







PREP-CHEM-SRC

A preprocessor of trace gas and aerosol emission fields for regional and global atmospheric chemistry models

User's Guide for version 1.8.3 March 2018

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1. Introduction

PREP-CHEM-SRC is a pollutant emissions numerical too developed at CPTEC/INPE whose function is to create data of atmospheric pollutant emissions from biomass burning, photosynthesis or other forest transformation processes, combustion of oil-based products by vehicles or industry, charcoal production, and many other processes.

The system is maintained and developed at CPTEC/INPE by the GMAI group, which not only updates versions of data such as EDGAR, RETRO, MEGAN, etc., but also implements new functionalities such as volcanic emissions which is present now in this version.

The purpose of this guide is to present how to install, compile and run the pre-processor. Finally, the steps for utilizing the emissions data in the CCATT-BRAMS, WRF-Chem and FIM-Chem models are presented.

We recommend that you read the article "PREP-CHEM-SRC – 1.0: a preprocessor of trace gas and aerosol emission fields for regional and global atmospheric chemistry models" (Freitas et al., 2010 - http://www.geosci-model-dev.net/4/419/2011/gmd-4-419-2011.pdf).

2. Structure

PREP-CHEM-SRC is comprised of 5 principal directories:

- a) aux_src contains modules and libraries from the BRAMS model on which the compilation of PREP-CHEM-SRC depends;
- b) **bin** contains the input file *prep_chem_sources.inp* and the *build* directory which contains the necessary files for compilation;
- a) **extra** contains files and programs that can be utilized by the users such as convert emiss for WRF-Chem;
- b) **src** contains the source code for the emissions model;
- c) **test** contains scripts files for generation of multiple emissions:

The README contains brief instructions on how to compile PREP-CHEM-SRC.

2. Install Libraries

Libraries for PREP-CHEM-SRC version 1.8.3

a) NetCDF

You may download file from ftp://ftp.unidata.ucar.edu/pub/netcdf/netcdf-4.1.3.tar.gz (newer versions not tested):

```
→ wget ftp://ftp.unidata.ucar.edu/pub/netcdf/netcdf-4.1.3.tar.gz
```

Go to a temporary directory and unzip the file netcdf-4.1.3.tar.gz.

```
→ tar -zxvf netcdf-4.1.3.tar.gz
```

Go to the netcdf-4.1.3 directory created in the process of unpacking.

```
→ cd netcdf-4.1.3
```

For the configuration process of the library, use the command:

```
\rightarrow FC=gfortran CC=gcc ./configure -prefix=/opt/lib-gfortran/netcdf-4.1.3 --enable-fortran --disable-netcdf-4 -disable-shared
```

Where:

- prefix must be an preferred user libraries directory, compiled with the preferred compiler (i.e. gfortran). Make sure you can write on this directory;
- FC: the fortran compiler;

For the compilation process:

```
→ make
```

→ make install

b) Zlib

You may download file from http://zlib.net/ (Please check last version)

```
→ wget http://zlib.net/zlib-1.2.8.tar.gz
```

Go to a temporary directory and unzip the file:

```
→ tar -zxvf zlib-1.2.8.tar.gz
```

Enter the zlib-1.2.8 directory created in the process of unpacking:

```
→ cd zlib-1.2.8.
```

For the configuration process of the library, use the command:

```
\rightarrow FC=ifort CC=icc ./configure -prefix=/opt/lib-gfortran/zlib-1.2.8 Where:
```

- prefix must be an preferred user libraries directory;
- FC: the fortran compiler;
- CC: the C compiler.

For the compilation process:

```
→ make
```

Please check the build.

→ make check

After going through all the tests without error messages, install the library.

```
→ make install
```

c) HDF5

You may download source code from http://www.hdfgroup.org/HDF5/release/obtain5.html,

choosing the last version of Stable builds, currently http://www.hdfgroup.org/ftp/HDF5/current/src/hdf5-1.8.16.tar (newer versions not tested yet)

Get the file:

```
→ wget http://www.hdfgroup.org/ftp/HDF5/current/src/hdf5-1.8.16.tar
```

Unzip the file:

```
→ tar -xvf hdf5-1.8.16.tar
```

Go to the directory hdf5-1.8.16 created in the process of unpacking.

```
→ cd hdf5-1.8.16
```

For the process of configuration and installation of the library is necessary for the zlib library is already properly installed.

