(LEN= 31), POINTER
INTEGER,
                   POINTER
                              :: ModelSpecIDs (:)
                              :: ModelSpecMW
REAL(hp),
                   POINTER
                                               (:)
                   POINTER
                              :: ModelSpecEmMW (:)
REAL(hp),
                              :: ModelSpecMolecRatio(:)
REAL(hp),
                  POINTER
                              :: ModelSpecKO
REAL(hp),
                  POINTER
                                               (:)
REAL(hp),
                              :: ModelSpecCR
                                               (:)
                  POINTER
                  POINTER
                              :: ModelSpecPKA (:)
REAL(hp),
INTEGER,
                  INTENT(OUT) :: RC
```

## **REVISION HISTORY:**

```
13 Sep 2013 - C. Keller - Initial Version
```

#### 3.2.6 Set\_Grid

SUBROUTINE SET\_GRID reads the grid information from the HEMCO standalone grid file and sets all HEMCO grid arrays accordingly. The grid file is expected to contain information on the grid edge lon/lat range, as well as the number of grid cells in longitude and latitude direction.

#### **INTERFACE:**

```
SUBROUTINE SET_Grid( am_I_Root, HcoState, RC )
```

### **USES:**

```
USE Grid_Mod, ONLY : DoGridComputation
```

USE inquireMod, ONLY : findFreeLUN

USE HCO\_ExtList\_Mod, ONLY : HCO\_GetOpt, GetExtOpt, CoreNr

USE HCO\_VertGrid\_Mod, ONLY : HCO\_VertGrid\_Define

#### INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root
```

## INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_STATE), POINTER :: HcoState INTEGER, INTENT(INOUT) :: RC
```

#### **REVISION HISTORY:**

10 Sep 2015 - C. Keller - Allow to provide mid-points instead of edges.

## 3.2.7 Get\_nnMatch

Subroutine Get\_nnMatch returns the number of species found in both the HEMCO configuration and the species input file.

## **INTERFACE:**

```
SUBROUTINE Get_nnMatch( am_I_Root, HcoConfig, nnMatch, RC )
```

```
USE HCO_Config_Mod, ONLY : Config_GetnSpecies
USE HCO_Config_Mod, ONLY : Config_GetSpecNames
```

## **OUTPUT PARAMETERS:**

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

INTEGER, INTENT( OUT) :: nnMatch ! Number of HEMCO species that are

! also species in the atm. model

## INPUT/OUTPUT PARAMETERS:

```
TYPE(ConfigObj), POINTER :: HcoConfig ! Config object
```

#### REVISION HISTORY:

```
13 Sep 2013 - C. Keller - Initial Version
```

## 3.2.8 Register\_Species

Subroutine Register\_Species registers all species in the HEMCO state object.

### **INTERFACE:**

```
SUBROUTINE Register_Species( am_I_Root, HcoState, RC )
```

#### **USES:**

```
USE HCO_LogFile_Mod, ONLY : HCO_SPEC2LOG
```

#### INPUT PARAMETERS:

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

## INPUT/OUTPUT PARAMETERS:

```
TYPE(HCO_STATE), POINTER :: HcoState
```

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

## **REVISION HISTORY:**

```
13 Sep 2013 - C. Keller - Initial Version
```

## 3.2.9 Define\_Diagnostics

Subroutine Define Diagnostics defines all diagnostics to be used in this simulation.

#### **INTERFACE:**

```
SUBROUTINE Define_Diagnostics( am_I_Root, HcoState, RC, SetDefault )
```

```
USE HCO_EXTLIST_MOD, ONLY : GetExtNr
```

## INPUT PARAMETERS:

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

TYPE(HCO\_STATE), POINTER :: HcoState

LOGICAL, INTENT(IN ), OPTIONAL :: SetDefault ! Define default diagnostics?

## INPUT/OUTPUT PARAMETERS:

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

#### **REVISION HISTORY:**

```
13 Sep 2013 - C. Keller - Initial Version
05 Feb 2015 - C. Keller - Added SetDefault flag
```

# 3.2.10 Read\_Time

Subroutine READ\_TIME reads the time information for the HEMCO standalone from an input file.

### **INTERFACE:**

```
SUBROUTINE Read_Time( am_I_Root, HcoState, RC )
```

## **USES:**

```
USE inquireMod, ONLY : findfreeLUN
```

USE HCO\_Extlist\_Mod, ONLY : HCO\_GetOpt, GetExtOpt, CoreNr

#### INPUT PARAMETERS:

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

TYPE(HCO\_State), POINTER :: HcoState

!INPUT/OUTPUT PARAMETERS

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

## **REVISION HISTORY:**

