WRF/Chem Version 3.3 User's Guide

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WRF/Chem Version 3.3 User's Guide

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WRF/Chem Version 3.3 User's Guide

WRF/Chem Overview

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1.1 Introduction

The WRF/Chem user's guide is designed to provide the reader with information specific to the chemistry part of the WRF model and its potential applications. It will provide the user a description of the WRF/Chem model and discuss specific issues related to generating a forecast that includes chemical constituents beyond what is typically used by today's meteorological forecast models. For additional information regarding the WRF model, the reader is referred to the WRF model User's Guide (http://www.mmm.ucar.edu/wrf/users/docs/user_guide_V33/contents.html).

Presently, the WRF/Chem model is now released as part of the Weather Research and Forecasting (WRF) modeling package. And due to this dependence upon WRF, it is assumed that anyone choosing to use WRF/Chem is very familiar with the set-up and use of the basic WRF model. It would be best for new WRF users to first gain training and experience in editing, compiling, configuring and using WRF before venturing into the more advanced realm of setting up and running the WRF/Chem model.

The WRF/Chem model package consists of the following components (in addition to resolved and non resolved transport):

- Dry deposition, coupled with the soil/vegetation scheme
- Four choices for biogenic emissions:
  - No biogenic emissions included.
  - Online calculation of biogenic emissions as in Simpson et al. (1995) and Guenther et al. (1994) includes emissions of isoprene, monoterpenes, and nitrogen emissions by soil.
  - Online modification of user specified biogenic emissions - such as the EPA Biogenic Emissions Inventory System (BEIS) version 3.13. The user must provide the emissions data for their own domain in the proper WRF data file format.
  - Online calculation of biogenic emissions from MEGAN.
- Three choices for anthropogenic emissions:
  - No anthropogenic emissions

    - User-specified anthropogenic emissions such as those available from the EPA NEI-05 data inventory. The user must provide the emissions data for their own domain in the proper WRF data file format.
    - Global emissions data from the one-half degree RETRO and ten degree EDGAR data sets.
- Several choices for gas-phase chemical mechanisms including
    - RADM2, RACM, CB-4 and CBM-Z chemical mechanisms.
    - The use of the Kinetic Pre-Processor, (KPP) to generate the chemical mechanisms. The equation files (using Rosenbrock type solvers) currently available for RADM2, RACM, RACM-MIM, SAPRC-99, MOZART chemical mechanisms as well as others.
- Three choices for photolysis schemes:
    - Madronich scheme coupled with hydrometeors, aerosols, and convective parameterizations. This is a computationally intensive choice, tested with many setups.
    - Fast-J photolysis scheme coupled with hydrometeors, aerosols and convective parameterizations.
    - F-TUV photolysis scheme. This scheme is also from Sasha Madronich. Faster, but does not work with all aerosol options.
- Three choices for aerosol schemes:
    - The Modal Aerosol Dynamics Model for Europe - MADE/SORGAM.
    - The Model for Simulating Aerosol Interactions and Chemistry (MOSAIC - 4 or 8 bins) sectional model aerosol parameterization.
    - A total mass aerosol module from GOCART.
- Aerosol direct effect through interaction with atmospheric radiation, photolysis, and microphysics routines. In version 3.3 this is available for GOCART, MOSAIC or MADE/SORGAM options.
- Aerosol indirect effect through interaction with atmospheric radiation, photolysis, and microphysics routines. In V3.3 this options is available for MOSAIC or MADE/SORGAM.
- A tracer transport option in which the chemical mechanism, deposition, etc. has been turned off. The user must provide the emissions data for their own domain in the proper WRF data file format for this option. May be run parallel with chemistry.
- A plume rise model to treat the emissions of wildfires.

1.2 WRF/Chem software

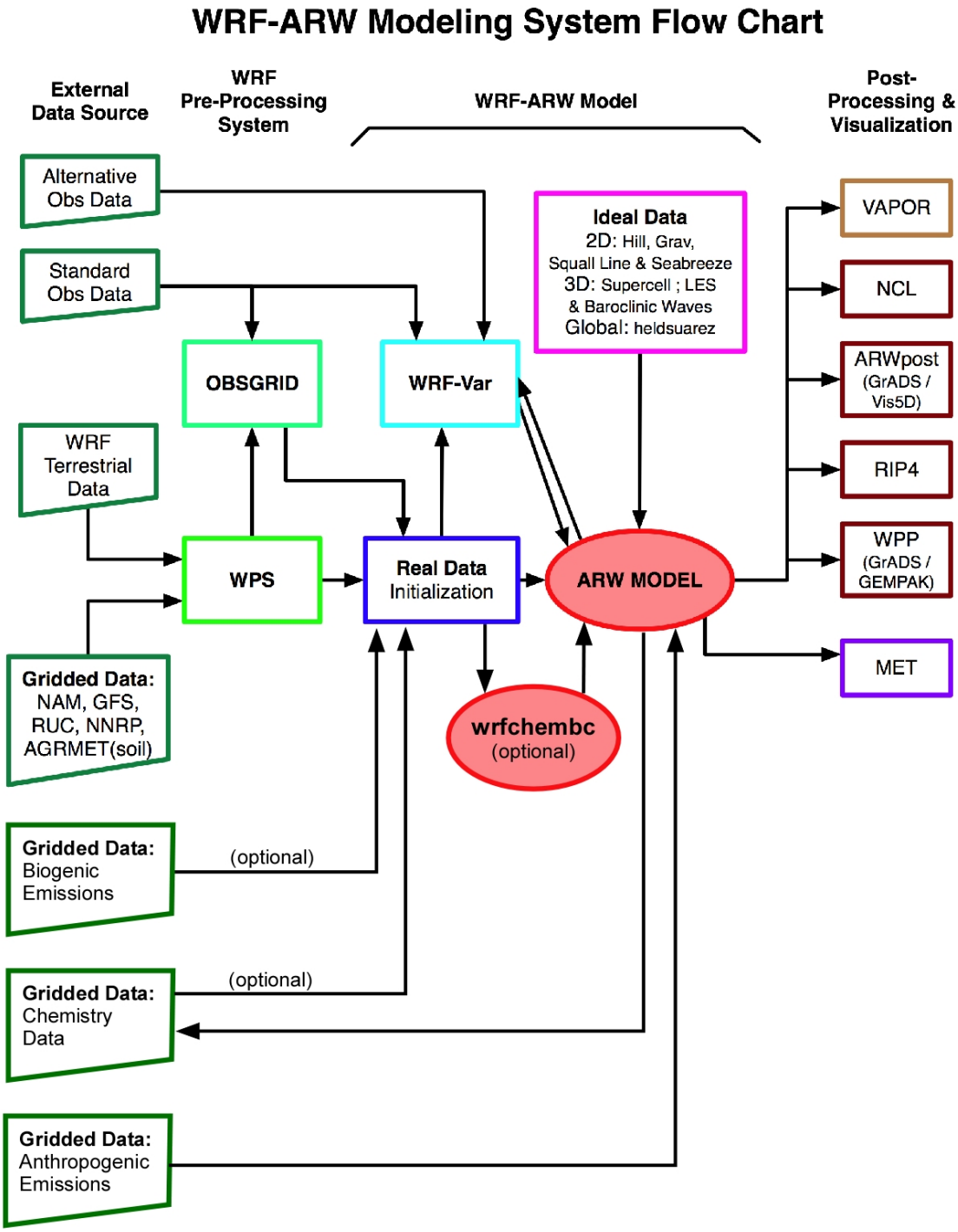
The chemistry model has been built to be consistent with the WRF model I/O Applications Program Interface (I/O API). That is, the chemistry model section has been built following the construction methodology used in the remainder of the WRF model. Therefore, the reader is referred to the WRF software description in the WRF User's Guide (Chapter 7) for additional information regarding software features like the build mechanism and adding arrays to the WRF registry.

1.3 Possible applications of the current modeling system

- Prediction and simulation of weather, or regional or local climate.
- Coupled weather prediction/dispersion model to simulate release and transport of constituents.
- Coupled weather/dispersion/air quality model with full interaction of chemical species with prediction of O_3 and UV radiation as well as particulate matter (PM).
- Study of processes that are important for global climate change issues. These include, but are not restricted to the aerosol direct and indirect forcing.

1.4 The WRF/Chem modeling system overview

The following figure shows the flowchart for the WRF/Chem modeling system version 3.3.



As shown in the diagram, the WRF/Chem modeling system follows the same structure as the WRF model by consisting of these major programs:

- The WRF Pre-Processing System (WPS),

- WRF-Var data assimilation system,
- WRF solver (ARW, o r NMM core) including chemistry,
- Post-processing and visualization tools.

Chapter 2: WRF/Chem Software Installation

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2.1 Introduction

The WRF modeling system software (including chemistry) installation is straightforward on the ported platforms. The package is mostly self-contained, meaning that WRF requires no external libraries that are not already supplied with the code. One exception is the netCDF library, which is one of the supported I/O API packages. The netCDF libraries or source code are available from the Unidata homepage at http://www.unidata.ucar.edu (select DOWNLOADS, registration required, to find the netCDF link).

The WRF/Chem model has been successfully ported to a number of Unix-based machines. We do not have access to all tested systems and must rely on outside users and vendors to supply required configuration information for compiler and loader options of computing architectures that are not available to us. See also chapter 2 of the User's Guide for the Advanced Research WRF for a list of the supported combinations of hardware and software, required compilers, and scripting languages as well as post-processing software. It can not be guaranteed that chemistry will build successfully on all architectures that have been tested for the meteorological version of WRF.

Note that this document assumes *a priori* that the reader is very familiar with the installation and implementation of the WRF model and its initialization package (e.g., the WRF Standard Initialization program, or WPS). Documentation for the WRF Model and its initialization package can be found at (http://www.mmm.ucar.edu/wrf/users/pub-doc.html). With this assumption in place, the remainder of this chapter provides a quick overview of the methodology for downloading the WRF/Chem code, setting the required environmental variables, and compiling the WRF/Chem model. Subsequent chapters assume that the user has access to the WRF/Chem model and emission data sets for their region of interest and has them readily available so that a full weather and chemical transport simulation can be conducted.

2.2 Building the WRF-chemistry code

2.2.1 Getting the code

- Download, or copy to your working space, the WRF zipped tar file
  - The WRF model and the chemistry code directory are available from the WRF model download web site (http://www.mmm.ucar.edu/wrf/users).
  - The chemistry code is a separate download from the WRF model download web page and can be found under the WRF-Chemistry code title.
  - Always get the latest version if you are not trying to continue a long project.
  - Check for known bug fixes for both, WRF and WRF-Chem.

- Unzip and untar the file
  - > gzip –cd WRFV3-Chem-3.3.TAR | tar –xf –
  - Again, if there is a newer version of the code use it, 3.3 is used only as an example.
  - > cd WRFV3

Remember that bug fixes become available on a regular basis and can be downloaded from the WRF/Chem web site (http://www.wrf-model.org/WG11). You should check this WEB page frequently for updates on bug fixes. This includes also updates and bug fixes for the meteorological WRF code (http://www.mmm.ucar.edu/wrf/users/).

2.2.2 UNIX environment settings for WRF/Chem

Before building the WRF/Chem code, several environmental settings are used to specify whether certain portions of the code need to be included in the model build. In c-shell syntax, the important environmental settings are:

setenv WRF_EM_CORE 1
setenv WRF_NMM_CORE 0

explicitly defines which model core to build. These are the default values which are generally not required. The environmental setting

setenv WRF_CHEM 1

explicitly defines that the chemistry code is to be included in the WRF model build, and is required for WRF/Chem. This variable is required at configure time as well as compile time.

optionally,

setenv WRF_KPP 1,
setenv YACC '/usr/bin/yacc –d',
setenv FLEX_LIB_DIR /usr/local/lib

explicitly defines that the Kinetic Pre-Processor (KPP) (Damian et al. 2002, Sandu et al. 2003; Sandu and Sander 2006) is to be included in the WRF/Chem model build using the flex library (libfl.a). In our case the flex library is located in /usr/local/lib and compiles the KPP code using the yacc (yet another compiler compiler) location in /usr/bin. This is optional as not all chemical mechanisms need the KPP libraries built during compilation. The user may first determine whether the KPP libraries will be needed (see chapter 6 for a description of available options). One should set the KPP environmental variable to zero (setenv WRF_KPP 0) if the KPP libraries are not needed.

2.2.3 Configuring the model and compiling the code

The WRF code has a fairly complicated build mechanism. It tries to determine the architecture that you are on, and then present you with options to allow you to select the preferred build method. For example, if you are on a Linux machine, the code mechanism determines whether this is a 32-or 64-bit machine, and then prompts you for the desired usage of processors (such as serial, shared memory, or distributed memory) and compilers. Start by selecting the build method:

- > ./configure

- Choose one of the options
  - Usually, option "1" is for a serial build. For WRF/Chem, **do not use the shared memory OPENMP option (smpar, or dm + sm),** these are not supported. The serial build is a preferred choice if you are debugging the program and are working with very small data sets (e.g. if you are developing the code). Since WRF/Chem uses a lot of memory (many additional variables), the distributed memory options are preferred for all other cases.
- You can now compile the code using
  - > ./compile em_real >& compile.log
- If your compilation was successful, you should find the executables in the "main" subdirectory. You should see ndown.exe, real.exe, and wrf.exe listed.

  - > ls -ls main/*.exe

2.2.4 Building the WRF-chemistry emissions conversion code

After building the WRF-Chemistry model, you can then compile the conversion programs that will allow you to run the anthropogenic and biogenic emissions programs.

These programs are used to convert "raw" anthropogenic and biogenic data files into WRF netCDF input data files. In the WRFV3 directory, type the following commands:

- > ./compile emi_conv

- > ls -ls WRFV3/chem/*.exe
  - You should see the file convert_emiss.exe listed in the chemistry directory. This file should already be linked to the WRFV3/test/em_real directory.

- > ls -ls WRFV3/test/em_real/*.exe
  - You should see the files ndown.exe, real.exe, wrf.exe, convert_emiss.exe, listed in the em_real directory.

Chapter 3: Generation of WRF/Chem Emissions Data

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3.1 Introduction

One of the main differences between running with and without chemistry is the inclusion of additional data sets describing the sources of chemical species. At this time, these files need to be prepared externally from the WRF/Chem simulation due to the wide variety of data sources. This places the WRF/Chem user in a position of needing to understand the complexity of their emissions data as well as having the control over how the chemicals are speciated and mapped to their simulation domain. While this can be a daunting task to the uninitiated, the following section will attempt to illustrate the methodology through which emissions data is generated for a forecast domain.

3.2 Preparation of anthropogenic emissions for use with WRF/Chem

At this time there is no single tool that will construct an anthropogenic- emissions data set for **any domain and any chemical mechanism** that you select. **This places the requirement upon you to construct the anthropogenic-emissions data set for your particular domain and desired chemistry.** However, several programs and data sets are

provided that you may use to create an emissions data set, if your domain and your choice of chemical mechanism follow some restrictions. These programs are described in the following two subsections. Note that you must know *a priori* the preferred domain location and chemistry options that will be used in the simulation. The "raw" anthropogenic-emissions data set described next can be used if the domain is located over the 48 contiguous states of the United States. The next section shows the suggested methodology for constructing your own anthropogenic-emissions data set.

3.2.1 The standard 4km resolution data set (2005 NEI emissions data for USA only)

Anthropogenic-emissions data is currently available for the contiguous 48 states of the United States, southern Canada and northern Mexico based upon the U.S. Environmental Protection Agency (EPA) National Emissions Inventory (NEI) 2005 inventory. Area type emissions are available on a structured 4-km grid, while point type emissions are available by latitude and longitude locations and with stack parameters needed for plume-rise calculations. This data is discussed later in this section and can be found online at http://ruc.noaa.gov/wrf/WG11/anthropogenic.htm. For those who desire to conduct simulations over other regions of the world, the reader is referred to the section in the appendix that describes the use of a global anthropogenic-emissions inventory for the WRF/Chem model. The methodology for transferring an anthropogenic-emissions data set to the WRF model is discussed in the following section.

3.2.1.1 Anthropogenic-emissions construction methodology for WRF/Chem

The methodology for constructing your own anthropogenic-emissions data set is:

- Obtain the "raw" anthropogenic-emissions data. This data could come from a variety of data sources and be on multiple map projections and/or domains.
    - A 4-km emissions data set (area) and point source is available for the U.S. (see below). Use of this data is recommended when the simulation domain has a horizontal grid spacing of 12 km or greater.
- Specify, or make a table listing that relates "raw" emissions to the speciation of the desired chemical mechanism and PM mechanism (see following section)
    - The provided routines (emiss_v03.F) assume that the RADM2 chemical mechanism and MADE/SORGAM modal aerosol models are being used in the simulation.
- Prepare the 3-D (or 2-D) anthropogenic emissions data set
    - Account for rise of emissions from stack, biomass burning, etc.
    - Output data in an intermediate format (binary for the U.S. NEI05 case). You can change format to match your needs in module_input_chem_data.F
- Convert the emissions data to a WRF netCDF data file
    - Convert intermediate format (binary) emissions to 4-D WRF netcdf files (with executable of convert_emiss.F subroutine)
    - Input data format must match that used in the conversion routine (see module_input_chem_data.F)

- Map data (extracted from the header in file wrfinput_d01) is needed for some plotting routines to function properly.

- If running WRF/Chem with a carbon bond type mechanism (CBM4, CBMZ, etc.) be sure to use the correct emiss_inpt_opt setting for the chemical mechanism. The WRF/Chem code will assume the emissions are in RADM2 form and will repartition the emitted species to the appropriate carbon bond mechanism unless you specify a different choice with the emiss_inpt_opt. In addition, the SORGAM emissions will be converted to the 4 or 8 size bins for use in the MOSAIC aerosol routines.

3.2.1.2 Construction of an anthropogenic-emissions-inventory conversion table

Begin with a list of known chemical species that are emitted in the domain of interest. These species may need to be translated into a list of chemical species that are used by your particular photochemical and aerosol mechanisms within the WRF-Chemistry model. If you are uncertain about the names and units of the emissions data, the registry.chem file in the WRFV3/Registry subdirectory contains the names and dimensions of the chemical species used within the WRF/Chem model.

The translation from "raw" to WRF/Chem species emissions will often result in either lumping several emitted chemical species into one simulated species, or the partitioning of one emitted species into fractions of several simulated species. As an example, the following emission assignment table (Table. 3.2) translates the "raw" NEI05 based emission species into the WRF/Chem RADM2 species. The columns contain the following information:

- names of the emitted species in the "raw" data derived from the EPA NEI05 inventory, VOC speciation is that used in the SAPRC-99 chemical mechanism.
- names of the emitted species used in the WRF-Chemistry model, Variable names (e.g. e_co) must match the WRF/Chem Registry names of the emission variables.
- the fractional amount of the "raw" emitted species assigned to the model emission name,
- the molecular weight (used as a switch in emiss_v03.F – applies only to primary NOx, SO_2, CO and NH_3 emissions),
- the technical name of the "raw" emitted species

Table 3.2. Conversion table within emiss_v03.F used to produce input-emissions data for a WRF-chemistry simulation. This table lists the "raw" emission name, the emissions field name used in the WRF model, the weight factor applied to the chemical field, the molecular weight of the species (NOx, SO_2, CO and NH_3 only) and the full species name. The fields are then converted to an emissions speciation suitable for use with the RADM2 chemical mechanism (+MADE/SORGAM aerosol module).