For the configuration process of the library, use the command:

```
\rightarrow FC=ifort F77=ifort F90=ifort CC=icc CXX=icpc ./configure - prefix=/opt/lib-gfotran/lib/hdf5-1.8.16 --with-zlib=/opt/lib-gfotran/zlib-1.2.8 --disable-shared —enable-fortran
```

Where:

- prefix must be an preferred user libraries directory;
- FC: the fortran compiler: i.e. gfortran
- F77: the fortran 77 or compatible compiler: i.e. gfortran
- F90: the fortran 90 or compatible compiler: i.e. gfortran
- CC: C compiler: i.e. gcc
- CCX: C++ compiler: i.e. g++

For the compilation process:

→ make

Please check the build.

→ make check

After going through all the tests without error messages, install the library.

3. Step-by-step installation:

- a) PHASE I Download the PREP-CHEM-SRC-1.8.3 and the input files
 - Download the PREP-CHEM-SRC-1.8.3.tar.gz at: http://brams.cptec.inpe.br/downloads/
 - Surface and some emission data for testing could be downloaded at: http://brams.cptec.inpe.br/input-data/
- b) PHASE II compile PREP-CHEM-SRC
 - Go to the bin/build directory:

```
→ cd PREP-CHEM-SRC-1.8.3/bin/build
```

• Edit the include.mk.gfortran file (or include.mk.intel, or include.mk.pgi, depending on which compiler was used):

```
→ gedit include.mk.gfortran
```

• Alter the following variables¹:

```
NETCDF = /opt/lib-gfortran/netcdf-4.1.3
NETCDF_LIBS =-L$(NETCDF)/lib -lnetcdff -lnetcdf

HDF5=/opt/lib-gfortran/hdf5-1.8.16
HDF5_INC=-I$(HDF5)/include
HDF5_LIB=-L$(HDF5)/lib -lhdf5hl_fortran -lhdf5_fortran -lhdf5_hl
-lhdf5 -L/opt/lib-gfortran/zlib-1.2.8/lib -lz -ldl
F_COMP = gfortran
C_COMP = gcc
LOADER = gfortran
C_LOADER = gcc
```

Compile the code by running Makefile

For BRAMS:

```
→ make OPT=gfortran CHEM=RELACS_TUV AER=SIMPLE
```

For BRAMS with MATRIX:

```
→ make OPT= gfortran CHEM=RELACS MX AER=MATRIX
```

^{1&}lt;sup>1</sup> For advanced modifications, consult the table in appendix A.

For WRF-Chem/FIM-Chem:

```
→ make OPT=gfortran.wrf CHEM=RADM WRF FIM AER=SIMPLE
```

- c) PHASE III verifying and running PREP-CHEM-SRC
 - Go to the bin directory
 - → cd bin
 - Create a symbolic link to the UserData directory (in source files directory):
 - → ln -s /Data/source/PREP-CHEM-SRC-1.8.3/extra/UserData
 - Download chemical data from http://brams.cptec.inpe.br/input-data/ at Chemical section.
 - Move the extracted data files in a directory, i.e. /Data/datain
 - Create a symbolic link to data files (/Data/datain). This link will be used in prep chem sources.inp:
 - → ln -s /Data/datain datain

NOTE: observe 2 files in particular:

- prep_chem_sources.inp input namelist. It contains the grid configurations, input
 data and other resources for the creation of the emissions map used in the BRAMS
 model;
- prep_chem_sources_<chemical mechanism>.exe executable created by the compilation conducted in phase II;
 - Verify the content of the prep_chem_sources.inp input file:
 - → gedit prep chem sources.inp

```
!----- if \ the \ output \ data \ is \ for \ use \ in \ CATT-BRAMS \ model, \ provide \ at \ least \ one \ analysis \ file \\ !----- of \ this \ model
   rams_anal_prefix = '../ANL/OPQUE',
!----- date of emission
    ihour=00,
    iday=25,
    imon=07
    iyear=2007,
use edgar =3, ! 0 - not, 1 - Version 3, 2 - Version 4 for some species
   edgar_data_dir ='./datain/EMISSION_DATA/EDGAR/hdf/edgar-htap',
   use_gocart =0,
   gocart_data_dir ='./datain/EMISSION_DATA/GOCART/emissions',
   use streets =0,
   streets\_data\_dir="./datain/BRAMS\_5.2/EMISSION\_DATA/STREETS",
   seac4rs_data_dir='./datain/EMISSION_DATA/SEAC4RS',
   use fwbawb =0,
   fwbawb_data_dir ='./datain/EMISSION_DATA/Emissions_Yevich_Logan',
   use_bioge =0, ! 1 - geia, 2 - megan
   ! ######
   ! # BIOGENIC = 1
   bioge_data_dir ='./datain/EMISSION_DATA/biogenic_emissions',
! # MEGAN = 2
   !bioge_data_dir='./datain/EMISSION_DATA/MEGAN/2000',
   ! ######
  use gfedv2 =0,
  gfedv2_data_dir ='./datain/EMISSION_DATA/GFEDv2-8days',
  use_bbem =2,
   use_bbem_plumerise =1,
!----- if the merging of gfedv2 with bbem is desired (=1, yes, \theta = no)
  merge_GFEDv2_bbem =0,
!----- Fire product for BBBEM/BBBEM-plumerise emission models
  bbem_wfabba_data_dir = './datain/Emission_data/fires_data/GOES/f',
bbem_modis_data_dir = './datain/Emission_data/fires_data/MODIS/Fires',
bbem_inpe_data_dir = './datain/Emission_data/fires_data/DSA/Focos',
bbem_fre_data_dir = './datain/Emission_data/Fre/f',
   bbem_extra_data_dir ='NONE',
!----- veg type data set (dir + prefix)
  veg_type_data_dir
                          ='./datain/surface_data/GL_IGBP_MODIS_INPE/MODIS',
!----- vcf type data set (dir + prefix)
 use\_vcf = 0,
 vcf_type_data_dir
                          ='./datain/surface_data/VCF/data_out/2005/VCF',
!----- Carbon density data ------!--- New Olson''s data set (dir + prefix)
 olson_data_dir
                      ='./datain/Emission_data/OLSON2/OLSON',
!----- Old Olson''s data set carbon_density_data_dir='./datain/surface_data/GL_OGE_INPE/OGE',
!----- carbon density data set for Amazon (dir + prefix)
  fuel_data_dir ='./datain/Emission_data/Carbon_density_Saatchi/amazon_biomass_final.gra',
!----- gocart background
  use\_gocart\_bg = 0,
```

```
gocart_bg_data_dir='./datain/Emission_data/GOCART',
!----- volcanoes emissions
   use volcanoes =0,
    volcano index =1143, !REDOUBT
   use these values='NONE',
dise_these_values= NoNe;

! define a text file for using external values for INJ_HEIGHT, DURATION,
! MASS ASH (units are meters - seconds - kilograms) and the format for
! a file 'values.txt' is like this:
! 11000. 10800. 1.5e10
! use_these_values='values.txt'
   begin_eruption='201303280000', !begin time UTC of eruption YYYYMMDDhhmm
!----- degassing volcanoes emissions