```
13 Sep 2013 - C. Keller - Initial Version
```

#### 3.2.11 ExtState\_SetFields

Subroutine ExtState\_SetFields fills the ExtState data fields with data read through the HEMCO configuration file.

#### **INTERFACE:**

```
SUBROUTINE ExtState_SetFields ( am_I_Root, HcoState, ExtState, RC )
```

```
USE HCO_ARR_MOD, ONLY: HCO_ArrAssert
USE HCO_GEOTOOLS_MOD, ONLY: HCO_GetSUNCOS
USE HCO_GEOTOOLS_MOD, ONLY: HCO_CalcVertGrid
USE HCOX_STATE_MOD, ONLY: ExtDat_Set
USE HCO_CLOCK_MOD, ONLY: HcoClock_First
```

#### INPUT PARAMETERS:

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

TYPE(HCO_STATE), POINTER :: HcoState

TYPE(EXT_STATE), POINTER :: ExtState

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

#### **REVISION HISTORY:**

```
28 Jul 2014 - C. Keller - Initial Version
06 Oct 2014 - M. Sulprizio- Remove PCENTER. Now calculate from pressure edges
09 Jul 2015 - E. Lundgren - Add MODIS Chlorophyll-a (CHLR)
26 Oct 2016 - R. Yantosca - Don't nullify local ptrs in declaration stmts
```

### 3.2.12 ExtState\_UpdateFields

Subroutine ExtState\_UpdateFields makes sure that all local variables that ExtState is pointing to are up to date. For the moment, this is just a placeholder routine as none of the ExtState fields is filled by local module fields. Content can be added to it if there are variables that need to be updated manually, e.g. not through netCDF input data.

#### **INTERFACE:**

```
SUBROUTINE ExtState_UpdateFields ( am_I_Root, HcoState, ExtState, RC )
USES:
```

#### INPUT PARAMETERS:

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

TYPE(HCO_STATE), POINTER :: HcoState

TYPE(EXT_STATE), POINTER :: ExtState

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

```
28 Jul 2014 - C. Keller - Initial Version
```

## 3.2.13 IsEndOfSimulation

Function IsEndOfSimulation returns true if the passed date is beyond the end of the simulation date.

#### **INTERFACE:**

```
FUNCTION IsEndOfSimulation(Yr, Mt, Dy, Hr, Mn, Sc) RESULT (IsEnd)
USES:
```

#### INPUT PARAMETERS:

```
INTENT(IN ) :: YR
 INTEGER,
                   INTENT(IN ) :: MT
 INTEGER,
                  INTENT(IN ) :: DY
 INTEGER,
                              ) :: HR
 INTEGER,
                  INTENT(IN
 INTEGER,
                  INTENT(IN ) :: MN
 INTEGER,
                   INTENT(IN ) :: SC
!OUTPUT PARAMETERS
 LOGICAL
                                :: IsEnd
```

# REVISION HISTORY:

```
08 Sep 2014 - C. Keller - Initial Version
13 Jul 2015 - C. Keller - Bug fix: now save YYYYMMDD and hhmmss in different variables to avoid integer truncation errors.
```

## 3.2.14 HCOI\_Sa\_InitCleanup

deallocates all local species arrays used during initialization.

#### **INTERFACE:**

```
SUBROUTINE HCOI_SA_InitCleanup ( am_I_Root, RC )
```

#### **USES:**

## INPUT PARAMETERS:

```
LOGICAL, INTENT(IN ) :: am_I_Root ! Are we on the root CPU?
!INPUT/OUTPUT PARAMETERS
INTEGER, INTENT(INOUT) :: RC ! Success or failure?
```

```
04 Feb 2016 - C. Keller - Initial Version
```

## 3.3 Fortran: Module Interface hemco\_standalone.F90

Program HEMCO\_StandAlone is the driver for HEMCO in in stand-alone mode. It receives the configuration file name as input argument and then calls the routine HCOI\_StandAlone\_Run (from module file hcoi\_standalone\_mod.F90) to repeatedly call HEMCO for one or more timesteps on the predefined grid.

## **INTERFACE:**

PROGRAM HEMCO\_StandAlone

## **USES:**

```
USE HCOI_STANDALONE_MOD, ONLY : HCOI_Standalone_Run
```

IMPLICIT NONE
INTRINSIC :: TRIM

```
16 Jul 2014 - R. Yantosca - Initial version
21 Jul 2013 - C. Keller - Now pass configuration file name as argument
```