"raw" name	WRF/Chm name	Weight	MW	Species name

CO	e_co	1.00	28	Carbon monoxide
NOX	e_no	1.00	46	Nitrogen Oxides (NO or NO_2)
SO2	e_so2	1.00	64	Sulfur dioxide
NH3	e_nh3	1.00	17	Ammonia
HC02	e_eth	1.00	00	Alkanes with kOH<500/ppmv/min (Ethane)
HC03	e_hc3	1.00		Alkane500<kOH<2500 (exclude C3H8, C2H2, organic acids)
HC04	e_hc3	1.11	00	Alkane2500<kOH<5000 (exlude butanes)
HC05	e_hc5	0.97	00	Alkane 5000<kOH<10000 (exlude pentanes)
HC06	e_hc8	1.00	00	Alkane kOH>10000
HC07	e_ol2	1.00	00	Ethylene
HC08	e_olt	1.00	00	Alkene kOH <20000 /ppm/min
HC09	e_oli	1.00	00	Alkene kOH >20000 /ppm/min
HC10	e_iso	1.00	00	Isoprene
HC12	e_tol	1.00	00	Aromatic kOH <20000 /ppm/min (exclude benzene and toluene)
HC13	e_xyl	1.00	00	Aromatic kOH >20000 /ppm/min (exclude xylenes)
HC14	e_hcho	1.00	00	Formaldehyde
HC15	e_ald	1.00	00	Acetaldehyde
HC16	e_ald	1.00	00	Higher aldehydes
HC17	e_ald	1.00	00	Benzaldehyde
HC18	e_ket	0.33	00	Acetone
HC19	e_ket	1.61	00	Methylethyl ketone
HC20	e_ket	1.61	00	PRD2 SAPRC-99 species (ketone)
HC21	e_hc3	0.40	00	Methanol
HC22	e_ald	1.00	00	Glyoxal
HC23	e_ald	1.00	00	Methylglyoxal
HC24	e_ald	1.00	00	Biacetyl
HC25	e_csl	1.00	00	Phenols
HC26	e_csl	1.00	00	Cresols
HC27	e_ald	0.50	00	Methacrolein
HC27	e_olt	0.50	00	Methacrolein
HC28	e_ket	0.50	00	Methylvinyl ketone
HC28	e_olt	0.50	00	Methylvinyl ketone
HC29	e_ket	1.00	00	IPRD SAPRC-99 species (other ketones)
HC31	e_olt	1.00	00	Propylene
HC32	e_hc3	0.40	00	Acetylene
HC33	e_tol	0.29	00	Benzene
HC34	e_hc3	1.11	00	Butanes
HC35	e_hc5	0.97	00	Pentanes
HC36	e_tol	1.00	00	Toluene
HC37	e_xyl	1.00	00	Xylenes
HC38	e_hc3	0.57	00	Propane
HC39	e_oli	1.00	00	Dienes
HC40	e_olt	1.00	00	Styrenes
HC41	e_ora2	1.00	00	Organic Acids

PM01	e_pm25i	0.20	01	Unspeciated primary PM2.5 - nuclei mode
PM01	e_pm25j	0.80	01	Unspeciated primary PM2.5 - accumulation mode
PM02	e_so4i	0.20	01	Sulfate PM2.5 - nuclei mode
PM02	e_so4j	0.80	01	Sulfate PM2.5 - accumulation mode
PM03	e_no3i	0.20	01	Nitrate PM2.5 - nuclei mode
PM03	e_noj	0.80	01	Nitrate PM2.5 - accumulation mode
PM04	e_orgi	0.20	01	Organic PM2.5 - nuclei mode
PM04	e_orgj	0.80	01	Organic PM2.5 - accumulation mode
PM05	e_eci	0.20	01	Elemental Carbon PM2.5 - nuclei mode
PM05	e_ecj	0.80	01	Elemental Carbon PM2.5 - accumulation mode
PM10-PRI	e_pm10	1.00	01	Unspeciated Primary PM10

The next step is to construct a program that reads the "raw" anthropogenic emissions data, converts each chemical species to those used by the WRF/Chem model following the information from your particular conversion table and finally maps it onto the 3-dimensional simulation domain. Therefore, within this step any plume rise, or above surface anthropogenic emission placement needs to be specified. Particular attention to geospatial details, such as the WRF/Chem domain grid locations, and the elevation of model vertical levels relative to the "raw" emissions data-set must be considered.

Provided on the WRF/Chem ftp site is a program that can be used with the NEI-05 U.S. anthropogenic emissions inventory - emiss_v03.F. While your application may not use the "raw" emissions data for your simulation, it is provided as an example of the adopted methodology. The product of the program is a binary data file containing three-dimensional emissions data, output at each hour, that is mapped to a specified simulation domain. The data format in the provided program is provided in Table 3.2.

Table 3.2. Converted or "intermediate binary" emission data used to produce input emissions data for a WRF-chemistry simulation. This table lists each output variable, its variable declaration, dimensions, and any additional information. The output-data fields are specific to the RADM2 -chemical mechanism (+MADE/SORGAM aerosol module).

File variable	declaration	dimensions	comments
nv	integer	1	Number of chemical species
ename	character*9	30	Name of each emissions field in model
hour	integer	1	Hour of the emissions data (begin loop)
so2	real	(nx,nz,ny)	
no	real	(nx,nz,ny)	
ald	real	(nx,nz,ny)	
hcho	real	(nx,nz,ny)	
ora2	real	(nx,nz,ny)	
nh3	real	(nx,nz,ny)	

hc3	real	(nx,nz,ny)	
hc5	real	(nx,nz,ny)	
hc8	real	(nx,nz,ny)	
eth	real	(nx,nz,ny)	
ora2	real	(nx,nz,ny)	
nh3	real	(nx,nz,ny)	
co	real	(nx,nz,ny)	
ol2	real	(nx,nz,ny)	
olt	real	(nx,nz,ny)	
oli	real	(nx,nz,ny)	
tol	real	(nx,nz,ny)	
xyl	real	(nx,nz,ny)	
ket	real	(nx,nz,ny)	
csl	real	(nx,nz,ny)	
iso	real	(nx,nz,ny)	
pm2.5i	real	(nx,nz,ny)	
pm2.5j	real	(nx,nz,ny)	
so4i	real	(nx,nz,ny)	
so4j	real	(nx,nz,ny)	
no3i	real	(nx,nz,ny)	
no3j	real	(nx,nz,ny)	
orgi	real	(nx,nz,ny)	
orgj	real	(nx,nz,ny)	
eci	real	(nx,nz,ny)	
ecj	real	(nx,nz,ny)	
pm10	real	(nx,nz,ny)	(end loop)

For spatial partitioning, the emiss_v03.F program implicitly assumes the WRF/Chem grid has a horizontal grid resolution larger that 4 km, and simple grid dumping from the "raw" 4 km domain into the specified WRF/Chem domain is appropriate. Currently no plume rise calculations directly couple WRF dynamics to anthropogenic point emissions. The emiss_v03.F routine includes some plume rise from the Brigg's formulation due to momentum lift from direct injection, and a specified horizontal wind climatology. Emissions within nested domains are also handled within emiss_v03.F by specifying mother domain map parameters, the nested domain grid resolution, and beginning x and y locations of the nested domain within the mother domain. These variable names are listed, and described further in the following section.

We assume that the anthropogenic emissions data is updated at an hourly interval. However, the update interval is arbitrary and can be specified by you for your individual application. In addition, if the given binary format of the output data from emiss_v03.F is not functional for your needs, the data format can be modified within the program. However, if the output data format is changed, the WRF/Chem program convert_emiss.F will also need to be modified so that the converted raw emissions data can be read into the program correctly and converted.

Both surface and elevated point source emissions of gas-phase species are in units of *mole per square kilometer per hour,* and in *microgram per square meter per second* (microgram m^{-2} s^{-1}) for the aerosol species. These are the units assumed within the WRF/Chem input processor for the emissions files, and the convert_emiss.F processing step that generates the netcdf emission file(s) described further below. (Conversion of gas-phase emissions into the mixing ratio increases at each grid is handled within module_emissions_anthropogenic.F . Aerosol increases due to emissions are handled in individual aerosol mechanism modules.)

It is entirely incumbent upon the user to specify location and time of emissions from the "raw" emissions for their own applications within this intermediate step of the emissions processing.

3.2.1.3 Additional details for running emiss_v03.F with the NEI-05 anthopogenic-emissions data set

The "raw" anthropogenic-emissions data for the 48 contiguous states as well as select regions of Canada and Mexico have been made available for download by the NOAA/Earth Systems Research Laboratory, Chemical Sciences Division. The process to create anthropogenic-emissions input data files from this data is as follows:

- Before generation of the anthropogenic-emissions data file can begin, the real.exe program should be used to create the wrfinput_d01 and wrfbdy_d01 data files for your desired domain. There are two reasons for doing this. The first is so that you know exactly where the simulation domain is located. The second is because the emissions conversion program (convert_emiss.exe) will read the netCDF header information from the wrfinput_d01 data file and write this information into the WRF-chemical-emissions data files. If the wrfinput_d01 data file does not exist, the program will abort with an error.

- Download the raw-emissions data tar file from the anonymous ftp server (ftp://aftp.fsl.noaa.gov/divisions/taq/emissions_data_2005/em05v2_file*.tar) and extract the data into its own directory (e.g., $home/emissions_data).

- Download the emiss_v03.F program from the anonymous ftp server.

- Modify emiss_v03.F to set map and grid parameters for your particular domain as well as the directory that contains the "raw" emissions data. For the provided test domain you should have the following settings:

Model variable	Value	Description
Il	40	east-west grid spacing (ix2+1) of mother domain and west_east_stag dimension on your WRF domain
Jl	40	north-south grid spacing (jx2+1) of mother domain and south_north_stag dimension on your WRF domain
Ix2	39	x-dimension of user domain output data (IL-1)
Jx2	39	y-dimension of user domain output data (JL-1)
Kx	19	z-dimension of user domain output data or kemit on your WRF

		domain. The vertical dimension can equal or be less than that used in the WRF domain.
Inest1	0	nesting or no nesting flag (no nesting => inest1 = 0)
Dx	60.E3	horizontal grid spacing (m) of user domain
Dxbigdo	60.E3	Horizontal grid spacing on mother domain (m)
Xlatc	38.00	grid center latitude of mother domain
Xlonc	-80.00	grid center longitude of mother domain
Clat1	38.001	Northern most reference latitude of projection (mother domain)
Clat2	38.000	Southern most reference latitude of projection (CLAT1 > CLAT2 for Lambert Conformal, CLAT2 not used for polar stereographic)
Iproj	1	projection type (see WRFSI information)
Rekm	6370.	Earth radius (km)
XNESSTR	1.	x-location in mother domain of southwest corner point of the (1,1) grid in the user domain. Not used if Inest1=0 .
YNESSTR	1.	y-location in mother domain of southwest corner point of the (1,1) grid in the user domain. Not used if Inest1=0 .
Datadir	/data	Path to directory holding emissions input data (character string)
Zfa	(See below)	Elevation (m) at the top of each computational cell
KWIN	20	Number of vertical levels in the horizontal wind profile
WSP		Wind speed at level height(m) specified by REFWZ
REFWZ		Elevation (m) of the specified horizontal wind profile

```
DATA ZFA/  0.,  255.,  515.,  781., 1054., 1335.,  &
        1527., 1824., 2130., 2553., 2994., 3454.,  &
        4059., 4967., 6741., 8723.,10992.,14084.,  &
       16461.,20346./
```

Note: the model ZFA height levels have been determined separately by processing the wrfinput_d01 file generated by real.exe to add the vertical domain levels in meters.

- Compile emiss_v03.F (single processor mode) with the command "pgf90 –Mfree –byteswapio –o emiss_v03.exe emiss_v03.F" and run emiss_v03exe. This program, using raw emissions data, maps the emissions data to your specified domain and generates binary emissions data files (file names are set in emiss_v03.F to be wrfem_00to12Z and wrfem_12to24Z).

3.2.2 Using the global emissions data set

The use of a global emissions data set has recently been added to WRF/Chem options. The global emissions data comes from the REanalysis of the TROpospheric (RETRO) chemical composition over the past 40 years (http://retro.enes.org/index.shtml) and Emission Database for Global Atmospheric Research (EDGAR) (http://www.mnp.nl/edgar/introduction). Both RETRO and EDGAR provide global annual emissions for several greenhouse gases (e.g., CO2, CH4 and N2O) as well as some precursor gases on a .5x.5 degree (RETRO) or a 1x1 degree (EDGAR) grid.

A simple grid mapping program has been made available to WRF/Chem users. This program, called prep_chem_sources, was developed at CPTEC, Brazil and is

available to WRF/Chem users. The program will map the global anthropogenic emissions data to a WRF forecast domain using a polar stereographic or Lambert conformal projection. See appendix (B) for more information regarding the prep_chem_sources routine.

3.2.3 Wildfire emissions

The prep_chem_sources program (see appendix B) is capable of providing biomass burning, or wildfire, emissions to the WRF/Chem forecast. The geostationary NOAA weather satellite (GOES) provides half-hourly fire data for the Western Hemisphere. Specifically, GOES-12 provides coverage for North and South America while GOES-11 covers North America only. Data files containing the WFABBA fire location are distributed by the University of Wisconsin-Madision (http://cimss.ssec.wisc.edu/goes/burn/wfabba.html). The archived WF-ABBA data are available at this time from two different web sites; http://www.firedetect.noaa.gov and http://www.nrlmry.navy.mil.flambe/index.html. Additional wild fire location data is available from MODIS at the University of Maryland web site: http://firefly.geog.umd.edu/firms. The prep_chem_sources reads this data, the WFABBA data files all being in one directory and MODIS from the same or different directory, and maps the point source data to the WRF domain. It is also not too difficult to include other sources for wildfire emissions.

In the WRF/Chem model, the wildfire emissions data is obtain from the wrffirechemi_d01 emissions data file. It computes the plume rise of the wildfire smoke based upon the environmental wind and temperature profile. The emissions to the forecast are then provided as a vertical distribution based upon the results from the plume rise calculation.

3.3 Generating the netcdf emissions data sets

The final step in the process is to produce a WRF/Chem netCDF emissions input data file containing all of the required metadata (map projection data, simulation start time, etc.) for the simulation. Ideally the metadata contained in the WRF/Chem emissions file would be generated by the previous step. However, if not provided by the user, the WRF input data file (e.g., wrfinput_d01) can be read and the metdata information added to the anthropogenic emissions input data file. The name of the final netcdf data file(s) can be either wrfchemi_<hour>_d<domain_id> or wrfchemi_d<domain_id>_<date/time> depending upon your intent (io_style_emissions option in namelist). The latter intent is designed for daily varying emissions (io_style_emissions=2), and in this case the date/time specified in the WRF/Chem-emissions data file must match the simulation date/time or no emissions data will be read and a run-time error will result. The first intent (io_style_emissions=1) assumes you are creating two netcdf 4-D emission files named wrfchemi_00z_d<domain_id> and wrfchemi_12z_ d<domain_id> that contain hourly emissions from 00:00 to 11:00 UTC, and 12:00 to 23:00 UTC, respectively. This is the format generated by convert_emiss.F that matches the provided NEI-05 inventory.

The NEI-05 inventory is representative of a "typical ozone season day" by the U.S. EPA, and is typically used for all days within multi-day WRF/Chem simulations.

- Before the conversion from "binary intermediate" to netcdf file emissions can begin, you need to change the namelist.input file in the WRFV3/test/em_real directory to the emissions data file settings. The settings that will generate 24 hours of hourly-emissions (i.e., io_style_emissions=2) data are:

```
 &time_control
 run_days                  = 1,
 run_hours                 = 0,
 run_minutes               = 0,
 run_seconds               = 0,
 start_year                = 2008,
 start_month               = 07,
 start_day                 = 14,
 start_hour                = 00,
 start_minute              = 00,
 start_second              = 00,
 end_year                  = 2008,
 end_month                 = 07,
 end_day                   = 15,
 end_hour                  = 12,
 end_minute                = 00,
 end_second                = 00,
 auxinput6_inname          = 'wrfbiochemi_d<domain>,
 auxinput7_inname          = 'wrffirechemi_d<domain>,
 auxinput8_inname          = 'wrfchemi_gocart_bg_d<domain>,
 auxinput5_interval_m      = 60,
 auxinput7_interval_m      = 1440,
auxinput8_interval_m       = 1440,
io_form_auxinput2          = 2,
 io_form_auxinput5         = 2,
 io_form_auxinput6         = 2,
 io_form_auxinput7         = 2,
io_form_auxinput8          = 2,
io_form_auxinput12         = 0,

&chem
 chem_opt                  = 1,
 emiss_opt                 = 3,
 chem_in_opt               = 0,
 bio_emiss_opt             = 1.
```

Starting with version 3.3, you should note that the namelist setting for the auxiliary input port time interval is now dependent upon each input stream. That is, for the emissions conversion program convert_emiss.exe, the settings for

each auxiliary input port specifies whether it is turned on, the IO format, the time interval for the emissions data updates and the number of frames in each file (not shown).

- We assume that you have already configured and compiled the WRF/Chem model. So now build the emissions conversion program with the command "compile emi_conv" in WRFV3 directory.

- Run convert_emiss.exe for 24 hours starting at 0000 UTC and ending at 0000 UTC and save the netCDF wrfchemi_d01 data file as wrfchemi_d01_2008-07-14_00:00:00. The filename(s) need to match the name of the input data file in mediation_integrate.F (see convert_emiss.F program inside the WRFV3/chem directory). The file(s) should be transferred (or linked) to your WRFV3/test/em_real directory.

- Once the "wrfchemi" files are generated it is best to plot fields, or use a program like ncview to examine the files that have been generated. Look at the files and confirm that the emissions appear to match the WRF forecast domain you previously generated. When looking at anthropogenic emissions (e.g., co) the surface emissions should look similar to a map with cities and possibly roads showing. Be sure to confirm that the fields are consistent with your expected emissions fields in both space (vertically) as well as in time. If the emissions do not match, then a dimension error is likely happened in your namelist.input file.

3.4 Construction and preparation of tracer emissions

At this time there is no single program available that will allow the user to construct tracer emissions for their domain and directly import them into the simulation. However, there are relatively simple methodologies that can be undertaken to allow the user to generate their tracer emissions.

Probably the most simple way to produce tracer emissions it to modify the program emiss_v03.F to suit your needs. Upon examination of the emiss_v03.F program one will see that it can be modified to skip the reading of the NEI emissions data sets and instead fill the output array. The output array (i.e., EM3RD(I,K,J,N)) can be filled with user specified values at the desired grid location with the user specified emitted tracer amount. The user needs to be aware of not only where the emitted species are to be located in their simulation domain (grid indexes I,K and J)), but also which chemical emissions index, N, corresponds to the emitted species used as a tracer in their simulation. To get the emissions correct, start by examining the registry.chem file to determine which species are used in the tracer package (chem._opt=13). Then use the array ENAME in the emiss_v03.F program to get the name and order of the emitted species. Then one can set the emissions for the correct chemical index in the output array. Once the modified program has been compiled and run the binary intermediate file containing the emitted tracer data will need to be converted to a WRF netCDF input file using the convert_emiss.F program discussed in the previous section.

Another methodology is for the user to build their own tracer emissions data file and use the convert_emiss.F program as is, or modified as needed, to read the tracer data file and produce a tracer emissions input file. This option allows users to use pre-existing data files and to modify the tools available with the chemistry to produce input, or output files for their needs depending upon the emissions options selected.