   use_degass_volcanoes =0,
    degass_volc_data_dir ='./datain/Emission_data/VOLC_SO2',
!------ User specific emissions section below -----
!----- Update for South America megacities
    ! (set 'NONE' if you do not want to use ) user_data_dir='.../extra/UserData/',
!----- Urban emissions file name
    ! ".asc" file in user_data_dir (set 'NONE' if you do not want to use ) cites_mobile_urban_emissions_file = 'SA_citiesMobileUrbanEmissions.asc',
!----- Streets Inventory
   ! Enables Local inventory information for streets
! Use 'NONE' or leave it blank to not use streets inventory
! Cities implemented: "RJ" - Rio Olympic Games update
streets_inventory_region = 'RJ',
!----- User specific emissions section end -----
   pond=1, ! mad/mfa 0 -> molar mass weighted
                                1 -> Reactivity weighted
!----- for grid type 'll' or 'gg' only
   grid_resolucao_lon=0.2,
    grid_resolucao_lat=0.2,
   \begin{array}{lll} nlat=&320, & ! \ if \ gg \ (only \ global \ grid) \\ lon\_beg & = & -180., \ ! \ (-180.:+180.) \ long\_begin \ of \ the \ output \ file \\ lat\_beg & = & -90., \ ! \ (-90.:+90.) \ lat \ -begin \ of \ the \ output \ file \\ delta\_lon & = & 360, \ ! \ total \ long \ extension \ of \ the \ domain \ (360 \ for \ global) \\ delta\_lat & = & 180, \ ! \ total \ lat \ extension \ of \ the \ domain \ (180 \ for \ global) \\ \end{array}
!----- For regional grids (polar or lambert)
   NGRIDS = 1,
                                    ! Number of grids to run
    NNXP
               = 150,50,86,46,
                                                ! Number of x gridpoints
                                           ! Number of y gridpoints
! Grid number which is the next coarser grid
               = 90, 50, 74, 46,
    NXTNEST = 0, 1, 1, 1,
   DELTAX = 111487.,
DELTAY = 111487.,
                                          ! X and Y grid spacing
    ! Nest ratios between this grid and the next coarser grid.
   NSTRATX = 1,2,3,4, \\ NSTRATY = 1,2,3,4,
                                         ! x-direction
                                             ! y-direction
    NINEST = 1, 10, 0, 0,
                                       ! Grid point on the next coarser
   NJNEST = 1, 10, 0, 0,
                                       ! nest where the lower southwest
                                      ! corner of this nest will start.
! If NINEST or NJNEST = 0, use CENTLAT/LON
, ! If polar, latitude/longitude of pole point
! If lambert, lat/lon of grid origin (x=y=0.)
    POLELAT = 85., !-89.99,
    POLELON = 0.,
                                      ! If polar for BRAMS, use 90.0 in STDLAT2
    STDLAT1 = 0.,
                                      ! If lambert, standard latitudes of projection
    STDLAT2 = -60.,
                                        !(truelat2/truelat1 from namelist.wps, STDLAT1 < STDLAT2)
                                      ! If mercator STDLAT1 = 1st true latitude
    STDLON = 0.0
                                      ! Standard longitude, used if lambert or polar
    CENTLAT = 85.,!-89.99, -23., 27.5, 27.5, CENTLON = 0., -46.,-80.5, -80.5,
```