3.5 Preparation of biogenic emissions

The WRF-chemistry model does have four options to compute the biogenic-emissions data. These options are:

3.5.1 No biogenic emissions

The first option is not to use an additional biogenic emissions input data file (bio_emi_opt= 0). The user could add the biogenic emission to the anthropogenic emissions data if it is desired. Be sure to do this for every time period in the emissions input data and not just the first time.

3.5.2 Guenther biogenic emissions

For the second option (bio_emi_opt= 1), the model calculates the biogenic emissions online using the USGS landuse classification, which is generated by WRF WPS and available for the meteorological and chemical model. The user does not prepare any biogenic emissions input data set.

3.5.3 BEIS 3.13 biogenic emissions

For the third option, the user specifies reference fields for the biogenic emissions, which are then modified online by a subroutine from the Biogenic Emissions Inventory System (BEIS) version 3.13. The land-use for this emissions inventory is obtained from the Biogenic Emissions Landuse Database version 3 (BELD3). The reference fields need to be provided as an additional input data file (wrfbiochemi_d01) for the real.exe program.

The BEIS3.13 model is publicly available through the CMAS (Community Modeling and Analysis System) at http://www.cmascenter.org/ as part of the SMOKE (Sparce Matrix Operator Kernel Emissions) software package (version 2-4). The physical parameterizations for temperature, light dependencies, and canopy light correction are contained within module_bioemi_beis313.F of WRF/Chem. Reference emission files (30°C, 1000 PAR) from BEIS3.13 rely on the BELD3 (Biogenic Emissions Landuse Database, version 3) available at http://www.epa.gov/ttn/chief/emch/biogenic/. This North American database contains fractional area information on 230 individual forest, grass and crop types at 1-km horizontal resolution. Tools for spatial allocation of BELD3 data into common user defined grids are also available at that web-site. As part of the reference emission pre-

processing, BEIS3.13 contains seasonal specific, and vegetation-specific information for emissions of 33 individual VOC species (including isoprene and 14 monoterpenes), biogenic/agricultural NO, and LAI (Leaf Area Index) information needed in the canopy light dependence calculations of isoprene, methanol and methyl-butenol.

The current version of module_bioemi_beis313.F is specific to reference emissions generated for the RADM2, or RACM chemical mechanism by NOAA/ESRL/CSD. Reference emissions for 15 VOC species within RACM, 3 NO emission classes, and the LAI field specific to isoprene are each output on a 2-dimensional grid for the defined WRF/Chem simulation grid as simple ASCII files having the dimensions of (nx-1,ny-1), in 12E9.2 format. This input format is defined, and modifiable within the input_ext_chem_beis3_file routine in WRFV3/chem/module_input_chem_bioemiss.F Units of emissions are in mole/km^2/hr within the ASCII files, the same as other gas-phase emissions. A list of biogenic emission variables specific to the RACM species assignment is given in table 3.3.

Table 3.3. List of biogenic emission variable names, and their RACM mechanism meaning.

File variable	comments
Iso	Isoprene
Oli	Internal Olefins
Api	Alpha Pinene
Lim	Limonene
Xyl	Xylene
hc3	Alkane500<kOH<2500 (propane)
Ete	Ethylene
Olt	Terminal Olefins
Ket	Ketones
Ald	Acetaldehyde (and higher aldehydes)
Hcho	Formaldehyde
Eth	Ethane
ora2	Acetic and higher organic acids
Co	Carbon Monoxide
Nr	Nonreactive VOC
noag_grow	Agricultural NO – fertilized growing
noag_nongrow	Agricultural NO – nonfertilized growing
Nononag	Nonagricultural NO
Slai	LAI for isoprene emissions

The program convert_emiss.F must be compiled, and the executable convert_emiss.exe must be run. A data file called wrfbiochemi_d01 (for domain 1) will be created if bio_emiss_opt = 2 in your namelist.input file. Run real.exe (with bio_emi_opt=2 in the

namelist) when creating the wrfinput data file - the biogenic emissions variables should now be included in the wrfinput data file.

3.5.4 MEGAN biogenic emissions

The final option for biogenic emissions is the use of the Model of Emissions of Gases and Aerosols from Nature (MEGAN). This global biogenic emissions data set has a horizontal spatial resolution of approximately 1 km so it can be used for nearly any WRF/Chem simulation. The use of this biogenic emissions option requires the user to download and compile a further utility from the National Center for Atmospheric Research (NCAR). The utility prepares MEGAN input data files for use in WRF-Chem – these files are named wrfbiochemi_d0x files – and a separate file is provided for each domain (d0x). The assimilation of MEGAN biogenic emissions into WRF-Chem is a matter of setting the correct namelist.input settings. Further instructions, including support contact details at NCAR, can be found in Appendix D.

3.6 Conversion of biogenic emission data files

The emissions-input data files for biogenic and biomass burning data also need to be in a WRF input data file format. This includes containing the correct header information related to your simulation domain. There is a program available that converts the emissions data from their respective intermediate data files to a WRF chemical emissions input file – convert_emiss.exe. This program is located under the WRFV3/chem directory and is compiled using the compile emi_conv command. The executable can be located in the WRFV3/test/em_real directory. The program will read the namelist.input file and convert the data files depending upon the options set by the user in the chemistry and time_control namelists.

3.7 Placement of chemical emission input data files

The emissions-input data files need to be located either in the run or the test/em_real directory. Often we place the data in the run directory and link it the test/em_real directory, since they will be used over and over again.

As you can see from this example, the WRF/Chem anthropogenic-emissions data file (wrfchemi_d01_2008-07-14_12:00:00) is located in the WRFV3/run directory and is linked to the WRFV3/test/em_real directory. Some advantages of this methodology is the reduced chance of accidentally removing the data files. It reduces disk space usage as only one data file is needed, and it could allow for one data file to be used for multiple simulations by changing the name of the linked data file.

Chapter 4: Running the WRF-Chemistry Model

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4.1 Introduction

After successful construction of the anthropogenic and biogenic-emission-input data files, it is time to run the model. This process is no different than running the meteorological version of the model. To make an air-quality simulation, change directory to the WRFV3/test/em_real directory. In this directory you should find links to the executables real.exe, and wrf.exe, other linked files, and one or more namelist.input files in the directory.

For larger domain simulations, one should use a DM (distributed memory) parallel system to make a forecast. This is of particular importance for WRF/Chem since much additional memory is required.

4.2 WRF/Chem namelist options: the choice of CHEM_OPT

The largest portion of the chemistry namelist options are related to the chemical mechanisms and aerosol modules selection. The mechanism used during the forecast is decided with the namelist parameter chem_opt that is described next. Some of these choices require other settings for other namelist options. The options that are printed with red lettering indicates those option that are not fully implemented and tested. Model users are discouraged from selecting those options as they are not fully supported and could produce erroneous, or in the extreme case, detrimental results. In addition, it should be pointed out that the model developers most often work with just a few options at one time (e.g., RADM2/MADE-SORGAM, CBMZ/MOSAIC). Not all of the other available options are tested during development, but often it is a trivial exercise to make the other options functional. Therefore, users are encouraged to determine their desired settings that works best for their simulation, test the namelist combination, improve the model code and then communicate the improvements to the WRF/Chem user community. The

chem_opt namelist parameter is organized according to the chemical mechanism that is used.

	&chem namelist variable	Description	Special Requirements
	chem_opt = 0	no chemistry	
ADM2)SSA hemistry	= 1	include chemistry using the RADM2 chemical mechanism - no aerosols	
	= 2	include chemistry using the RADM2 chemical mechanism and MADE/SORGAM aerosols.	No indirect effect To have radiative feed back with the chemistry/aerosols use ra_sw_physics = 2 (Goddard shortwave scheme). For dust and seasalt use dust_opt=2, seas_opt=2.
	= 5	CBMZ chemical mechanism with Dimethylsulfide, or DMS	
	= 6	CBMZ chemical mechanism without DMS	
	= 7	CBMZ chemical mechanism (chem_opt=6) and MOSAIC using 4 sectional aerosol bins.	No indirect effect To have radiative feed back with the chemistry/aerosols use ra_sw_physics = 2 (Goddard shortwave scheme) For dust and seasalt use dust_opt=2, seas_opt=2.
	= 8	CBMZ chemical mechanism (chem_opt=6) and MOSAIC using 8 sectional aerosol bins.	No indirect effect To have radiative feed back with the chemistry/aerosols use ra_sw_physics = 2 (Goddard shortwave scheme). For dust and seasalt use dust_opt=2, seas_opt=2.
	= 9	CBMZ chemical mechanism (chem_opt=6) and MOSAIC using 4 sectional aerosol bins including some aqueous reactions	For direct and indirect effect use: phot_opt=2; ra_sw_physics=2; progn=1; mp_physics=2; aer_ra_feedback=1;wetscav_onoff=1; cldchem_onoff=1 For dust and Seasalt use dust_opt=2, seas_opt=2.
	= 10	CBMZ chemical mechanism (chem_opt=6) and MOSAIC using 8 sectional aerosol bins including some aqueous reactions	For direct and indirect effect use: phot_opt=2; ra_sw_physics=2; progn=1; mp_physics=2; aer_ra_feedback=1; wetscav_onoff=1;

		cldchem_onoff=1. For dust and seasalt use dust_opt=2, seas_opt=2.
= 11	RADM2 chemical mechanism and MADE/SORGAM aerosols including some aqueous reactions	For direct and indirect effect use: phot_opt=2; ra_sw_physics=2; progn=1; mp_physics=2; aer_ra_feedback=1; wetscav_onoff=1; cldchem_onoff=1. For dust and seasalt use dust_opt=2, seas_opt=2.
= 12	RACM chemical mechanism and MADE/SORGAM aerosols including some aqueous reactions	This is a KPP option – not functioning correctly with V3.3 – watch for bug fixes on WEB site. Will have the same direct/indirect options as (11)
= 13	Run with 5 tracers with emissions, currently set-up for SO2, CO, no,ald,hcho,ora2	Use of tracer_opt suggested.
= 14	Single tracer run using tracer_1 array	Use of tracer_opt suggested.
= 15	Ensemble tracer option using 20 individual tracers and an ensemble tracer array	Use of tracer_opt suggested.
= 30	CBMZ chemical mechanism (chem_opt=6) and MADE/SORGAM modal aerosol.	No indirect effect
= 31	CBMZ chemical mechanism (chem_opt=6) and MOSAIC using 4 sectional aerosol bin with dms.	No indirect effect
= 32	CBMZ chemical mechanism with (chem_opt=6) and MOSAIC using 4 sectional aerosol bins with dms. Some aqueous reactions included.	No indirect effect
= 33	CBMZ chemical mechanism (chem_opt=6) and MOSAIC using 8 sectional aerosol bin with dms.	No indirect effect
= 34	CBMZ chemical mechanism with (chem_opt=6) and MOSAIC using 8 sectional aerosol bins with dms. Some aqueous reactions included.	No indirect effect
= 35	CBMZ chemical mechanism (chem_opt=6) and MADE/SORGAM modal aerosol. Some aqueous reactions included.	No indirect effect
= 101	RADM2 Chemistry using KPP library	Rosenbrock solver, can use larger timestep
= 102	RACM-MIM Chemistry using KPP library	Rosenbrock solver, can use larger timestep
= 103	RACM Chemistry using KPP library	Rosenbrock solver, can use larger timestep

= 104	RACM Chemistry and PM advection using KPP library	PM total mass. This was originally implemented for wildfires.
= 105	RACM Chemistry and MADE/SORGAM aerosols using KPP library	Rosenbrock solver, can use larger timestep
= 106	RADM2 Chemistry and MADE/SORGAM aerosols using KPP library	Rosenbrock solver, can use larger timestep
= 110	CB4 Chemistry using KPP library	Rosenbrock solver, can use larger timestep
= 111	MOZART Chemistry using KPP library	Rosenbrock solver, can use larger timestep. Use phot_opt=3.
= 112	MOZART Chemistry and GOCART aerosols (MOZCART) using KPP library	Rosenbrock solver, can use larger timestep. Use phot_opt=3
= 120	CBMZ Chemistry using KPP library	Rosenbrock solver, can use larger timestep
= 170	CBMZ Chemistry with MOSAIC aerosols using KPP library	Rosenbrock solver, can use larger timestep
= 195	SAPRC99 Chemistry using KPP library	Rosenbrock solver, can use larger timestep
= 198	SAPRC99 Chemistry with MOSAIC using KPP library. The MOSAIC aerosols uses 4 sectional aerosol bins and includes volatility basis set (VBS) for organic aerosol evolution.	Rosenbrock solver, can use larger timestep
= 200	NMHC9 Chemistry using KPP library	Only 18 variables, currently no direct or indirect effect supported. Optionally use dmsemis_opt=1, dust_opt=1, seas_opt=1
= 300	GOCART simple aerosol scheme, no ozone chemistry	Only 18 variables, currently no direct or indirect effect supported. Optionally use dmsemis_opt=1, dust_opt=1, seas_opt=1
= 301	GOCART coupled with RACM-KPP	Simple aerosol treatment, no direct or indirect effect supported yet. Optionally use dmsemis_opt=1, dust_opt=1, seas_opt=1.
= 302	RADM2 Chemistry and GOCART aerosols using KPP library	Simple aerosol treatment, no indirect effect supported yet. Optionally use dmsemis_opt=1, dust_opt=1, seas_opt=1
= 303	RADM2 Chemistry and GOCART aerosols	Simple aerosol treatment, no direct or indirect effect supported yet. Optionally use dmsemis_opt=1, dust_opt=1, seas_opt=1
= 400	Volcanic ash-fall and concentration only	Simple ash treatment with 10 ash size bins.

= 401	Dust concentration only	Simple dust treatment with 5 size bins.

4.3 Other chemistry namelist options

input_chem_inname = <string>		name of chemistry input file
emi_inname = <string>		name of the anthropogenic emissions input file. For example, wrfchemi_12z_d<domain> for io_style_emissions = 1, or wrfchemi_d<domain>_<date> for io_style_emissions = 2
chem_in_opt	= 0	use idealized profile to initialize chemistry
	=1	use previous simulation data to initialize chemistry. The input file name will have the structure wrf_chem_input_d<domain> and the data will be read in through auxiliary input port 12
io_style_emissions	= 0	no emissions data read
	= 1	two 12-h emissions data files used
	= 2	Date/time specific emissions data files used
chemdt	= 1.5	time step used by chemistry in minutes
bioemdt	= 30	update time interval used by biogenic emissions in minutes
kemit	= 8	number of vertical levels in the emissions input data file. (considering the domains namelist; 0 < kemit < e_vert)
kemit_aircraft	= 1	number of vertical levels for aircraft emissions.
photdt	= 30	update time interval used by photolysis routine in minutes
phot_opt	= 0	no photolysis
	= 1	use Madronich photolysis (TUV)
	= 2	use Fast-J photolysis
	= 3	use Madronich F-TUV photolysis (aerosol interaction is not hooked up with MOSAIC aerosols).
emiss_opt	= 0	no anthropogenic emissions
	= 2	use radm2 anthropogenic emissions
	= 3	use radm2/MADE/SORGAM anthropogenic emissions
	= 4	use CBMZ/MOSAIC anthropogenic emissions
	= 5	GOCART RACM_KPP emissions
	= 6	GOCART simple emissions
	= 7	MOZART emissions
	= 8	MOZCART (MOZART + GOCART aerosols) emissions
	= 13	SAPRC99 emissions
aircraft_emiss_opt	= 0	no aircraft emissions
	= 1	use aircraft emissions
gas_drydep_opt	= 0	no dry deposition of gas species
	= 1	include dry deposition of gas species
aer_drydep_opt	= 0	no dry deposition of aerosols
	= 1	include dry deposition of aerosols
bio_emiss_opt	= 0	no biogenic emissions
	= 1	calculate biogenic emissions online using the Gunther scheme
	= 2	include biogenic emissions reference fields in wrfinput data file

		and modify values online based upon the weather
	= 3	include MEGAN biogenic emissions online based upon the weather, land use data
emiss_inpt_opt	= 0	no emissions data read
	= 1	Emissions are speciation for RADM2/SORGAM. Recommended when using the NEI-05 or EDGAR/RETRO emissions speciated for RADM2 chemical mechanism.
	= 3	Emissions are speciation for GOCART_SIMPLE from NEI-05. This is a kludge and its use is not recommended.
	= 101	RADM2 emission speciation adapted after reading the data file to follow the CBMZ/MOSAIC framework
	= 102	RADM2 emission speciation adapted after reading data file to follow the RADM2/SORGAM framework (similar to 101, but with isoprene included)
	= 103	Carbon Bond 4 emission speciation adapted after reading the data file.
	= 111	RADM2 emission speciation adapted after reading data file to follow the MOZART framework.
biomass_burn_opt	= 0	No biomass burning emissions
	= 1	include biomass burning emissions and plume rise calculation
plumerisefire_frq	= 180	Time interval for calling the biomass burning plume rise subroutine.
dust_opt	= 0	No GOCART dust emissions included
	= 1	include GOCART dust emissions - need to provide fractional erosion map data
	=2,	MOSAIC and MADE/SORGAM dust emissions option (does not requires extra input data)
seas_opt	= 0	no GOCART sea salt emissions
	= 1	include GOCART sea salt emissions
	= 2	MOSAIC or MADE/SORGAM seasalt emissions
dmsemis_opt	= 0	no GOCART dms emissions from sea surface
	= 1	include GOCART dms emissions from sea surface - need to provide dms reference field (currently only working for GOCART options)
aer_op_opt	= 1	aerosol optical properties calculated based upon volume approximation
	= 2	aerosol optical properties calculated based upon Maxwell approximation
	= 3	aerosol optical properties calculated based upon exact volume approximation
	= 4	aerosol optical properties calculated based upon exact Maxwell approximation
	= 5	aerosol optical properties calculated based upon exact shell approximation
opt_pars_out	= 0	No optical properties output.
	= 1	include optical properties in output.

gas_bc_opt = 1	uses default boundary profile
= 101	uses modified default boundary profile – originally designed for use at Houston, TX
gas_ic_opt = 1	uses default initial condition profile
= 101	uses modified default initial condition profile – designed for use at Houston, TX
aer_bc_opt = 1	uses default boundary profile
= 101	uses modified default boundary profile – designed for use at Houston, TX
aer_ic_opt = 1	uses default initial condition profile
= 101	uses modified default initial condition profile – designed for use at Houston, TX
gaschem_onoff = 0	gas phase chemistry turned off in the simulation (useful for debugging)
= 1	gas phase chemistry turned on in the simulation (default)
aerchem_onoff = 0	aerosol chemistry turned off in the simulation (useful for debugging)
= 1	aerosol chemistry turned on in the simulation (default)
wetscav_onoff = 0	wet scavenging turned off in the simulation, also see the "chem_opt" parameter
= 1	wet scavenging turned on in the simulation, also see the "chem_opt" parameter
cldchem_onoff = 0	cloud chemistry turned off in the simulation, also see the "chem_opt" parameter
= 1	cloud chemistry turned on in the simulation, also see the "chem_opt" parameter
vertmix_onoff = 0	vertical turbulent mixing turned off in the simulation (useful for debugging)
= 1	vertical turbulent mixing turned on in the simulation (default)
chem_conv_tr = 0	subgrid convective transport turned off in the simulation (if no parameterization is used or for debugging)
= 1	subgrid convective transport turned on in the simulation (default)
have_bcs_chem = .false.	get lateral boundary data from idealized profile specified in chemistry routines (use caution when setting as the namelist variable is defined as a logical).
have_bcs_chem = .true.	get lateral boundary data from wrfbdy data file (use caution when setting as the namelist variable is defined as a logical).
have_bcs_tracer = .false.	do not use tracer lateral boundary data from wrfbdy data file (use caution when setting as the namelist variable is defined as a logical).
have_bcs_tracer = .true.	get tracer lateral boundary data from wrfbdy data file for tracer species.
aer_ra_feedback = 0	No feedback from the aerosols to the radiation schemes
= 1	Feedback from the aerosols to the radiation schemes turned on, see also chem_opt parameter
chemdiag = 0	Turns off chemical tendency diagnostics.

	= 1	Turns on chemical tendency diagnostics for equation budget analysis.

In the physics namelist there are options that are directly related to the chemistry, these include the options related to the aerosol direct and indirect forcing ra_sw_physics, progn, and mp_physics. In addition there is a cumulus radition feedback option, cu_rad_feedback, as well as online/offline cumulus cloud time average option, cu_diag. These options will only work with the GD or the G3 scheme (cu_phys=3 or 5). If the cu_rad_feedback is not turned on the radiation and photolysis schemes will not "see" parameterized clouds. If cu_diag is not turned on the time average cumulus cloud arrays will not be computed. These options will only work with WRF/Chem.

cu_rad_feedback	= .false.	No feedback from the parameterized convection to the atmospheric radiation and the photolysis schemes. (Use caution when setting as the namelist variable is defined as a logical.)
	= .true.	Feedback from the parameterized convection to the radiation schemes turned on. (Use caution when setting as the namelist variable is defined as a logical.)
cu_diag	= 0	Turns off time average cumulus cloud.
	= 1	Turns on time average cumulus clouds.
progn	= 0	Turns off prognostic cloud droplet number in the Lin et al. and Morrison microphysics.
	= 1	Prognostic cloud droplet number included in the Lin et al. and Morrison microphysics scheme. This effectively turns the Lin et al. scheme into a second-moment microphysical scheme. If set with chem._opt=0 a default prescribed aerosol concentration is used.

In the time_control namelist there are options that are directly related to the chemistry, these include the options related to the reading of the various emissions data through the WRF auxiliary input ports and the methodology to read and write data files.

auxinput5_interval = 3600	Input time interval for anthropogenic emissions data. Typical settings are hourly for NEI emissions and monthly for the RETRO/EDGAR data.
auxinput6_interval =	Input time interval for biogenic emissions data. Typically biogenic emissions are static fields and this setting is not used.
auxinput7_interval =	Input time interval for biomass burning (wildfire) emissions data. For forecasts the wildfire emissions are often static fields and this setting is not used. For retrospective simulations the data can be updated according to the availability of additional fire information.
auxinput8_interval =	Input time interval for GOCART background fields. Typically for forecasts the monthly background data are static fields and this

		setting is not used.
io_form_auxinput5	= 2	Anthropogenic emissions input (wrfchemi_00z_d01 and wrfchemi_12z_d01) data format is WRF netCDF
	= 11	Parallel netCDF
io_form_auxinput6	= 2	Biogenic emissions input (wrfbioemi_d01) data format is WRF netCDF. Can be used if bio_emiss_opt > 1
	= 11	Parallel netCDF. Can be used if bio_emiss_opt > 1
io_form_auxinput7	= 2	Biomass burning emissions input (wrffirechemi_d01) data format is WRF netCDF
	= 11	Parallel netCDF
io_form_auxinput8	= 2	GOCART background emissions input (wrf_gocat_bg_d01) data format is WRF netCDF.
io_form_auxinput12	= 2	Set to use previous simulation data to initialize chemistry (wrf_chem_input_d01). The data format is WRF netCDF.
	= 11	Parallel netCDF.

4.3.1 Running with only dust aerosols

The WRF-Chem code is now able to predict dust transport along with the meteorology. To run with dust only you need to obtain several input data file for the WRF Preprocessor System (WPS). These files include the dust erosion fields (erod) that are included in the WPS GEOG directory and the GEOGRIB.TBL_ARW_CHEM table file. These files are available for download at:

ftp://aftp.fsl.noaa.gov/divisions/taq/dust_emissions_v3.3

After downloading the files and placing them in the correct WPS directories the WPS can be run and the dust erosion fields will be included your meteorology input data files. The WRF model can be run using the dust only namelist settings (chem_opt=401). Be sure when running with the dust only option that the other chemistry namelist settings (e.g., gaschem_onoff, phot_opt, gas_drydep_opt, etc.) are turned off.

4.3.2 Tracers running with chemistry

The WRF-Chem code is now able to predict chemical tracers alongside reactive chemistry. **This tracer option is set in the namelist.input under the dynamics namelist and not the chemistry namelist.** This will allow a user to run WRF/Chem with chemistry *and* tracers simultaneously. To run with tracer edit your namelist.input file and add the following under the dynamics namelist section:

tracer_opt	= 0	No tracers
	= 1	Smoke tracer which must run with biomass burning
	= 2	Lateral boundaries, stratospheric, boundary layer, and surface tracers
	= 3	Same as tracer_opt=2 but surface tracer is replaced by the biomass

		burning tracer
	= 4	Same as as tracer_opt=2 with the addition of a Lightning-NOx (LNOx) tracer, so must have the lightning NOx parameterization turned on (see Appendix D).

tracer_adv_opt	= 0	Use positive definite advection for tracers
	= 1	Use positive definite and monotonic advection for tracers. (Recommended)

The biomass burning tracer (ppmv) gets carbon monoxide (CO) emissions from the biomass burning emissions input and provides this data as a tracer. Unlike the reactive species emitted from biomass burning, the tracer experiences passive transport. When activating the tracer species using the tracer_opt namelist option a pair of tracers is released in the run. The first tracer is considered completely passive, while the other has a first-order decay with a one-day lifetime. The lateral boundary data for each tracer sets the tracer concentration to a value of 1 and is advected into the model domain during the simulation. The stratosphere tracer is set to 1 above a specified minimum temperature at this time, but an update to using the World Meteorological Organization (WMO) tropopause definition is planned. The boundary layer tracer is set to 1 below the PBL height. And finally, the surface tracer is set to 1 at the lowest model level (k=1).

When setting tracer_opt=4 there will also be a pair of tracers produced for lightning-NOx (LNOx). The first tracer tracks NO produced from intra-cloud lightning; the second tracer tracks NO produced from cloud-to-ground lightning.

4.4 Typical choices for namelist options

The addition of chemistry to WRF is making the choice of namelist options much more complicated than for the meteorological version of WRF. Not all chemistry options are interchangeable with each other (e.g. not every chemical mechanism will work with every available aerosol module), not all physics options will work with all chemistry options. The namelist description in the previous sections gives the user an idea of what physics options have to be chosen when applying the modeling system to study the aerosol direct and indirect effect. Work is in progress to extend the list of radiation and microphysics routines that will work with the aerosol routines. Work is also in progress to generalize the aerosol direct/indirect effect with respect to all available aerosol modules (e.g. allowing GOCART routines to interact with the atmospheric radiation schemes and the photolysis routines as well as allowing the full indirect effect for the modal aerosol scheme).

Even for very simplistic chemical setups seemingly small changes in the namelist options can cause large differences in the results. For real-time and research applications, we commonly use (very different than in V3.0x):

chem_adv_opt = 2,

moist_adv_opt=2,
scalar_adv_opt=2,
diff_6th_opt = 0

The above options should always be used when running chemistry simulations. The WRF advection scheme has the tendency to overshoot and produce locally unrealistically low values (referred to at times as "digging holes") if those options are not turned on. This "digging" is stronger with stronger gradients like those found where there are high emission rates.

cu_phys = 3 or 5
cugd_avedx=1,
cu_rad_feedback=.true.
chem_conv_tr = 1,

The above options should be used if a convective parameterization is called for. The option chem_conv_tr will work with any other parameterization. However, cu_rad_feedback will only work with cu_phys=3 or 5. The latter option ensures that areas with convective precipitation will be seen by the atmospheric radiation scheme and the photolysis scheme. Not using any of the above convection-related options (chem_conv_tr=0) will underestimate the transport out of the boundary layer significantly. Setting false the cu_rad-feedback option will lead to photolysis rates that are unaffected by convection (too high), as well as skin and surface temperatures that are too warm. The cugd_avedx parameter should be to one (1), except for forecasts high resolution of dx larger than 2km, but smaller than 10km. It will turn on subsidence spreading over neighboring grid points from the convective parameterization. In that case, set cugd_avedx=3 and cu_phys = 5. Other values are currently not allowed.

sf_sfclay_physics = 1
sf_surface_physics=2
bl_pbl_physics =1

The choice of the PBL physics is the most contested. It might depend strongly on the users own preferences. The user must keep in mind that results can differ significantly depending on this choice. The YSU scheme will lead to the deepest boundary layers when using the above choices (1-2-1). The user may also go to 2-2-2, using the MYJ scheme. There is no sure way of telling which will work better. We also sometimes choose the RUC soil parameterization (2-3-2) in combination with either YSU or MYJ scheme. This may work fine when the input conditions come from the RUC. The question of what modeling system the input and boundary conditions come from (such as GFS,NAM,ECMWF, etc) and what type of physics are used in that modeling system can play a role too in determining the choice of PBL physics. The user may want to try to be consistent with the larger scale model, or chose the larger scale model based on his preferred choice of physics options – if possible. An additional consideration here is also the availability of an initial cloud analysis. This is available from the RUC, also the WRF based Rapid Refresh (RR) which will replace the RUC, and may be essential in reducing

spin-up. New PBL parameterizations are now also available. These show great promise. You may try the MYNN scheme. It was tested successfully with chemistry.

mp_zero_out = 2

We always choose this option if not using positive definite advection. It ensures that hydrometeor mixing ratios are not allowed to grow smaller than a threshold value (mp_zero_out_thresh), in particular qv as well as other moisture mixing ratios will never go negative.

chem_dt = 0 [sets chem_dt = time_step; remember that the units are in minutes]

If you are using chem_opt=1 or 2, we advise to use the timestep as is used by the meteorological part of the model. That is, set chem._dt = 0 and the chemistry will use the same time step as used by the meteorology dynamics part of the model. You can choose larger time steps for any of the other options of chem_opt, but may want compare your results to a control simulation with chem._dt=0.

4.5 Input fields for chemical constituents

Unless chemical fields are available from a modeling system (global model, larger scale model, or even another WRF/Chem run), an idealized vertical profile for each chemical species is provided to start the model simulation. This vertical profile, obtained when the model is initialized with chem_in_opt set equal to zero "0" in the namelist.input, is based upon northern hemispheric, mid-latitude, clean environment conditions. If modifications are required, the routine module_input_chem._data can be modified to produce the desired initial conditions. Note that if the initial fields are modified, the boundary conditions will probably also need to be modified (also located in module_input_chem_data).

The idealized profile is obtained from climatology in the routine module_input_chem._data with data based upon results from the NALROM numerical chemistry model. The profile is declared globally inside the routine so that the lateral boundary conditions for a chemistry simulation may also be derived from this idealized profile. For ease of use, please note that in this module, the variable "iref" is the reference index, and "fracref" is the reference fraction corresponding to iref. For example, the species number 1 for a WRF/Chem simulation is SO2. The first reference index for the idealized profile, iref(1), is set to the number 12 indicating that SO2 is taken from the 12^{th} species in the input data table. Not all chemical species matchup so cleanly. For example, the NALROM model calculates its chemistry using lumped OX (where OX = O3 + NO2 + HNO3 + ...) and a lumped NOX is obtained from (NOX = NO + NO2 + NO3 + 2N2O5 + HO2NO2 + HONO). However, the RADM2 chemical mechanism strictly uses O3, and NOx is a combination of NO + NO2 only. Therefore, fractions of chemical species based upon the values of fracref are used to separate the lumped chemical species into the chemical species used by the RADM2 chemical mechanism.

Short-lived species are initialized to steady-state equilibrium - since they are short-lived. The short-lived species within a lumped category (Ox , NOx, or NO3+N2O5 in our case) would be renormalized to the lumped class after the steady-state equilibrium concentrations are determined.

The following is the list of long-lived species provided by the NALROM chemistry model.

NAMEL(1)	OX
NAMEL(2)	NOX
NAMEL(3)	HNO3
NAMEL(4)	H2O2
NAMEL(5)	CH3OOH
NAMEL(6)	CO
NAMEL(7)	ISOPRENE
NAMEL(8)	CH2O
NAMEL(9)	CH3CHO
NAMEL(10)	PAN
NAMEL(11)	OTHER ALKA
NAMEL(12)	SO2
NAMEL(13)	BUTANE
NAMEL(14)	ETHENE
NAMEL(15)	PROPENE
NAMEL(16)	PPN
NAMEL(17)	MEK
NAMEL(18)	RCHO
NAMEL(19)	SO4
NAMEL(20)	MVK
NAMEL(21)	MACR
NAMEL(22)	HAC
NAMEL(23)	MGLY
NAMEL(24)	HPAN
NAMEL(25)	MPAN
NAMEL(26)	PROPANE
NAMEL(27)	ACETYLENE
NAMEL(28)	OH
NAMEL(29)	HO2
NAMEL(30)	NO3 + N2O5
NAMEL(31)	HO2NO2
NAMEL(32)	SUM RO2
NAMEL(33)	OZONE
NAMEL(34)	NOX

4.6 Using chemical boundary conditions from other modeling systems

At this time, tools to provide data for the lateral boundary have been provided by the user community. Most of these tools are still under development and are supported by the individual groups. Each of these tools are designed to provide larger scale data from models other then WRF as boundary and initial conditions to the WRF/Chem simulations.

4.6.1 The wrfchembc utility

One such utility program that is available from NOAA/ESRL is called wrfchembc. This program currently works with data – for a selected number of species - from the MPI-MATCH and RAQMS global chemistry models. You can download the latest version of the code from the ESRL ftp site. For example, the latest code might be named

ftp://aftp.fsl.noaa.gov/divisions/taq/broken_experimental/wrfchemv2.2_bcond_code_09Apr07.tar

You can then modify the Makefile to use your desired compile options and compile to generate the wrfchembc executable. You must also modify the wrfchembc_namelist.input file to have the correct data directories and species added to the wrfbdy file.

Run the wrfchembc program after real.exe and before wrf.exe to add the global model data to the lateral boundary data file (wrfbdy_d01). In addition, before running wrf.exe, modify the namelist.input to set have_bcs_chem = .true.

4.6.2 The mozbc utility

Another tool is provided by NCAR/ACD and is designed to create time-varying chemical boundary conditions from the MOZART global model to a WRF/Chem simulation. The mozbc utility is a single cpu code that maps species concentrations from MOZART datasets to WRF/Chem concentrations for initial condition and boundary condition datasets. The utility is setup for MOZART species concentrations to be in volume mixing ratio and converts the species units to WRF/Chem depending on whether it is a gas or aerosol. The mozbc utility allows for a versatile mapping to each WRF chemical species from MOZART species including multiple with choices for:

- An individual weight factor per MOZART species,
- An overall conversion factor per WRF/Chem species.

The mozbc utility requires users to have a WRF/Chem initial condition file (wrfinput_d<domain>) for each domain of interested and/or a WRF/Chem boundary

condition file (wrfbdy_d01) for the first WRF/Chem domain. The Mozart datasets are interpolated in space (bilinearly in longitude, longitude and linearly in pressure), **but not in time**. Therefore, users need to ensure that the times in the MOZART and WRF/Chem files are matching for the period of interest. Otherwise, if a non-matching time is found the mozbc will abort the run with an error statement.

4.7 Making a nested domain WRF/Chem simulation

Produce wrfinput files for both domains following Chapter 4 of WRF Users Guide.

Like the single domain WRF/Chem simulations, it is probably best to make a nested domain weather forecast (Chapter 4 of WRF Users Guide).

Generate the emissions files for both domains using the emiss_v03.F program (section 3 of Quick Step Guide, Chapter 2 of the user's guide). File names will be wrfem_00to12z_d01 and wrfem_00to12z_d02.

The convert_emiss.exe program is not currently designed to read the namelist.input file and generate the nested domain emissions files. Therefore, run the conversion program treating the nested domain as if it was actually the mother domain.

Follow the description in section 3 to generate wrfchemi_d01 for the coarse domain, move it to a save place. Change the namelist.input file. Moving the nested information to the mother domain column. Move the met wrfinput_d02 to wrfinput_d01, link the output from emisv03 (for the nested domain) to the required filenames and then run convert_emiss. Finally, move the resulting wrfchemi_d01 to wrfchemi_d02.

When running wrf.exe with more than one domain (e.g., 2-way nested simulation), nearly every chemistry namelist option needs to be set for each domain. A user should always examine the Registry/registry.chem file and check each of the chemistry namelist variables. Those variables that are dimensioned max_domains need to be set for each domain. The following example shows how the chemistry namelist variables might be configured for a simulation using more than one domain.

```
&chem
kemit                 = 19,
chem_opt              = 301, 301,
bioemdt               = 30, 30,
photdt                = 30, 30,
chemdt                = 2.0, 0.66666,
io_style_emissions    = 1,
emiss_opt             = 5, 5,
chem_in_opt           = 1, 1,
phot_opt              = 1, 1,
gas_drydep_opt        = 1, 1,
aer_drydep_opt        = 1, 1,
```

```
bio_emiss_opt        = 1, 1,
dust_opt             = 0,
dmsemis_opt          = 0,
seas_opt             = 0,
gas_bc_opt           = 1, 1,
gas_ic_opt           = 1, 1,
aer_bc_opt           = 1, 1,
aer_ic_opt           = 1, 1,
gaschem_onoff        = 1, 1,
aerchem_onoff        = 1, 1,
wetscav_onoff        = 0, 0,
cldchem_onoff        = 0, 0,
vertmix_onoff        = 1, 1,
chem_conv_tr         = 1, 1,
biomass_burn_opt     = 1, 0,
plumerisefire_frq    = 30, 0,
aer_ra_feedback      = 0, 0,
have_bcs_chem        = .false., .false.,
```

Chapter 5: Visualizing WRF/Chem Data files

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5.1 Introduction

The WRF modeling system has a number of visualization tools that are available to display data. Since the model output data is netCDF format, essentially any tool capable of displaying this data format can be used to display the WRF model data. Currently, NCAR currently supports 4 graphical tool packages (NCL, RIP4, WRF-to-GrADS and WRF-to-vis5d. A description of each of these tools is also available online at:

http://www.mmm.ucar.edu/wrf/users/graphics/WRF-post-processing.htm.

The WRF/Chem model, being part of the WRF modeling system, can likewise use any of the WRF netCDF visualization tools. A detailed description of all available visualization tools is beyond the scope of this user's guide. Instead this chapter will discuss a few of the tools that are being used to examine WRF/Chem input and output files – ncdump, ncview and RIP. However, each user is encouraged to explore the multitude of netCDF visualization tools that are available and use the one(s) that are best suited to their needs.

5.2 The ncdump application

The ncdump utility is distributed by Unidata and installed with the netCDF library. This application is a netCDF file viewer which can be used to generate ASCII representation of the data. There are some limits to what this program can do with point (e.g., surface station) data, but there are more options available for examining array data. However, ncdump can be cumbersome when examining large volumes of array data. The Unidata web page

http://www.unidata.ucar.edu/software/netcdf/docs/ncdump-man-1.html,

contains a detailed description of the ncdump command and examples of its usage.