- After the configuration of prep_chem_sources.inp: Set the chemical data directories and other parameters (check apendix B)
- Run the executable for the RELACS mechanism:

For BRAMS:

```
→ ./prep chem sources RELACS TUV SIMPLE.exe
```

For BRAMS with MATRIX:

```
→ ./prep_chem_sources_RELACS_MX_MATRIX.exe
```

For WRF-Chem/FIM-Chem:

```
→ ./prep chem sources RADM WRF FIM SIMPLE.exe
```

 List the files again and observe that some files were created (.ctl, .vfm and .gra)

```
→ ls
```

NOTE: if WRF-Chem output was selected (special_output_to_wrf = 'YES'), then the following binary files should be produced:

```
WRF-$year-$mo-$day-000000-g1-ab.bin (anthropogenic plus MEGAN climatology if use_bioge =2)
WRF-$year-$mo-$day-000000-g1-bb.bin (biomass burning)
WRF-$year-$mo-$day-000000-g1-gocartBG.bin (GOCART background)
```

 Open the .ctl and .gra files in GRADS in order to visualize some pollutants:

```
→ grads -blc "open created file.ctl"
```

Some basic commands in the GRADS program

| Command | Description |
|---------|-------------|
| | |

| d "parameter" (ex: d CO) | Plots the field generated on the display |
|---|---|
| set lat "latitude" / set lon "longitude" (ex: set lat -30; set lon -57) | Plots at a latitude and longitude of interest |
| set lat "starting latitude" "final latitude" set lat "starting longitude" "final longitude" (set lon -110 -77) (set lat -90 90) | Plots an area of interest |
| set lev "level" | Chooses a specify vertical level to display |
| clear | Clears the display |
| set gxout contour set gxout shaded set gxout grfill | Contour plot Shaded contour plot Same as shaded except that each grid box is filled |
| set mpdset mres | Plots the political map |
| set t "time" | Gives the last time of the currently open file |

d) PHASE IV – Using the emissions data in the BRAMS, WRF-Chem or FIM-Chem atmospheric models

• BRAMS

In order for the BRAMS model to be able to use the emissions model map, the .vfm file must be present in the directory specified in RAMSIN.

This can be done in two ways:

- 1) Moving the file or the files to the created datain/COND SRC directory, or
- 2) Creating symbolic links in the specific area of BRAMS to this directory.

In order to facilitate the use of the chemical mechanisms we suggest the second method.

WRF-Chem

In order to use the emissions data in WRF-Chem, the binary files produced by PREP-CHEM-SRC (*-ab.bin, *-bb.bin, *-gocartBG.bin) must be converted to netCDF using the convert_emiss program.

After compiling WRF-Chem, compile convert emiss.exe:

```
→ cd WRFV3.3
→ ./compile emi_conv
```

For each day (\$year-\$mo-\$day-00), run real.exe with chem_opt=0 and start and end time set to \$year-\$mo-\$day-00 to generate a wrfinput d01 file with timestamp for that day.

```
→ ./real.exe
```

Link PREP-CHEM-SRC-1.8.3 emissions to WRF run directory:

```
\rightarrow ln -sf PREP-CHEM-SRC-1.8.3/bin/WRF-$year-$mo-$day-000000-g1-gocartBG.bin wrf_gocart_backg \rightarrow ln -sf PREP-CHEM-SRC-1.8.3/bin/WRF-$year-$mo-$day-000000-g1-ab.bin emis-sopt3_d01 \rightarrow ln -sf PREP-CHEM-SRC-1.8.3/bin/WRF-$year-$mo-$day-000000-g1-bb.bin emissfire_d01
```

Run convert emiss:

```
→ ../chem/convert_emiss.exe
```

Rename output to include the date:

```
→ mv wrfchemi_d01 wrfchemi_d01_{$year}-$mo-${da}_00:00:00
→ mv wrffirechemi_d01 wrffirechemi_d01_{$year}-$mo-${da}_00:00:00
→ mv wrfchemi_gocart_bg_d01 wrfchemi_gocart_bg_d01_{$year}-$mo-$
{da}_00:00:00
```

Double-check your namelist settings:

```
&time control
                                     = 2 ; netCDF format for anthropogenic
 io form auxinput5
emissions
                                     = 2 ; netCDF format for biomass burning
io form auxinput7
emissions
                                    = 2 ; netCDF format for GOCART emissions
 io form auxinput8
                                   = 1440,1440 ; daily emissions
 auxinput5 interval m
auxinput7_interval_m
auxinput8_interval_m
                                   = 1440,1440
                                   = 1440, 1440
                              = 1,1 ; one file per day
 frames_per_auxinput7
 frames_per_auxinput7
                                  = 1, 1
 frames_per_auxinput8
                                  = 1, 1
&chem
 kemit
                             = 1, ; surface emissions only
io style emissions
                                         = 2, ; Date/time specific emissions
data files used
emiss inpt opt
                                         = 1, 1, ; RADM2/SORGAM specia-
tion
                                            = 5,
                                                    5, ; GOCART RACM KPP
 emiss opt
emissions
```

Now you are ready to run WRF-Chem.