5.3 Using NCL scripts

Among the many port-processing utilities to visualize WRF output is NCL. This section will briefly describe a script that can be used to generate a plot of chemical species. For additional information about NCL, the reader is directed to Chapter 8 in the WRF model User's Guide.

Following the NCL script examples, the following script has been generated to plot ozone for the 1 August 2000 at 0000 UTC. The user is required to set the date and run directory (direc) as well as the header for the file name (filnm) and field to be plotted in the script. The gas phase species can be converted to ppm from ppb for easier plotting and viewing. The script is as follows:

```
load "$NCARG_ROOT/lib/ncarg/nclscripts/csm/gsn_code.ncl"
load "$NCARG_ROOT/lib/ncarg/nclscripts/csm/gsn_csm.ncl"
load "$NCARG_ROOT/lib/ncarg/nclscripts/wrf/WRF_contributed.ncl"

begin

; read in wrfout file

   date = "08-01_00"

   direc = "./"

; filename=filnm

   filnm = addfile(direc+"wrfout_d01_2000-"+date+":00:00.nc","r")

; extract field to be plotted from file

   ozone = filnm->o3

; scale by 1000 (convert ppm to ppb)
   ozone = ozone*1000.
   ozone@units = "ppbv"

;=================================================================
; set up plotting parameters

; creating 2 workstations to plot both to screen (x11) and to a pdf file
  wks = gsn_open_wks("x11","ozone_lev50_"+date)
  wks_2 = gsn_open_wks("pdf","ozone_lev50_"+date)
  gsn_define_colormap(wks,"WhViBlGrYeOrRe")    ; choose colormap for wks
  gsn_define_colormap(wks_2,"WhViBlGrYeOrRe")  ; choose colormap for wks_2

; assign plotting resources

  res = True
  res@gsnMaximize     = True
  res@gsnSpreadColors = True              ; use full range of color map
  res@cnFillOn        = True              ; turn on color fill
```

```
  res@cnLinesOn       = False               ; turn off contour lines
  res@cnLineLabelsOn  = False               ; turn off contour line labels
  res@cnLevelSelectionMode = "ManualLevels"  ; set explicit contour levels
  res@cnMinLevelValF = 60
  res@cnMaxLevelValF = 110
  res@cnLevelSpacingF = 5
;
  res@tiMainString = "OZONE CONC. AT "+date+"UTC"

;=================================================================

; use WRF_contributed procedure to set map resources

    WRF_map_c(filnm,res,0)

; define lat, lon

    ozone@lat2d = filnm->XLAT(0,:,:)
    ozone@lon2d = filnm->XLONG(0,:,:)
;
; plot ozone at the lowest level

    plot = gsn_csm_contour_map(wks,ozone(0,0,:,:),res)
    plotpdf = gsn_csm_contour_map(wks_2,ozone(0,0,:,:),res)

end
```

By issuing the ncl execution command
ncl <script name>
The contour plot showing ozone concentration over the domain is generated (Figure 5.1).

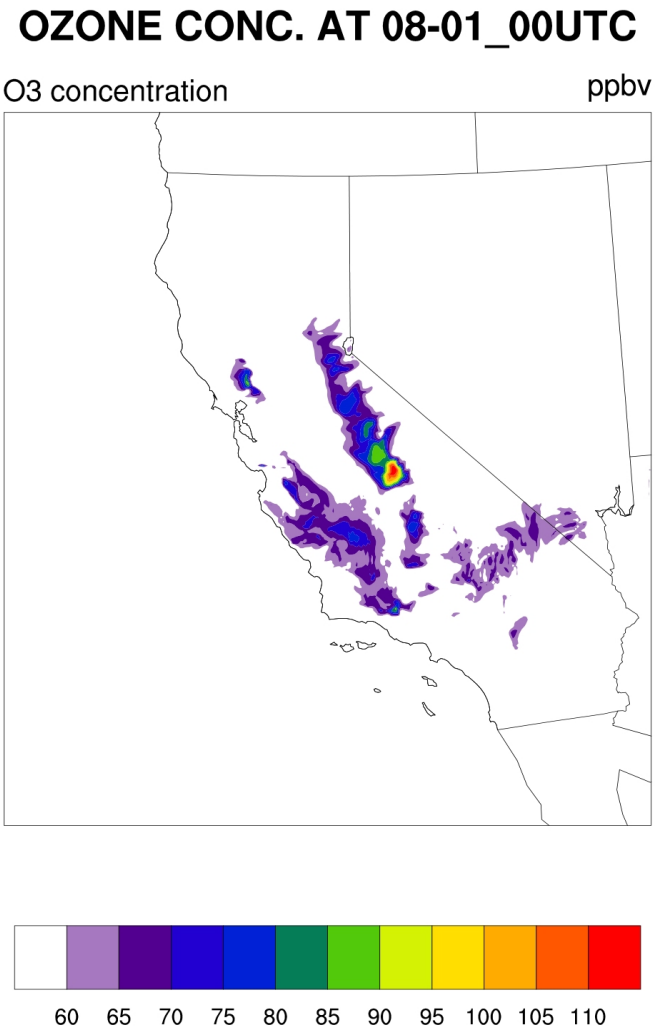

Fig. 5.1 A sample of a color-filled contour plot generated using the NCL script. The colored regions represent locations in which the surface ozone concentration (ppbv) is in the range indicated by the color-bar shown at the bottom of the figure.

5.4 The ncview application

The Ncview application is a visual browser for netCDF data developed by David W. Pierce of the Scripps Institution of Oceanography. Ncview reads the wrfout files (also all input files, including the emissions) directly using the simple command ">ncview wrfout….". This makes it a very useful tool for a quick look analysis or diagnosis of a problem with the model run, including problems with any of the input files. Ncview installs onto UNIX platforms under X11 and provides an easy, push-button method to examine the contents of a netCDF file (Fig. 5.2). When looking at the data you can change the color maps, invert the data, generate line plots, etc. In addition, if the file contains a time series, Ncview permits simple animation of the data. An additional information program as well as a link to download the source code is available online at:

http://meteora.ucsd.edu/~pierce/ncview_home_page.html.

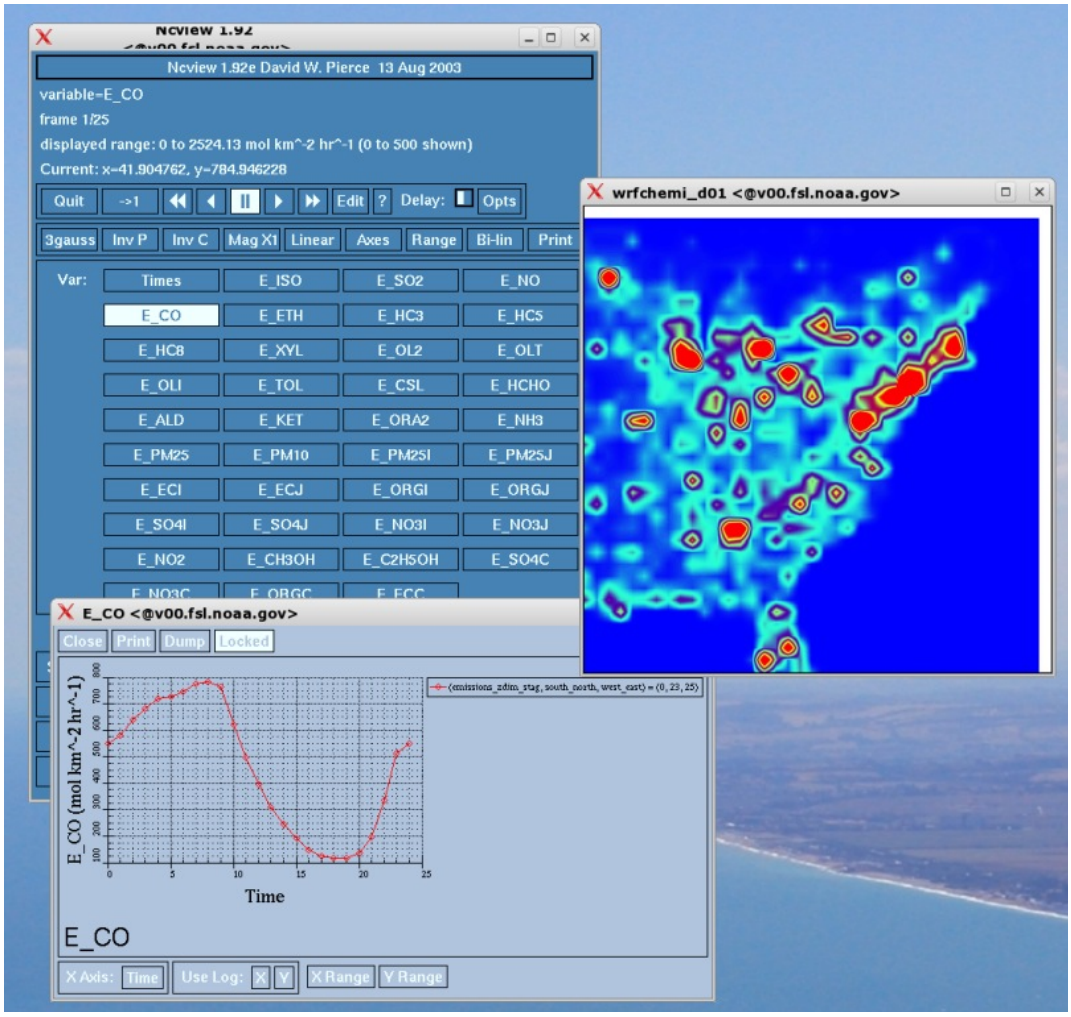

Fig. 5.2 A screen-capture image showing how the Ncview user interface allows the user to examine the WRF/Chem emissions input data file. The color image shows the surface emissions for carbon monoxide and the plot shows the temporal evolution of the surface CO emissions at a single point.

5.5 The RIP application

5.5.1 Downloading and installing the RIP program

The FORTAN program RIP (Read/Interpolate/Plot) invokes NCAR Graphics routines to produce two-dimensional images from gridded numerical model data.

Originally designed to work with the PSU/NCAR Mesoscale Model (*i.e.,* MM5), it has been modified by Mark Stoelinga to work with the WRF model. RIP is officially supported by the National Center for Atmospheric Research (NCAR) and functions on UNIX systems that have a FORTRAN 77/90 compiler and the NCAR Graphics Library. Documentation regarding the RIP program is available online at:

http://www.mmm.ucar.edu/wrf/users/docs/ripug.htm.

RIP is not fully interactive, but instead it requires the user to specify the desired plots through a formatted text file. NCAR Graphics CGM files are created when the RIP program is executed and these files can be viewed with any one of several different metacode translator applications (*i.e.,* idt, ctrans). Additional plots or modification of any existing plots is accomplished through changing the formatted text file and re-executing the RIP program.

5.5.2 Pre-processing data from WRF/Chem

Before using RIP to plot WRF/Chem output, one first needs to specify the location of the RIP executable by setting the environmental variable RIP_ROOT. In c-shell syntax, if the RIP code is located in /home/username/RIP, the command is:

setenv RIP_ROOT /home/username/RIP.

After setting the RIP_ROOT environmental variable, the WRF/Chem data files need to be converted to data files having the format expected by the RIP program. The RIP data preprocessor program, or rip_dp, is used to accomplish this task. Like RIP, a formatted text file is needed to specify what operations are to be performed. The rip_dp input data file (named ripdp.in for example) might look similar to the following example:

```
&userin
 ptimes=0,-
72,3,ptimeunits='h',tacc=30.,discard='QGRAUP','Q2','T2','TH2','AC0','AC
O3','ALD','ANTHA','CANWAT','cor','CORN','COSALPHA','CSL','CU_CO_TEN','D
CB','DEP_VEL','dmap','E','ECI','E_ECI','orgaro1j','orgaro2j','orgaro1i'
,'orgaro2i','orgba1i','orgba1j','orgba2i','orgba2j','orgba3i','orgba3j'
,'orgba4i','orgba4j','orgole1i','orgole1j','orgpai','orgpaj','p25i','p2
5j','nh4ai','nh4aj','no3ai','no3aj','E_NH3','E_ORGI','E_SO2','ETH','EXC
H_H','GLW','GLY','GRDFLX','h2o2','hc3','hc5','hc8','hfx','hno3','hno4',
'ho','ho2','hono','ISLTYP','ISO','IVGTYP','KET','LANDMASK','LH','MGLY',
'MU','MUB','n2o5','nh3','nu0','ol2','olt','onit','op1','op2','paa','pan
','rtc','rte','SEAS','SFROFF','SH2O01','SH2O02','SH2O03','SH2O04','SINA
LPHA','tol','tpan','UDROFF','xyl',
 iexpandedout=1
 &end
```

In this file the number of hours (72), the time interval (3) and the arrays that are to be excluded from preprocessing are specified.

The command to run the rip_dp program might look like the following:

```
ripdp_wrf –n ripdp.in /Data/wrfplots all /WRFV3/test/em_real/wrfout_d01_2008-07-14_12:00:00
```

The execution of the rip_dp program will produce many small Rip data files. These files are located in the Data directory and are named like the following files:

wrfplots_0000.00000_ALBEDO
wrfplots_0000.00000_V10
wrfplots_0000.00000_ALT
wrfplots_0000.00000_VEGFRA
wrfplots_0000.00000_TMN
wrfplots_0000.00000_SO2
…

5.5.3 Generating NCAR GKS plots using RIP

Before generating the NCAR graphics data files, the user needs to provide all of the specific details in RIP user input data file, rip.in. The first part of this data file consists of 2 namelists: the userin namelist which holds the general input specifications and the trajcalc namelist which controls the creation of trajectories plots. The second part of the rip.in file holds a specification table that controls the generation of the plot(s). The reader should examine the online RIP documentation for a more detailed explanation.

For the generation of a horizontal plot showing the fine particulate matter (PM2.5) and the horizontal winds at the surface and placed on a map of the simulation domain, the rip.in data file would look similar to the following:

```
 &userin
 idotitle=1,title='PM2.5 Level 1',titlecolor='def.foreground',
 ptimes=${hour},
 ptimeunits='h',tacc=180,timezone=-7,iusdaylightrule=1,
 iinittime=1,ivalidtime=1,inearesth=0,
 flmin=.09, frmax=.92, fbmin=.10, ftmax=.85,
 ntextq=0,ntextcd=0,fcoffset=0.0,
 idescriptive=1,icgmsplit=0,maxfld=10,itrajcalc=0,imakev5d=0
 &end
 &trajcalc
 rtim=15,ctim=6,dtfile=3600.,dttraj=600.,vctraj='s',
 xjtraj=95,90,85,80,75,70,65,80.6,80.6,80.6,80.6,80.6,80.6,
 yitraj=50,55,60,65,70,75,80,77,77,77,77,77,77,
 zktraj=.9,.9,.9,.9,.9,.9,.9,.99,.9,.8,.7,.6,.5,
 ihydrometeor=0
 &end
=========================================================================
--------------------    Plot Specification Table    --------------------
=========================================================================
feld=PM_2.5_DRY; ptyp=hc; vcor=s; levs=b1; cint=.5; cmth=fill;>
   smth=2;cosq=.0,violet,2.,dark.blue,4.,blue,6.,green,>
        8.,light.green,10.,dark.yellow,15.,yellow,>
```

```
        20.,red,30.,red.coral,40.,orange,50.,tan,>
        60.,light.gray,70.,med.gray,80.,black,100.,white
feld=uuu,vvv; ptyp=hv; nttl;vcmx=-1; colr=black;linw=2
feld=map; ptyp=hb
feld=tic; ptyp=hb
==========================================================================
```

Generation of a NCAR CGM data file is done by issuing the command:

${RIP_ROOT}/rip rip.in wrfplots

In the /Data directory. With the successful execution, a file named wrfplots.cgm is created. As mentioned previously, the CGM data file can be viewed using any of the CGM file viewers like ctrans. For example, to use ctrans to view the CGM file, issue the command:

${NCARG_ROOT}/bin/ctrans -d X11 wrfplots.cgm.

The product from executing this command will be an image like the one shown in Fig. 5.3.

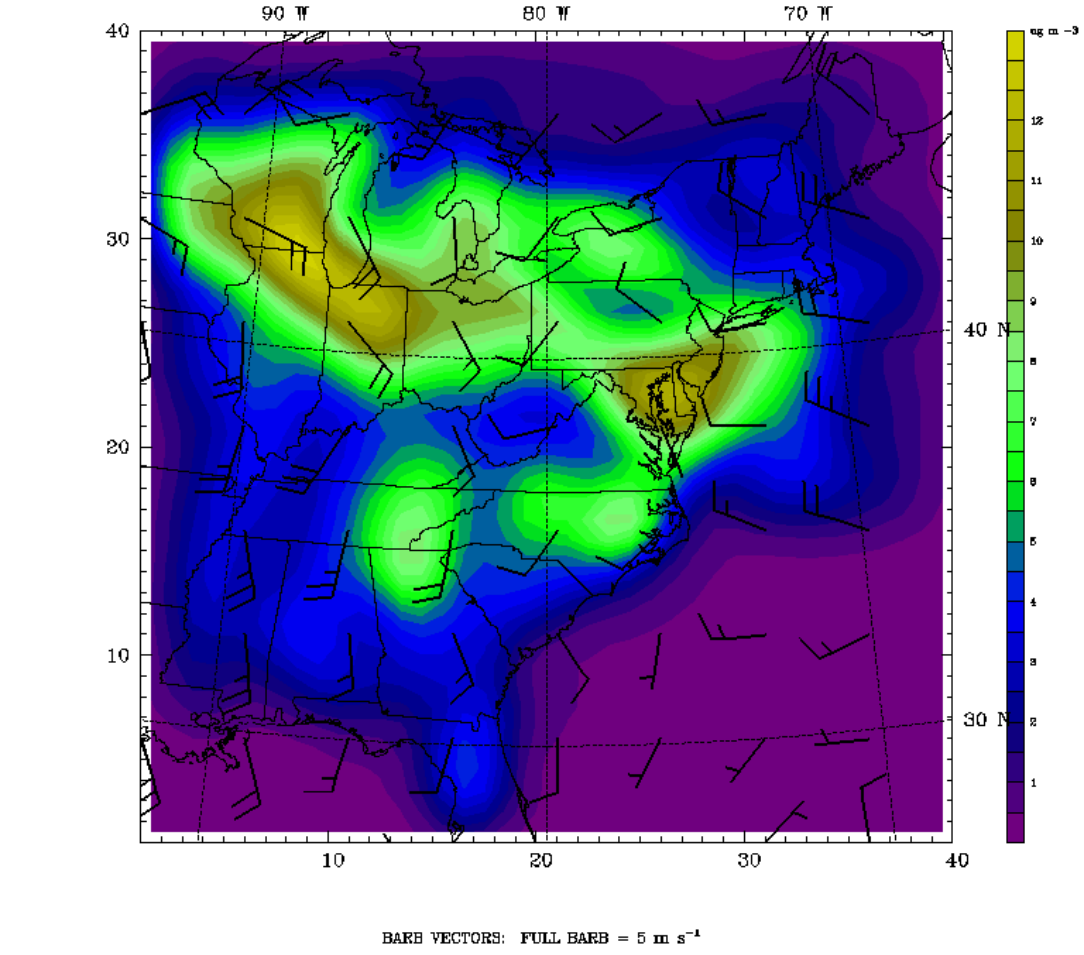

Fig. 5.3. An NCAR GKS figure produced using by the RIP visualization tool. The image shows the surface fine particulate matter (PM2.5) concentration (micrograms per cubic meter) and the horizontal surface winds (barbs).

With the successful visualizing of the results from a WRF/Chem simulation, one could add additional fields to plot by making additional RIP user input data files for each individual plot, or modify the previous image specifications in a user-input data file. After modifying the user-input data file(s), you would only need to (re)create the NCAR CGM file(s).

Chapter 6: WRF/Chem KPP Coupler

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6.1 Introduction

Coupled state of the art meteorology/chemistry models such as WRF/Chem typically include hundreds of reactions and dozens of chemical species. Solving the corresponding huge systems of ordinary differential equations requires highly efficient numerical integrators. In the case of hard-coded manually "tuned" solvers, even minor changes to the chemical mechanism, such as updating the mechanism by additional equations, often require recasting the equation system and, consequently, major revisions of the code. This procedure is both extremely time consuming and error prone.

In recent years, automatic code generation has become an appreciated and widely used tool to overcome these problems. The Kinetic PreProcessor (KPP) is a computer program which reads chemical equations and reaction rates from an ASCII input file provided by the user and writes the program code necessary to perform the numerical integration (Damian et al. 2002; Sandu et al. 2003; Sandu and Sander 2006). Computational efficiency is obtained by automatically reordering the equations in order to exploit the sparsity of the Jacobian. While still in a developmental stage, KPP Version 2.1 has been sucessfully implemented into WRF/Chem. Furthermore, a preprocessor for WRF/Chem has been developed that automatically generates the interface routines between the KPP-generated modules and WRF/Chem, based on entries from the WRF/Chem registry files and the KPP input files. This WRF/Chem-KPP coupler, WKC hereafter, is automatically executed during code compilation and considerably reduces the effort to add chemical compounds and/or reactions to existing chemical mechanisms. Likewise, the effort needed to construct new chemical mechanisms code has been greatly reduced due to the addition of KPP into WRF/Chem.

The WRF/Chem KPP Coupler, or WKC, was discussed by Salzmann and Lawrence (2006) at the WRF-User Workshop. The abstract is for the presentation is available with the KPP documentation in the WRF/Chem code (WRFV3/chem/KPP/documentation/abstr_wkc.pdf). A more complete set of

documentation for KPP (Kinetic PreProcessor) is also provided on line by Adrian Sandu at:

http://people.cs.vt.edu/ asandu/Software/Kpp/.

References for the KPP are Damian et al. (2002), Sandu et al. (2003), Sandu and Sander (2006) and it is requested that these references are cited when presenting results from the KPP generated code. KPP and WKC are distributed under the GNU General Public License (GPL). Constructive comments and suggestions regarding the coupler and/or this documentation are welcome. Only a limited number of all KPP features are available for use with WKC, but more features may be added in the future.In the remainder of this chapter, the WKC as implemented into the WRF/Chem model is described. Since the coupler has been only recently added to the WRF repository, it is possible that some design details could change based upon response from the WRF model developers as well as the WRF/Chem user community.

6.2 KPP requirements

KPP requires the UNUX tool programs flex, yacc, and sed to be installed on your system before compiling the code. Check with your system administrator if these programs are not installed. The path to the flex library (either libfl.a or libfl.sh) is specified by the environment variable FLEX_LIB_DIR. The default path for these libraries is assumed to be /usr/lib. If the library libfl.a (or libfl.sh) is not located in /usr/lib on your system, the variable FLEX_LIB_DIR should be set prior to compiling WRF/Chem. The C compiler is set by configure_kpp based on the settings in configure.wrf.

6.3 Compiling the WKC

The WKC, and therefore KPP as well, are compiled and executed automatically when WRF/Chem is compiled with the WRF_KPP environmental variable set (setenv WRF_KPP 1). The WKC copies the KPP generated code to the WRFV3/chem directory and automatically modifies the chemistry Makefile so that the KPP generated code is compiled and linked with the model. The KPP and WKC generated modules in the chem directory contain the string “kpp” in their file names. Running the clean script removes these modules.

6.4 Implementing chemical mechanisms with WKC

KPP files for chemical mechanisms which have already been implemented with WKC are located in subdirectories of WRFV3/chem/KPP/mechanisms. The corresponding packages are declared in the WRFV3/Registry/registry.chem file and contain the suffix “kpp” in their name. In order to use one of these mechanisms with WRF/Chem, set the chem_opt variable in the namelist.input file to the appropriate value. The following mechanisms are currently available:

- RACM/SORGAM
- RACM (Stockwell et al., 1997).
- RACM-MIM (Geiger et al., 2003)
- RACM/SORGAM

These WKC implemented mechanisms have chem_opt greater than 100. The methodology for implementing additional mechanism(s) using KPP is discussed later in this chapter.

6.5 Layout of WKC

WKC reads KPP species input files with suffix .spc and the file Registry/registry.chem and automatically generates the Fortran 90 interface routines between WRF/Chem and the KPP generated code (see Fig. 6.1). It is in parts based on the WRF registry mechanism. The WKC related files are located in the chem/KPP directory. This directory contains:

- a subdirectory mechanisms which holds directories with KPP input files for different mechanisms.
- a compile and a clean script for WKC (which are executed from the WRF/Chem compile script).
- a version of KPP v2.1 in the kpp subdirectory. This version of KPP was adapted to produce code which can directly be used with WRF/Chem (using the #WRF Conform option in the .kpp file).
- the source code of WKC in the util/wkc subdirectory.
- module wkpp_constants.F which allows to specify input to kpp such as RTOL and ATOL (likely to be extended in the future).
- a subdirectory inc containing files which are included during compile time (using "#include" statements). The files in chem/KPP/incare not removed by the WKC clean script. Their purpose is to allow user modifications to WKC generated code.

At the heart of WKC is the routine gen kpp.c, which is located in the util/wkc directory.

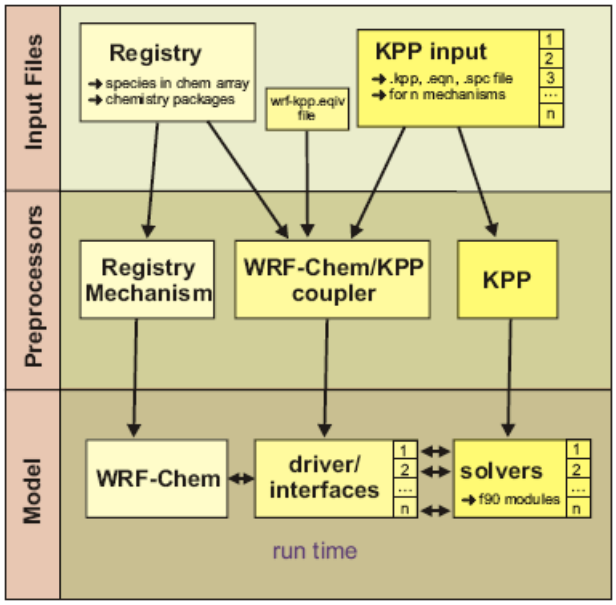

Fig. 6.1. Schematic showing the flow structure of KPP in the WRF/Chem model. Flowing down from the top, the Registry and KPP input data files (ASCII) are preprocessed into Fortran 90 and C code which is coupled to the WRF/Chem solvers.

6.6 Code produced by WKC, User Modifications

The code produced by WKC is called from the chem driver (see schematic call tree in Fig. 6.2). Since parts of the code are generated automatically, manual changes will be lost when recompiling WRF/Chem (as indicated by a warning in the header of the corresponding files). There are, however, a number of "#INCLUDE" preprocessor statements in the WKC generated code. The files included (in the .f files) are located in the chem/KPP/inc directory. These files are not removed by the clean script and can be used to inline user supplied code. In case this should not be enough, there are two ways to edit automatically generated files permanently: The files can either be renamed in such a way that they won't be removed by the clean kpp script, or the C code which generated the files (either KPP or WKC) can be edited. The latter is generally the better solution. However, the method of using include files in the chem/KPP/inc directory is strongly recommended.

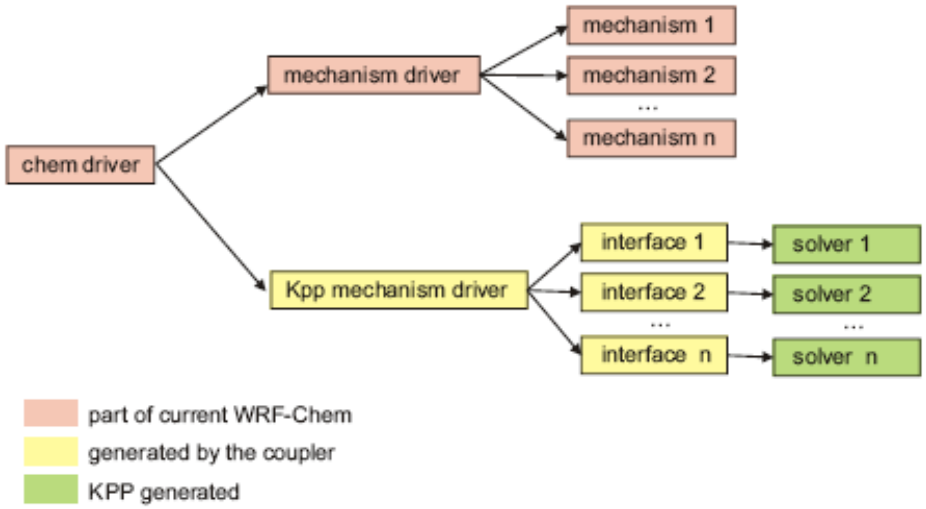

Figure 6.2: Schematic of the KPP call tree. Here the chem_driver routine in WRF/Chem calls a separate mechanism driver for each chemical mechanism implemented with KPP. This model configuration requires only one additional subroutine to be added to WRF/Chem so that the user can switch between the different implemented chemical mechanisms.

6.7 Available integrators

References for the chosen integrator can e.g. after compiling WRF/Chem with KPP be found in the chem directory in module kpp my mechanism Integrator.f90, where ‘‘my mechanism’’ refers to the chemical mechanism chosen in the WRF/Chem namelist. Currently, only Rosenbrock type integrators are available for the use with the WKC. on the methodology to add additional integrators to the WKC will be discussed in a later section.

6.8 Adding additional mechanisms with WKC

When implementing new mechanisms, it is often necessary to calculate additional photolysis rates, include new emission datasets, specify initial and boundary conditions, calculate additional dry deposition rates, specify Henry’s law coefficients for soluble trace gases and carry them through the wet deposition routines, etc., in addition to the following steps.

The following basic steps are necessary in order to add an additional mechanism:

- edit the registry file Registry.EM_CHEM to
  - add additional species to the chem array structure (if necessary).
  - add a package (a mechanism) with a name ending on “_kpp”, e.g., my_mechanism_kpp.

- provide input files my_mechanism.eqn, my_mechanism.spc, my_mechanism.kpp for KPP in a sub-directory of WRFV3/chem/KPP/mechanisms named after the package (i.e. my_mechanism, not my_mechanism_kpp).
- optionally provide a file (my_mechanism_wrfkpp.equiv) for mapping variable names in WRF/Chem to variable names in KPP (e.g. HO to OH).

For additional examples, you can examine the chemical mechanisms that have already been implemented. You should note that when copying one of the directories in WRFV3/chem/KPP/mechanisms to another directory it is necessary to change the name of #Model in the .kpp file and the names of the .eqn and the .spc file in the .def file. When introducing a "new" .kpp file you should set the #INTEGRATOR to an integrator contained in the directory WRFV3/chem/KPP/kpp/kpp-2.1/int/WRF_conform. For example, set

#INTEGRATOR WRF conform/rosenbrock

and add the line

#WRFCONFORM

to your new .kpp file. You should remember that not all KPP options are supported by the WKC. Also, the WKC is currently not able to handle comments in the .spc file!

6.9 Adapting KPP equation files

The process of adapting a KPP equation file for the use with WRF/Chem involves renaming a few variables in the equation file:

	KPP equation file	Equation file units	Registry
Photolysis rate	J(Pj_no2)	s^{-1}	ph_no2
Temperature	TEMP	K	t_phy
Third body concentration	C_M	(molecular moist air) cm^{-3}	Calculated from density
Water vapor concentration	C_H20	Molecules cm^{-3}	Calculated from qvapor

```
#EQUATIONS { racm-mim }
{001} NO2+hv=O3P+NO : j(Pj_no2) ;
{002} O3+hv=O1D{+O2} : j(Pj_o31d) ;
…
{242} MACP+HO2=MAHP : ARR2( 1.82e-13 , -1300.0, TEMP ) ;
{243} MACP+MACP=HACE+MGLY+0.5 HCHO+0.5 CO+HO2 : 2.00e-12 ;
{244} MSACP+NO2=MPAN : TROE( 9.70e-29 , 5.6 , 9.30e-12 , 1.5 , TEMP, C_M) ;
…
```

Example File 1: Excerpt from the KPP equation (.eqn) file for the RACM-MIM (Geiger et al., 2003) mechanism.

Photolysis rates, temperatures, third body concentrations, and water vapor concentrations are passed down from the WRF/Chem KPP interface routines. Photolysis rates are stored pointwise in a 1-D array and addressed by pointers defined in the automatically generated interface routine. For example, the NO2 photolysis rate ph no2 in the Registry. EM CHEM becomes j(Pj no2) in the KPP equation file (see example in Example File 1). Additional variables (e.g. user calculated N2O5 hydrolysis rates) can be passed down by modifying .inc files in the WRFV3/chem/KPP/inc directory.

6.10 Adapting additional KPP integrators for WKC

As previously mentioned, only Rosenbrock type solvers are currently available for use with the WKC. Introducing additional integrators which come with KPP into WRF/Chem is rather straight forward, but the process can be very time consuming. The integrator files which come with KPP are located in the directory chem/KPP/kpp/kpp2.1/int. Integrators which have been adapted for WRF/Chem are located in a subdirectory of chem/KPP/kpp/kpp2.1/int named WRF_Conform. The methodology for adapting an additional solver for WRF/Chem is as follows:

- Copy the .f90 and the .def file to the WRF_Conform directory.
- Add KPP ROOT as a prefix to the names of the subroutines in all subroutine and end subroutine statements.
- Change the arguments in the SUBROUTINE (KPP_ROOT_)INTEGRATE statements to match the calling routine (see the existing integrator routines for an example).

Remove all the USE statements in which non-constant data is used. Instead pass down the data in the subroutine statements. And you should be aware that, depending on the chosen solver, there may be additional required steps that have not been mentioned above.

Chapter 7: Summary

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7.1 Summary

Presented in this user's guide is version 3.3 of the WRF/Chem model. This guide is not intended to be an exhaustive report about all that is needed to setup and use the WRF/Chem model. While it attempts to provide the latest and most accurate information about the setup and running of WRF/Chem, errors or incomplete information may have been presented. Also, due to the complexity of the model and the diverse needs of each user, there may be insufficient information for your particular research or operational application.

As was stated in beginning chapters, you will need to consider your needs and/or requirements for the domain of interest before beginning the simulation. This includes, but is not limited to the available meteorological and anthropogenic emissions data sets. Also, the WRF model, and likewise the WRF/Chem model, is being continuously updated. Therefore, you are advised to stay involved in the WRF/Chem user community to be made aware of any and all updates to or issues with the code.

You are also advised to link your web browser to the WRF/Chem user group web page (http://www.wrf-model.org/WG11) and periodically scan the pages for changes and/or updates to the model. These web pages contain answers to frequently asked questions, or FAQ's. So this is a good place to start when you have a question regarding the setup, use, or performance of the WRF/Chem model. Finally, this web page contains a list of relevant publications regarding the WRF/Chem model. When presenting, or publishing your results from the WRF/Chem model, it is requested that you cite the Grell et al. (2005) and Fast et al. (2006) manuscripts provided in the relevant publications section of this chapter. For any application that uses the indirect effect, please also cite Gustafson et al. (2007). A more detailed model description with a series of papers is in the works and may appear in a new journal that is intended for model description papers only.

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Appendix A : WRF/Chem Quick Start Guide

1. Compiling WRF/Chem and the emission converter

a. Download the WRF and then the WRF/Chem from the NCAR WEB site http://www.mmm.ucar.edu/wrf/users/download/get_sources.htm

b. Set the environmental variables
   i. setenv WRF_CHEM 1
   ii. setenv EM_CORE 1
   iii. setenv FLEX_LIB_DIR /usr/lib (optional)
   iv. setenv WRF_KPP 1 (optional)
   v. setenv YACC '/usr/bin/yacc –d' (optional)

c. Compile WRF/Chem using the command:
   compile em_real >& compile.log

d. Compile convert_emiss using the command:
   compile emi_conv >& emcompile.log

2. Running WRF/Chem with the chemistry turned off

a. Decide which emissions preprocessor you will need to run (step 3 or step 6, see also section 2 in the WRF/Chem User's Guide). This is important, since step 6 requires the user to select a polar stereographic projection for the forecast domain.

b. Produce meteorological input files (wrfinput_d01 and wrfbdy_d01) for the domain of your choice (save these, they will be needed later). Use the WPS to do this. Be sure to choose the map projection based upon your desired emissions data set.

c. First run a meteorology-only simulation to verify the domain you want is functioning correctly, the code has compiled properly and no issues exist from the meteorological part of the model (set chem_opt=0 in the namelist).

   i. Modify the namlist.input file (to fit your needs and be sure to set chem_opt=0)

   ii. Run real.exe to produce a wrfinput and wrfbdy file

   iii. Run wrf.exe to produce a forecast

iv. Check the resulting output files to verify your forecast results

3. Producing an emissions input file for your forecast domain using the NEI-05 emissions data set available from the ESRL FTP site (USA only)

a. Download the emiss_v03.F program and the emission data from the ESRL anonymous ftp site, or through your web browser by setting the URL to: ftp://aftp.fsl.noaa.gov/divisions/taq/emissions_data_2005

b. Modify the emiss_v03.F program file to correspond to your domain setup (see also section 2 of the user guide).

c. Compile emiss_v03.F
   i. Using pgi, the suggested compile commands would be
      > pgf90 –w –byteswapio –Mfree –Mlfs –o emiss_v03.exe emiss_v03.F

d. Run emiss_v03.exe to produce an emissions file for a domain located over the contiguous states. Two binary data files will be produced called wrfem_00to12Z and wrfem_12to24Z. You can re-name them after the simulation run, or edit the emiss_v03.F to have the program produce a name that suits your liking.

e. Move the output files with the prefix "wrfem" from where you have run the program to WRFV3/run for use later on by the convert_emiss.exe program.

f. Go to the test/em_real directory and link the binary emissions files from (3e) to the files that are used by the WRF/Chem code
   i. ln –sf wrfem_00to12Z wrfem_00to12z_d01
   ii. ln –sf wrfem_12to24Z wrfem_12to24z_d01

g. Modify the namelist.input file to have the correct update time interval (auxinput5_interval_m, auxinput6_interval_m, etc.) for each auxiliary input stream as those output from the emiss_v03 program. Default output from emiss_v03 is 3600s. You should also set the correct emission input option (emiss_opt) for the anthropogenic emissions and your choice of chem_opt (see section 3.2 of the users guide).

h. Run the convert_emiss program. Run this program with one processor only. It is acceptable if the program was compiled with the distributed memory option, but do not run it with more than 1 processor. Required input files are: wrfinput_d01 (2a), wrfem_00to12z_d01 and/or wrfem_12to24z_d01 (3f), and namelist.input.

i. Check whether the program successfully produced the emissions input (wrfchemi_d01_xxz or wrfchemi_d<domain>_<date>). These are netcdf files, you can check them with ncview or ncbrowse.