FIM-Chem

4. IMPORTANT NOTES:

- When changing the compiler for the PREP-CHEM-SRC compilation (in case one uses a different version from the tutorial) make the change in the *include* mentioned in phase II;
- Always remember to use the same chemical mechanism in all phases (SPACK (for BRAMS), PREP-CHEM-SRC and the atmospheric model -BRAMS, WRF-Chem or FIM-Chem);
- Question, bug reports and suggestions can be send to brams_help@cptec.inpe.br

Appendix A

Table 1: Variables related with the compilation configuration.

| Variables | Description and comments |
|------------------------|---|
| MAKE | Defines the make utility to be used. |
| | Ex:/usr/bin/make |
| BASE | Base directory of the model. |
| LIBUTILS | Base directory of the internal libraries of the model. |
| NCARG_DIR (deprecated) | Base directory of the NCAR library |
| LIBNCARG (deprecated) | Name with which the NCAR library should be constructed. |
| HDF5_LIBS | Path to the HDF libraries and their dependencies. |
| CMACH | Defines the utilized architecture. Necessary for optimizations in some compilers. |
| _ | Compiler responsible for generating objects based on the Fortran source code. |
| | Ex: /usr/bin/ifort |
| C_COMP | Compiler responsible for generating objects based on the C source code. |
| | Ex: /usr/bin/gcc |
| LOADER | Compiler responsible for linking the generated objects. |
| | Ex: /usr/bin/ifort |
| MOD_EXT | |
| F_OPTS | Fortran compilation flags. |
| | *Important* some flags can cause system malfunction. |
| C_OPTS | C compilation flags. |
| | *Important* some flags can cause system malfunction. |
| LOADER_OPTS | Fortran compilation flags. |

| | *Important* some flags can cause system malfunction. | | |
|----------|--|--|--|
| PAR_DEFS | Informs the use of the mpicc and mpif90 scripts | | |
| ARCHIVE | Utility for the generation of libraries. | Utility for the generation of libraries. | |
| | Ex: ar rs | | |

APPENDIX B

NOTE: Observe that this file has various input parameters for PREP-CHEM-SRC:

| Parameters and examples | Description and comments |
|---|---|
| grid_type= 'polar', | This parameter (character) defines the grid projection on which the emission fields will be generated. The options are: |
| | 'polar' = polar stereographic grid |
| | 'gg' = Gaussian grid |
| | 'll' = rectangular projection grid |
| | 'lambert'= Lambert conformal grid |
| | 'FIM' = FIM model icosahedral grid |
| | 'mercator' = Mercator grid |
| | |
| ihour=0, | The emission date using GMT time. All |
| iday=12, | parameters are integers. |
| imon=7, | |
| iyear=2004, | |
| use_retro=1, | To select the anthropogenic sources |
| retro_data_dir='./Emission_data/RETRO/anthro', | datasets to be used (1 = yes, 0 = not) and to provide the directory path where |
| | the corresponding input data is located. |
| use edgar=1, | The parameters are integers and |
| edgar_data_dir='./Emission_data/EDGAR/anthro', | characters. |
| use_gocart=1, | To define if GOCART emissions of OC, |
| gocart_data_dir='./Emission_data/GOCART/emissions', | BC, SO2 and DMS will be used (1) or not (0) and the path where the raw data |