4. **Running WRF/Chem (multiple processors may be necessary due to large memory requirements, depending on your domain size)**

   a. Modify the namelist to suit your needs (check Chapter 3 of the user guide to select your namelist options, and chapter 4 as guidance for some typical setups)

   b. Run real.exe to produce the wrfinput file that includes chemistry. Check the output using ncview or ncbrowse or similar programs.

   c. Confirm that you have the emissions files for the simulation in the run directory. If necessary, rename your emissions files (or link them) to the files wrfchemi_00z_d01 and wrfchemi_12z_d01 (for io_style_emissions=1).

   d. Run wrf.exe.

   e. Inspect the model results to make sure your namelist.input settings were correct.

5. **Output can be visualized with various packages, including ncview, NCL, RIP, ncbrowse, GRADS**.

   The output from the WRF/Chem model is a standard WRF output netCDF data file. Therefore, your favorite netCDF data file viewer can be used to examine results. For example, the ncview program will allow the users to quickly view the model output.

Additional Options

6. **Using the global emissions data sets and/or wildfire emissions: When using one of these options you must set up your domain in lambert conformal or polar stereographic projection (required also for step 2a) If you want mix wildfire with emissions from step 3 you will also need to use one of these two projections.**

    a. Get the latest version of the prep_sources_chem_cptec tar files from the ESRL WEB site, including the documentation. ftp://aftp.fsl.noaa.gov/divisions/taq/global_emissions

    b. Compile prep_sources_chem_cptec_wrf following the instructions in the Guide-Prep-Sources-Chem.pdf document and/or the WRF/Chem User's Guide.

    c. Modify the prep_sources_chem.inp file for correct domain, and choice of input data.

    d. Run prep_sources_chem to generate emissions data file.

    e. From your WRF/Chem run directory, link output files (e.g., WRF-2008-07-15 files) from prep_sources_chem_cptec_wrf
        i. ln –sf Prep_sources_chem_cptec_wrf/WRF-2008-07-15-000000-g1-gocartBG.bin wrf_gocart_backg
        ii. ln –sf Prep_sources_chem_cptec_wrf/WRF-2008-07-15-000000-g1-ab.bin emissopt3_d01
        iii. ln –sf Prep_sources_chem_cptec_wrf/WRF-2008-07-15-000000-g1-bb.bin emissfire_d01

    f. Edit your namelist.input to reflect the switch to global emissions data and run convert_emiss.exe. Typically this will require a change to the update interval, the emissions option and possibly the vertical dimension for the emissions. For example, the global data is updated on a monthly basis and is surface data only. So for a typical simulation of a couple of days the emissions data will not be updated (auxiliary input port time intervals are set to a very large number of seconds) and the namelist modified for surface only emissions (kemit =1).

7. Special biogenic emissions files

There are four choices in the model for biogenic emissions.

a. The first option is not to use an additional biogenic emissions input data file (bio_emi_opt= 0). The user could add the biogenic emission to the anthropogenic emissions data if it is desired. Be sure to do this for every time period in the emissions input data and not just the first time.

b. For the second option (bio_emi_opt= 1), the model calculates the biogenic emissions online using the USGS landuse classification, which is generated by WRF WPS and available for the meteorological and chemical model.

c. For the third option, the user specifies reference fields for the biogenic emissions, which are then modified online by a subroutine from the Biogenic Emissions Inventory System (BEIS) version 3.13. The land-use for this emissions inventory is obtained from the Biogenic Emissions Landuse Database version 3 (BELD3). The reference fields need to be provided as an additional input data file (wrfbiochemi_d01) for the real.exe program.

d. The final option is the use of MEGAN, which again requires the preparation of reference fields (Appendix C of the users guide)

8. Nesting

a. Produce wrfinput files for both domains following Chapter 4 of WRF User's Guide.

b. Like the single domain WRF/Chem simulations, it is probably best to make a nested domain weather forecast (Chapter 5 of WRF User's Guide).

c. Generate the emissions files for both domains using the emiss_v03.F program (section 3 of Quick Step Guide, Chapter 2 of the WRF/Chem User's Guide). File names will need to differentiate between the domains (e.g., wrfem_00to12z_d01 and wrfem_00to12z_d02).

d. The convert_emiss.exe program is not currently designed to read the namelist.input file and generate the nested domain emissions files. Therefore, run the conversion program treating the nested domain as if it was actually the mother domain.

    i. Follow 3f – 3i to generate wrfchemi_d01 for the coarse domain, move it to a safe place so that they will not be over written.

ii. Change the namelist.input file. Moving the nested information to the mother domain column

iii. Move the met wrfinput_d02 to wrfinput_d01

iv. Link the output from emisv03 (for the nested domain) to the required filenames (see 3h)

v. Run convert_emiss.exe

vi. Move the resulting wrfchemi_d01 to wrfchemi_d02.

e. Modify the namelist.input file to set the chemistry namelist variables for the nested domain.

9. Boundary conditions from larger scale models

At this time, tools are still under development to provide larger scale data from models other then WRF as boundary and initial conditions to the WRF/Chem simulations. One such utility program that is available from NOAA/ESRL is called wrfchembc. This program currently works with data from the MPI-MATCH and RAQMS global chemistry models. See also section xx of the WRF/Chem Users Guide).

a. Download the latest version of the code from the ESRL ftp site. For example, the latest code might be named

   ftp://aftp.fsl.noaa.gov/divisions/taq/broken_experimental/wrfchemv2.2_bcond_code_09Apr07.tar

b. Modify the Makefile to use your desired compile options and compile to generate the wrfchembc executable

c. Modify the wrfchembc_namelist.input file to have the correct data directories and species added to the boundary data file (wrfbdy_d01).

d. Run the wrfchembc program after real.exe and before wrf.exe to add the global model data to the lateral boundary data file (wrfbdy_d01)

e. Before running wrf.exe, modify the namelist.input to set have_bcs_chem = .true.

f. Make a forecast using wrf.exe and inspect the model results to make sure your namelist.input settings were correct.

Appendix B : Using prep_chem_sources V1

Emission data generator package

- Fortran 90 code, easily configured.
- Gridded daily emissions fluxes (kg m^{-2}) using several types of map projection (currently polar stereographic, lambert conformal, Gaussian, regular lat-lon) with flexible resolution. Also for non-structured grids (only polar stereographic).
- Easy inclusion of local updates for mega-cities, point and line sources, etc.
- Biomass burning / wildfires emissions:
- Brazilian Biomass Burning Emission Model (Freitas et al., 2005; Longo et al., 2007): plume rise mechanism, daily and model resolution.
- GFEDv2 (van der Werf et al., 2006): 8 days/monthly – 1x1 degree.
- Emission Factors from Andreae and Merlet, 2001.
- 110 chemical species, 6 types of biomes burned
- Anthropogenic sources:
- RETRO (0.5^0 x0.5^0, monthly), EDGAR (1^0 x 1^0, annually)
- Biogenic sources (GEIA inventory 1 x 1 degree)
- Charcoal production, waste burning, ... (Harvard)
- GOCART 1x1 degree emission for OC, BC, SO2, DMS as well as 3d background fields for model initialization of OH, O2H2, NO3.
- There is an option for WRF-CHEM output (binary format), including plume rise stuff, for RACM chemical mechanism and aerosols (OC, BC, PM10, PM2.5).

Contact: First try wrfchemhelp.gsd@noaa.gov for help. The developers of this preprocessor are Saulo R. Freitas (saulo.freitas@cptec.inpe.br) and Karla Longo (karla.longo@dge.inpe.br), web http://meioambiente.cptec.inpe.br/.

Description of the routines:

--Anthropogenic emissions

- retro_emissions.f90
- edgar_emissions.f90
- fwb_awb_emissions.f90
- cetesb_update.f90
- convert_retro_to_racm.f90
- extrapolacao_update.f90
- gocart_emissions.f90
- gocart_backgound.f90

--- Biomass burning emissions

- AeM_emission_factors.f90

- convert_AeM_to_racm.f90
- emission_fields.f90
- gfedv2_8days_emissions.f90
- gfedv2_8days_plumerise.f90
- gfedv2_emissions.f90
- 3bem_emissions.f90
- 3bem_plumerise.f90
- fire_properties.f90

--- Biogenic emissions:

- biogenic_emissions.f90
- convert_bioge_to_racm.f90

--- Main routines

- prep_chem_sources.f90
- prep_chem_sources_utils.f90
- chem1_list.f90

--- Auxiliary routines

- grid_dims_output.f90
- var_tables.f90
- io_params.f90
- vtab_fill.f90
- mem_grid.f90
- node_mod.f90
- rconstants.f90
- lllc_utils.f90
- adap_init_prepchem.f90
- grid_dims.f90
- gridset_prepchem.f90
- rams_grid.f90
- anheader.f90

Utils/ Misc.

- numerical
- I/O routines

Generating emissions input with Prep_chem_sources

Step 1: Compiling the emissions preprocessor

Library: libutils-2.0-opt.a
From the directory: Prep_sources_chem_cptec_wrf
cd utils/bin
set up the Fortran/C compilers (file: include.mk)
make –f Make_utils
cd ../bin
set up the Fortran/C compilers (file: include_prep_chem_src.mk)
make –f Makefile
(If you get an error message, try running “make” a second time.)

Step 2: Editing the input file (namelist): prep_chem_sources.inp

```
 RP_INPUT
!---------------- grid_type of the grid output
  grid_type= 'polar',    !  'polar' = polar stereo. grid output
                                      !  'gg'  = gaussian grid output
                                      !  'll'  = lat/lon grid output
                                      !  'lambert'  = lambert conformal grid output
!---------------- date of emission
   ihour=0,
   iday=14,
   imon=7,
   iyear=2008,
!---------------- select the sources datasets to be used:   1 = yes, 0 = not
  use_retro=1,
  retro_data_dir=' /Emission_data/RETRO/anthro',

  use_edgar=1,
  edgar_data_dir=' /Emission_data/EDGAR/anthro',

  use_gocart=1,
  gocart_data_dir=' /Emission_data/GOCART/emissions',

  use_bioge=1,
  bioge_data_dir=' /Emission_data/biogenic_emissions',
```

```
use_fwbawb=0,
fwbawb_data_dir=' /Emission_data/Emissions_Yevich_Logan',

use_gfedv2=0,
gfedv2_data_dir=' /Emission_data/GFEDv2-8days',

use_bbem=1,
use_bbem_plumerise=1,
!---------------- if  the merging of gfedv2 with bbem is desired (=1, yes, 0 = no)
  merge_GFEDv2_bbem =0,

!---------------- Fire product for 3BEM/3BEM-plumerise emission models
bbem_wfabba_data_dir=' /Emission_data/fires_data/WF_ABBA_v60/filt/f',
bbem_modis_data_dir    =' /Emission_data/fires_data/MODIS/Fires.',
bbem_inpe_data_dir     =' /Emission_data/fires_data/DSA/Focos',
bbem_extra_data_dir    =' /Emission_data/fires_data/xxxxx,

!---------------- veg type data set (dir + prefix)
  veg_type_data_dir      =' /surface_data/GL_IGBP_MODIS_INPE/MODIS',

!---------------- carbon density data set (dir + prefix)
carbon_density_data_dir=' /surface_data/GL_OGE_INPE/OGE',
fuel_data_dir      =' /surface_data/fuel/glc2000_fuel_load.nc',

!---------------- gocart background
  use_gocart_bg=1,
  gocart_bg_data_dir=' /Emission_data/GOCART',

!---------------- for grid type 'll' or 'gg' only
  grid_resolucao_lon=0.1,  ! degree
  grid_resolucao_lat=0.1,   ! degree

  nlat=320,                  ! if gg (only global grid)
  lon_beg = -115.,          ! (-180.:+180.) long-begin of the output file
  lat_beg =  40.,            ! ( -90.:+90. ) lat -begin of the output file
  delta_lon= -115.,           ! total long extension of the domain (360 for global)
  delta_lat= 40.,           ! total lat  extension of the domain (180 for global)

!---------------- For regional grids (polar)
  NGRIDS   = 1,                    ! Number of grids to run

  NNXP     = 40,50,86,46,       ! Number of x gridpoints
  NNYP     = 40,50,74,46,       ! Number of y gridpoints
  NXTNEST  = 0,1,1,1,            ! Grid number which is the next coarser grid
  DELTAX   = 60000.,              ! X and Y grid spacing
```

```
  DELTAY   = 60000.,              ! X and Y grid spacing

  ! Nest ratios between this grid and the next coarser grid.
  NSTRATX  = 1,2,3,4,          ! x-direction
  NSTRATY  = 1,2,3,4           ! y-direction
! For polar, POLELAT/POLELON are the geographical coordinates
!   of the point of tangency between the projection plane and the
!   Earth surface.  They will coincide with the grid center
!   (nnxp/2,nnyp/2) if they are equal to centlat and centlon
! For Lambert POLELAT/POLELON are the location of the grid center.
  POLELAT  = 45.,
  POLELON  = -115.,


  STDLAT1  = 45.,           ! If polar, unused
  STDLAT2  = 35.,          ! If lambert, standard latitudes of projection

  CENTLAT  =  45.,  -23., 27.5,  27.5,       ! center  (Latitude, degrees) of each grid
  CENTLON  = -115.,  -46.,-80.5, -80.5,   ! center  (longitude, degrees) of each grid

!---------------- project  grid  to lat/lon: 'YES' or 'NOT' (only set up for GrADS
visualization)
  proj_to_ll='YES',

!---------------- model output domain for each grid (only set up for GrADS visualization)
  lati =  -90.,  -90.,   -90.,
  latf =  +90.,  +90.,   +90.,
  loni = -180., -180.,  -180.,
  lonf =  180.,  180.,   180.,

!---------------- output file prefix (may include directory)
  chem_out_prefix = 'WRF-Tutorial',

  chem_out_format = 'vfm', ! don't change this

!---------------- convert to WRF/CHEM (yes,not) – ONLY FOR RACM
 convert_to_wrf = 'yes',

END
```

STEP 3: Run the program (> Prep_chem_sources.exe)

Output filenames will be, based upon the output names and the date/times shown above, the following files:

WRF-Tutorial-2008-07-14-120000-g1-ab.bin
WRF-Tutorial-2008-07-14-120000-g1-bb.bin
WRF-Tutorial-2008-07-14-120000-g1-gocartBG.bin
WRF-Tutorial-2008-07-14-120000-g1.ctl
WRF-Tutorial-2008-07-14-120000-g1.gra
WRF-Tutorial-2008-07-14-120000-g1.vfm
WRF-Tutorial-2008-07-14-120000-g1

The important binary data files from the list are the first three. These files are the binary intermediate files containing anthropogenic emissions, biomass burning emissions information and the GOCART aerosol scheme background fields, respectively. These files will need to be copied or linked to your WRF run directory (e.g., WRFV3/test/em_real) and then converted to WRF emissions input files. The anthropogenic emissions files linked to a file named emissopt3_d01, the biogenic emissions file linked to a file named emissfire_d01 and the GOCART aerosols linked to a file named wrf_gocart_backg.

```
ln -s WRF-Tutorial-2008-07-14-120000-g1-ab.bin ../WRFV3/test/em_real/emissopt3_d01
ln -s WRF-Tutorial-2008-07-14-120000-g1-bb.bin ../WRFV3/test/em_real/emissfire_d01
ln -s WRF-Tutorial-2008-07-14-120000-g1-gocartBG.bin ../WRFV3/test/em_real/wrf_gocart_backg
```

To convert the global anthropogenic emissions to WRF chemistry emissions data files, emiss_opt needs to be set to a GOCART aerosol option (e.g., chem._opt=301 and emiss_opt=5). To use the NEI data set emiss_opt to another option like RADM2/SORGAM (chem._opt=2 and emiss_opt=3).

Description of the datasets in directory :

(1) /Emission_data

Biogenic Emissions from GEIA (http://www.geiacenter.org/)

biogenic_emissions

- ACETONE_BIO.TXT
- C2H4_BIO.TXT
- C2H4_OCEANS.TXT
- C2H6_BIO.TXT
- C2H6_OCEANS.TXT
- C3H6_BIO.TXT
- C3H6_OCEANS.TXT
- C3H8_BIO.TXT
- C3H8_OCEANS.TXT

- CH3OH_BIO.TXT
- CO_BIO.TXT
- CO_OCEANS.TXT
- ISOPRENE_BIO.TXT
- NO_SOILS.TXT
- NVOC.TXT
- TERPENES_BIO.TXT

Anthropogenic emissions from "Emission Database for Global Atmospheric Research (EDGAR)" http://www.mnp.nl/edgar
Resolution 1^0 x 1^0, annually
EDGAR/anthro:

- edg_CH4_2000_total.txt
- edg_CO_2000_total.txt
- edg_CO2_2000_total.txt
- edg_N2O_2000_total.txt
- edg_NMVOC_2000_total.txt
- edg_NOX_2000_total.txt
- edg_SF6_2000_total.txt
- edg_SO2_2000_total.txt
- edg_SULF_2000_total.txt

Woodfuels burning (including both fuelwood and charcoal burning), residue and dung used as biofuels and burning of residues in the fields

- From: Yevich, R. and J.A. Logan, An assessment of biofuel use and burning of agricultural waste in the developing world, Global Biogeochemical Cycles, 2003

- Emissions_Yevich_Logan:
- BIF.1x1
- CMB.1x1
- WDF.1x1

Anthropogenic emissions from
"REanalysis of the TROpospheric
chemical composition over the past 40 years"
(http://retro.enes.org/)
RETRO/anthro:

- RETRO_edg_anthro_ACIDS_2000.0.5x0.5.txt
- RETRO_edg_anthro_ALCOHOLS_2000.0.5x0.5.txt
- RETRO_edg_anthro_BENZENE_2000.0.5x0.5.txt
- RETRO_edg_anthro_C2H2_2000.0.5x0.5.txt
- RETRO_edg_anthro_C2H4_2000.0.5x0.5.txt

- RETRO_edg_anthro_C2H6_2000.0.5x0.5.txt
- RETRO_edg_anthro_C3H6_2000.0.5x0.5.txt
- RETRO_edg_anthro_C3H8_2000.0.5x0.5.txt
- RETRO_edg_anthro_C4H10_2000.0.5x0.5.txt
- RETRO_edg_anthro_C5H12_2000.0.5x0.5.txt
- RETRO_edg_anthro_C6H14_PLUS_HIGHER_ALKANES_2000.0.5x0.5.txt

- RETRO_edg_anthro_CHLORINATED_HYDROCARBONS_2000.0.5x0.5.txt
- RETRO_edg_anthro_CO_2000.0.5x0.5.txt
- RETRO_edg_anthro_ESTERS_2000.0.5x0.5.txt
- RETRO_edg_anthro_ETHERS_2000.0.5x0.5.txt
- RETRO_edg_anthro_KETONES_2000.0.5x0.5.txt
- RETRO_edg_anthro_METHANAL_2000.0.5x0.5.txt
- RETRO_edg_anthro_NOX_2000.0.5x0.5.txt
- RETRO_edg_anthro_OTHER_ALKANALS_2000.0.5x0.5.txt
- RETRO_edg_anthro_OTHER_AROMATICS_2000.0.5x0.5.txt
- RETRO_edg_anthro_OTHER_VOC_2000.0.5x0.5.txt
- RETRO_edg_anthro_TOLUENE_2000.0.5x0.5.txt
- RETRO_edg_anthro_TRIMETHYLBENZENES_2000.0.5x0.5.txt
- RETRO_edg_anthro_XYLENE_2000.0.5x0.5.txt
- SantiagoInventory_CO.txt