| | is located. |
|---|--|
| use_streets=1, | |
| streets_data_dir='./Emission_data/STREETS', | |
| use_seac4rs=1, | |
| seac4rs_data_dir='./Emission_data/SEAC4RS', | |
| use_bioge=1, | To select the biogenic sources datasets |
| bioge_data_dir='./Emission_data/biogenic_emissions', | to be used (0=not, 1=GEIA, 2=MEGAN) and the path where the original data is located. |
| use_fwbawb=0, | To define if biofuel use and agricultural |
| fwbawb_data_dir='./Emission_data/ fwbawb ', | waste burning emissions will be used (1) or not (0), and the path where the raw data is located. |
| use_gfedv2=0, | To define if the GFEDv2 biomass |
| gfedv2_data_dir='./Emission_data/GFEDv2-8days', | burning inventory is to be used (=1) or not (=0) and the path where the raw data is located. |
| use_bbem=1, | To define if the 3BEM biomass burning |
| use_bbem_plumerise=1, | inventory and smoke plume rise parameters will be used (=1) or not(=0). |
| merge_GFEDv2_bbem=0, | Defines if the merging of GFEDV2 with 3BEM is desired (integer: 1=yes, 0=no). If yes, 3BEM is used over South America instead of GFEDv2. |
| bbem_wfabba_data_dir='./Emission_data/fires_data/WF_ABBA_v60/filt/f', | Fire products for 3BEM/3BEM-plumerise emission models: |
| bbem_modis_data_dir='./Emission_data/fires_data/MODIS/Fires.', | Path of WF_ABBA fire product. The filtered fire product is recommended. The last letter 'f' is the prefix of the file name. |
| bbem_inpe_data_dir='./Emission_data/fires_data/DSA/Focos | Path of MODIS fire product and the prefix of the file name ("Fires."). |
| ' , | Path of INPE/DSA fire product and the prefix of the file name ("Focos"). |
| bbem_fre_data_dir='./datain/Emission_data/Fre/f', | Path of Fre Metodology and the prefix |
| bbem_extra_data_dir='./Emission_data/fires_data/xx, | ("f") |
| | Additional fire product provided by the user. |
| veg_type_data_dir='./surface_data/GL_IGBP_MODIS_INPE/ | Only for 3BEM: |
| MODIS | Land cover data set (dir + prefix) |
| carbon_density_data_dir='./surface_data/GL_OGE_INPE/O | Only for 3BEM: |
| GE', | Carbon density data set (dir + prefix) |
| fuel_data_dir='./surface_data/fuel/glc2000_fuel_load.nc', | Only for 3BEM: fuel load data provided by the user (dir + full file name). |
| USE_GOCART_BG=1, | GOCART background data for H2O2, |

| GOCART_BG_DATA_DIR='./Emission_data/GOCART', | OH and NO3 (only for WRF-Chem/FIM models with GOCART aerosol module) |
|--|---|
| USE_VOLCANOES=1, | This section is to control emission of |
| VOLCANO_INDEX=1450, | ASH by eruptive volcanoes. The data is based on Mastin et al. (2009). |
| USE_THESE_VALUES='NONE', | |
| BEGIN_ERUPTION='201004161200', | USE_VOLCANOES:1=yes,0=no (integer). |
| | VOLCANO_INDEX: the reference number (integer) of the volcano listed at Mastin et al. (2009) database. This number will provide trough a look up table a set of default parameters for injection height, duration and emission of ash. |
| | USE_THESE_VALUES: (character) if 'none', Mastin et al. (2009) database will be used. If the user want to use a different set of numbers, them must be in text file with inj_height, duration, mass ash (units are meters - seconds - kilograms). As example, a file named 'values.txt' with the text line: 11000. 10800. 1.5e10 |
| | will replace the default values by these numbers by setting USE_THESE_VALUES='./values.txt' |
| | BEGIN_ERUPTION= begin time UTC of eruption YYYYMMDDhhmm |
| USE_DEGASS_VOLCANOES=0, DEGASS_VOLC_DATA_DIR='./Emission_data/VOLC_SO2', | This section is to control emission of SO2 by eruptive and non-eruptive volcanoes. The data is based on Diehl, 2009 and 2010 papers. |
| | USE_DEGASS_VOLCANOES=1=yes, 0=no (integer). |
| | DEGASS_VOLC_DATA_DIR: character designing the path of the directory where the raw data is. |
| CITES_MOBILE_URBAN_EMISSIONS_FILE | This new parameter, avaiable in version 1.8.3 allows to choose the .asc file for Urban emissions, eg: SA_citiesMobileUrbanEmissions.asc |
| | SA_citiesMobileUrbanEmissionsUse rDefined.asc, and so on. Before version 1.8.3 the file name was fixed |
| | as |

| | SA_citiesMobileUrbanEmissions.asc |
|---|---|
| STREETS_INVENTORY_REGION | During the Olympic Games in Rio de Janeiro in 2016, the "Streets Inventory" functionality was implemented, which allows the use of parameterization of emission-generating streets for the city of Rio de Janeiro. However, to enable such functionality, you had to enable the parameter in the code. In order to be able to change the parameter without the need to recompile the code, the parameter "streets_inventory_region" was created. Until the current version it may receive the values "RJ" or "NONE". The value "RJ "enables functionality for Rio de Janeiro, and the value" NONE "keeps the functionality disabled. As it was implemented, the parameter allows to implement other configurations of cities, which can be determined in the parameter. |
| GRID_RESOLUCAO_LON=0.1, GRID_RESOLUCAO_LAT=0.1, | This section is only for grid_type 'll' or 'gg'. The parameter 'nlat' is integer, all others are real. |
| NLAT=320, LON_BEG = -170., LAT_BEG = 40., | GRID_RESOLUCAO_LON and GRID_RESOLUCAO_LAT are the grid spacing in degrees. |
| DELTA_LON= 90., | NLAT is the number of grids on the latitudinal direction for a Gaussian grid. |
| DELTA_LAT= 40., | LON_BEG and LAT_BEG are the longitude and latitude in degrees of the 1st grid box. The ranges are -180 to +180 and -90 to +90, respectively. |
| | DELTA_LON and DELTA_LAT are the total extension of the domain in degrees. Set 360 and 180 degrees for global domains, respectively. |
| NGRIDS = 1, | This section is only for regional grids. |
| NNXP = 275,50,86,46, | NGRIDS (integer) is the number of grids to generate emissions. |
| NNYP = 250,50,74,46, NXTNEST = 0,1,1,1, | NNXP, NNYP (integer) are the number of x,y gridpoints for each desired grid. |

| DELTAX = 5000., | NXTNEST (integer) is grid number |
|--|--|
| DELTAY = 5000., | which is the next coarser grid. |
| NSTRATX = 1,2,3,4, | DELTAX, DELTAY (real) are the X and Y grid spacing (meters). |
| NSTRATY = 1,2,3,4, | NSTRATX, NSTRATY (integer) are the |
| NINEST=1,10,0,0, | nest ratios between this grid and the |
| NJNEST=1,10,0,0, | next coarser grid. |
| POLELAT = 65., | NINEST, NJNEST (integer) are the grid point on the next coarser nest where the |
| POLELON = -150., | lower southwest corner of this nest will |
| STDLAT1 = 65., | start. If NINEST or NJNEST =0, use |
| STDLAT2 = 65., | CENTLAT/CENTLON parameters. |
| CENTLAT = 65.,-23., 27.5, 27.5, | POLELAT, POLELON (real) are, if grid type is polar, the latitude (in degrees) of |
| NTLON = -150., -46.,-80.5, -80.5, | pole point. If lambert, lat/lon of grid origin (x=y=0.) |
| | STDLAT1, STDLAT2 (real, only for Lambert-Conformal) are standard latitudes of projection in degrees. |
| | CENTLAT, CENTLON are the center (latitude, longitude, in degrees) of each grid. |
| PROJ_TO_LL='YES', LATI = -90., -90., -90., | This section is only for visualization using GrADS software. |
| LATF = +90., +90., +90., | PROJ_TO_LL (character) is to define if |
| LONI = -180., -180., -180., | a rectangular projection is desired: 'YES' or 'NOT'. |
| LONF = 180., 180., 180., | LATI, LATF, LONI, LONF (real, degrees) are the corners of the emission output domain for each grid. |
| CHEM_OUT_PREFIX = 'TEST-RACM', | CHEM_OUT_PREFIX: output file prefix |
| CHEM_OUT_FORMAT='vfm', CONVERT_TO_WRF = 'yes', | (may include directory path) |
| | CHEM_OUT_FORMAT: the format of the output: use 'vfm' for CCATT-BRAMS, |
| | WRF-CHEM or FIM. Binary is also |
| | available by setting 'bin' or 'txt' for a text file. NetCDF is under implementation. |
| | CONVERT_TO_WRF: convert to WRF/CHEM ('yes' or 'not', character). |