Biomass burning emissions from
"REanalysis of the TROpospheric
chemical composition over the past 40 years"
(http://retro.enes.org/)
Resolution: 0.5^0 x 0.5^0, monthly

- RETRO_edg_FIRES_2000_ACETONE_total.txt
- RETRO_edg_FIRES_2000_BC_total.txt
- RETRO_edg_FIRES_2000_BENZENE_total.txt
- RETRO_edg_FIRES_2000_CH2O_total.txt
- RETRO_edg_FIRES_2000_CH3CHO_total.txt
- RETRO_edg_FIRES_2000_CH3OH_total.txt
- RETRO_edg_FIRES_2000_CH4_total.txt
- RETRO_edg_FIRES_2000_CO2_total.txt
- RETRO_edg_FIRES_2000_CO_total.txt
- RETRO_edg_FIRES_2000_ETHANE_total.txt
- RETRO_edg_FIRES_2000_ETHENE_total.txt
- RETRO_edg_FIRES_2000_ETHYNE_total.txt
- RETRO_edg_FIRES_2000_H2_total.txt

- RETRO_edg_FIRES_2000_ISOPRENE_total.txt
- RETRO_edg_FIRES_2000_MONOTERPENES_total.txt
- RETRO_edg_FIRES_2000_N2O_total.txt
- RETRO_edg_FIRES_2000_NH3_total.txt
- RETRO_edg_FIRES_2000_NOX_total.txt
- RETRO_edg_FIRES_2000_OC_total.txt
- RETRO_edg_FIRES_2000_PM2_5_total.txt
- RETRO_edg_FIRES_2000_PROPANE_total.txt
- RETRO_edg_FIRES_2000_PROPENE_tota**l.txt**
- RETRO_edg_FIRES_2000_SO2_total.txt
- RETRO_edg_FIRES_2000_TC_total.txt
- RETRO_edg_FIRES_2000_TOLUENE_total.txt
- RETRO_edg_FIRES_2000_TPM_total.txt
- RETRO_edg_FIRES_2000_XYLENE_total.txt

GOCART emissions & background
Emissions for OC, BC and SO2
Resolution: 1x1 degree

- BC_anthro_noship_2006.nc
- OC_anthro_noship_2006.nc
- SO2_anthro_noship_2006.nc

DMS reference field
1x 1.25 degree (monthly)

- dms_1x1.25.nc

Background chemistry fields for GOCART runs

- GAO_source_3cl.nc includes NO3, H2O2 and OH
- 3d field (1x1.25 degree, monthly)
- gmi_2006MM.nc

Biomass Burning emissions from " Global Fire Emissions Database"
http://daac.ornl.gov/VEGETATION/guides/global_fire_emissions_v2.1.html
Global data of biomass consumed, 1 x 1 degree and 8-day time resolution
From year 2001 to 2005.

GFEDv2-8days:

- C_2001_JD001.txt
- C_2001_JD009.txt
- C_2005_JD337.txt

- (...)
- C_2005_JD345.txt
- C_2005_JD353.txt
- C_2005_JD361.txt

(2) Fire emission formats used by the preprocessor

Biomass burning emissions from
Brazilian Biomass Burning Emission Model
Emission Factors from Andreae and Merlet (2001).

(3) Fire location and properties from Wildfire Automated Biomass Burning Algorithm (WF_ABBA)

http://cimss.ssec.wisc.edu/goes/burn/abba.html. **Only for Americas**.

fires_data/WF_ABBA_v60/filt:

f20081940000.namer.v60.g10.filt
f20081940015.namer.v60.g12.filt
f20081940030.namer.v60.g10.filt
f20081940045.namer.v60.g12.filt
f20081940100.namer.v60.g10.filt

Format (ASCII, with header):

GOES-12 WF_ABBA (vs 6.0) Experimental Filtered Fire Product
Note: This product is preliminary and has not been quality controlled
Date: 2008194 Time: 1200 UTC Filtered file: 12 hours 24 files

Longitude	Latitude	T4(K)	T11(K)	Size(km2)	Temp(K)	Ecosystem	Fire Flag
-104.34	57.78	309.2	277.8	-9.0000	-9.	21	3
-96.17	56.38	308.1	296.5	.1931	481.	21	0
-88.27	48.60	300.2	274.4	-9.0000	-9.	21	4
-89.00	47.95	300.6	275.3	-9.0000	-9.	23	5
-89.05	47.88	301.5	274.6	-9.0000	-9.	23	5

Change routine ‘read_abba’ in the 3bem_emissions.f90 in case of different format.

Fire location and properties from Brazilian Institute for Space Research (INPE, www.queimadas.cptec.inpe.br).
Only for Central and South Americas.

(4) fires_data/AVHRR:

Focos20020901.txt
Focos20020902.txt
Focos20020903.txt
Focos20020904.txt
Focos20020905.txt

Format (ASCII, no header)

LAT	LONG	DATE	TIME	
-10.4283	-51.8000	2002-09-05	200621	NOAA-12
-10.4267	-51.8610	2002-09-05	200621	NOAA-12
-10.4267	-51.8550	2002-09-05	200621	NOAA-12

Only the first 2 columns are actually used

Change routine 'read_inpe' in the 3bem_emissions.f90 in case of different format.
Fire location and properties from MODIS

(5) fires_data/MODIS:

Fires.20020901.txt
Fires.20020902.txt
Fires.20020903.txt
Fires.20020904.txt
Fires.20020905.txt

Format (ASCII, no header)

Long	Lat			
-119.6177770642	37.7314428691	9	T	h08v05
-119.6094325631	37.7314428691	9	T	h08v05
-120.1852031388	36.9808173478	9	T	h08v05
-120.1768586377	36.9808173478	9	T	h08v05
-120.1685141366	36.9808173478	8	T	h08v05
-120.1601696355	36.9808173478	8	T	h08v05

Only the first 2 columns are actually used
Change routine 'read_modis' in the 3bem_emissions.f90 in case of different format.

(6) Directory /surface_data

- GL_IGBP_MODIS_INPE : 1 km global vegetation map from MODIS/INPE used for determination of the type of vegetation burnt by fires

- GL_OGE_INPE : 0.5 degree global carbon in live vegetation used for estimate the aboveground biomass density of the vegetation burnt by fires.

- Fuel: glc2000_fuel_load.nc = > 1 x 1 km above ground biomass

Appendix C: Using prep_chem_sources V1.1.1

Source Distribution Layout

The top level of the source code distribution contains the following subdirectories:

bin -- Scripts for maintenance, execution, compilation.
src -- Source codes
aux_src -- Auxiliary codes.

Third Party Software Requirements

JPEG distribution release 6b(libjpeg.a). You may download the software from http://www.hdfgroup.org/release4/obtain.html.
ZLIB 1.2.1(libz.a) or later distribution. You may download the software from the http://www.gzip.org/ site.
HDF4 4.2.5 (libmfhdf.a, libdf.a) or later distribution. You may download the software from http://www.hdfgroup.org/release4/obtain.html.
NetCDF 4.0.1 (libnetcdf.a). You may download the software from http://www.unidata.ucar.edu/downloads/netcdf/netcdf-4_0_1/index.jsp

Configuring/Installing HDF4

When compiling PREP-CHEM-SRC codes on a Linux system using the PGI (Intel) compiler, make sure the netCDF and HDF* library has been installed using the same PGI (Intel) compiler.

```
./configure --prefix=path_hdf4    \
--with-jpeg=path_jpeg \
                --with-zlib=path_zlib \
                --disable-netcdf
make && make install
```

Configuring/Installing the prep_chem_sources code

To compile the version 1.1.1 code one needs to change directory to the bin/build directory

cd bin/build

and then issue the make command with the compiler option (e.g., Intel, PGI) and the chemistry option (ie., RADM_WRF_FIM, RACM)

make OPT=opt.pgi CHEM=RACM

Using PREP-CHEM-SRC-1.1.1 with WRF-Chem V3.3

To run the prep_chem_sources executable one must first edit and the namelist input fields. Most of the settings are like the previous versions with the exception of the map projection settings. But fortunately the map projection settings correspond to the map projection settings used in the WPS input file namelist.wps. That is:

NINEST=i_parent_start,
NJNEST=j_parent_start,
POLELAT=ref_lat,
POLELON=ref_lon,
STDLAT1=truelat1,
STDLAT2=truelat2.

The prep_chem_sources settings CENTLAT and CENTLON are not used for WRF, but are most often the latitude and longitude of the central grid point for your domain.

After setting the prep_chem_sources namelist one can run the PREP-CHEM-SRC-1.1.1 executable (e.g., prep_chem_sources_RADM_WRF_FIM.exe) for each day to produce the intermediate data files. These files are the anthropogenic and biogenic emissions file (ending with -ab.bin), the biomass burning emissions file (ending with -bb.bin), and the GOCART background data (ending with -gocartBG.bin).

Once the prep_chem_sources executable has been run, the methodology for converting the binary intermediate files is the same as in previous versions. *But please note that version 1.1.1 data files are not backward compatible with earlier versions. That is, use version 1.1.1 output files with the updated version 3.3 code.*

The process to convert the binary intermediate files is outlined in section 3.2 of this user's guide, but it will be quickly recapped here. For each day that you are going to use the global emissions data you need to run the convert_emissions program. This program will also need a wrfinput data file for the desired date as well. So to begin, one can run the real.exe with chem_opt=0 and start and end time set to your year, month, day and start hour generate a wrfinput_d01 file. Then the output from prep_chem_sources is linked to the WRF running directory (e.g., WRFV3/test/em_real) with commands similar to the following:

```
ln -sf WRF-2011-07-14-000000-g1-gocartBG.bin ../../WRFV3/test/em_real/wrf_gocart_backg
ln -sf WRF-2011-07-14-000000-g1-ab.bin       ../../WRFV3/test/em_real/emissopt3_d01
ln -sf WRF-2011-07-14-000000-g1-bb.bin       ../../WRFV3/test/em_real/emissfire_d01
```

And then before one can run the convert emissions program convert_emiss (convert_emiss.exe) the namelist.input settings for the chemistry needs to be turned back on (e.g., chem_opt=301). Be sure to double check your other namelist settings as well or you might not get the desired data files.

```
&time_control
 io_form_auxinput5               = 2
 io_form_auxinput7               = 2
 io_form_auxinput8               = 2
 auxinput5_interval_m            = 1440,1440
 auxinput7_interval_m            = 1440,1440
 auxinput8_interval_m            = 1440,1440
 frames_per_auxinput7            = 1,1
 frames_per_auxinput7            = 1,1
 frames_per_auxinput8            = 1,1
/
&chem
 kemit                       = 1,
 io_style_emissions              = 2,
 emiss_inpt_opt                  = 1,       1,
 emiss_opt                       = 5,       5,
 biomass_burn_opt                = 1,       1,
 plumerisefire_frq               = 120,     120
```

And when complete and the data files are verified you can 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
```

Appendix D: Using MEGAN with WRF/Chem

Introduction

The University Corporation for Atmospheric Research (UCAR) provides Fortran source code files to create MEGAN (Model of Emissions and Gases from Nature) biogenic emission data for importing into WRF-Chem. MEGAN is a global emissions dataset, at one kilometer spatial resolution, compiled for 2003. A users guide and descriptions of the data set are provided at http://bai.acd.ucar.edu/Megan/.

The MEGAN toolkit for WRF-Chem preprocesses the MEGAN data set, and creates wrfbiochem_d0x (x = domain number) input files for ingestion into WRF-Chem at model run time.

The following instructions assume that real.exe and wrf.exe have been compiled normally and that an initial meteorology only wrfinput_d0x file(s) have been created post WPS. These instructions also assume you are using the provided 2003 MEGAN data files. The tar file from UCAR includes a helpful readme file which expands on the instructions below.

Compiling

1) Download the MEGAN preprocessor Fortran source code and data set from http://www.acd.ucar.edu/wrf-chem/. You will be asked to register some contact details – subsequently click the "bio-emiss" button on the user registration page to download the MEGAN Fortran source code, makefile and MEGAN data input files. The files can be downloaded to a directory of your choice – note that the process of using MEGAN needs to access the WRF run directory and the wrfinput_d01 file during MEGAN data preprocessing.

2) un-tar the files downloaded in the MEGAN directory by issuing the commands:

   >tar –xvf bio_emiss.tar

   This creates two other tar files, un-compress and un-tar these files:

   >tar –xvf megan_bio_emiss.tar
   >tar –zxvf megan.data.tar.gz

3) Ensure the correct environment variables for your Fortran compiler and netCDF libraries are set correctly by editing the make_util script file if necessary.

4) Compile the MEGAN source code in the MEGAN directory by issuing the command:

   >make_util megan_bio_emiss

   This will create the executable file – megan_bio_emiss

Preprocessing

5) Run real.exe for meteorology only to produce files that will contain WRF headers. This step is similar for all emissions input creation. This step will create a file named wrfinput_d01 that does not contain any input for MEGAN. The following MEGAN pre-processing steps utilize the wrfinput_d01for geographical and temporal parameters necessary for the production of wrfbiochem_d0x files.

6) Adjust the text file; megan_bio_emiss.inp, for:
   1. domains – the number of domains used in your WRF model,
   2. start_lai_month - this should be set as the month before the month in which your WRF run is set to start,
   3. end_lai_month – this should be set as the month in which your WRF run is set to end,
   4. wrf_dir – the directory where the associated wrfinput_d01 resides, and
   5. megan_dir – the directory in which the MEGAN data files exist.

   Note – lai (or leaf area index) parameter data files are provided in the MEGAN preprocessing download – one file exists for each month.

7) Create MEGAN bioegenic emissions data for your domain and time frame by issuing the command:

   >megan_bio_emiss < megan_bio_emiss.inp > megan_bio_emiss.log

   Note – this serial process can take some time depending on a range of factors (perhaps 10 minutes for a lambert conformal projection).

   Check megan_bio_emiss.log for any errors or problems.

8) The files created are wrfbiochemi_d0x files which should be copied (or linked) into the associated WRF run directory.

   You might review the wrfbiochemi_d0x files with ncview to ensure the correct geographical bounds have been applied and that the MEGAN data sets are included.

   Note – the MEGAN data elements in the wrfbiochemi_d0x files are:
   - MSEBIO_ISOP amount of isoprene (mol km^{-2} hr^{-1}),
   - PFTP_BT percentage of broad leaf,
   - PFTP_NT percentage of needle leaf,
   - PFTP_SB percentage of shrubs,
   - PFTP_HB percentage of herbaceous biota,
   - MLAI monthly leaf area index,
   - MTSA monthly air temperature (K), and
   - MSWDOWN monthly download short wave radiation (W m^{-2}).

Running WRF-Chem with MEGAN

9) To create the WRF-Chem boundary and combined emission files, run real.exe like normal in a directory that contains the files wrfbiochemi_d0x (from step 8), but with bio_emiss_opt=3. With bio_emiss_opt=3, real.exe will create wrfinput_d01 containing inputs required for running MEGAN online.

   Note - wrfbiochemi_d01 and wrfinput_d01 will also include variables for running BEIS3.13, but the values for BEIS variables will all be all zero; you'll need to create a different wrfbiochemi_d01 file if you want to use bio_emiss_opt=2.

10) Now, you can run wrf.exe with MEGAN emissions calculated online using bio_emiss_opt=3.

    Note – the process of using wrf_biochemi_d0x files in WRF-Chem model runs will depend on how many WRF-Chem domains you have in mind. For a single domain one wrf_biochemi_d01 file will be produced. Using more than one domain (therefore wrf_biochemi_d0x files, where x = 1, 2 to the maximum domain number) involves careful application of model processes as documented elsewhere in this manual. It can be complex using MEGAN data files for 2 way or 1 way (n-down or 2 way with feedback to the coarse domain switched off) nesting WRF-Chem processes. However, assuming the wrfinput_d0x files are setup correctly before preprocessing MEGAN data files, the wrf_biochemi_d0x files will match the geographical extent of the wrfinput_d0x files. There is slightly less complicated than the process needed to compile the baseline wrfchemi_d0x files.

    Note – when using MEGAN the bioemdt parameter of the &chem namelist.input section must be set to the same number of minutes as the model time step seconds (for each domain).

Appendix E: Using MOZART with WRF/Chem

Introduction

The National Center for Atmospheric Research (NCAR) provides Fortran source code to prepare additional data files to support the MOZART (Model for OZone And Related chemical Tracers) gas phase chemistry scheme in WRF-Chem. These files are needed to update WRF-Chem parameters suitable for MOZART. MOZART gas phase chemistry can be combined with GOCART aerosol treatment – known as MOZCART in this manual.

When setting up WRF-Chem to use MOZART/MOZCART the user should select the FTUV photolysis option (phot_opt=3) in the namelist.input file. NCAR advises the FTUV code has been updated to read in O_3 and O_2 climatological atmospheric column values rather than fixed values. This requires an additional input file for each domain – exo_coldens_d<nn> (nn = domain number). The exo_colden utility (for single CPU) reads WRF and MOZART input files and produces netCDF files for each WRF domain.

When using dry deposition in WRF-Chem (gas_drydep_opt=1) combined with MOZART (and MOZCART) scheme in WRF-Chem, NCAR advises an additional file for each domain is required – wrf_season_wes_usgs_d<nn> (nn = domain number). The wesely utility (for single CPU) reads WRF and MOZART input files and produces netCDF files for each WRF domain.

The tar file from NCAR includes a helpful readme file which expands on the instructions below. NCAR provides some information at http://www.acd.ucar.edu/wrf-chem/MOZCART_UsersGuide.pdf which provides a table mapping MOZART emissions species to EPA/NEI species as well as contact details at NCAR for further support.

Compiling

1) Download the MOZART preprocessor Fortran source code from http://www.acd.ucar.edu/wrf-chem/. You will be asked to register some contact details – subsequently click the "preprocessor" button on the user registration page to download the MOZART Fortran source code, makefile and MOZART data input files. The files can be downloaded to a directory of your choice – note that the process of using MOZART needs to access the WRF run directory and the wrfinput_d01 file during MOZART data preprocessing.

2) Un-tar the files downloaded in a directory of your choice by issuing the commands:
   >tar –xvf wes_coldens.tar

3) Compile the MOZART source code by issuing the commands:
   >make_util wesely
   >make_util exo_coldens

This will create the executable files – wesely and exo_coldens.

Preprocessing

5) The wesely program reads WRF wrfinput_d<nn> files and a MOZART data file containing dry emission parameters - season_wes_usgs.nc (found in the tar file above). Adjust the text file wesely.inp for:
   1. domains – the number of domains used in your WRF model,
   2. pft_flnm – season_wes_usgs.nc,
   3. wrf_dir – the directory where the associated wrfinput_d<nn> resides, and
   4. pft_dir – the directory in which the MOZART data file exists.

6) To create the wesely data files for MOZART, issue the command:
   >wesely < wesely.inp > wesely.out

   This creates a file for each domain wrf_season_wes_usgs_d<nn> which should be copied to the WRF run directory for use in WRF-Chem MOZART/MOZCART model runs.

7) The exo_colden program reads WRF wrfinput_d<nn> files and a MOZART data file exo_coldens.nc (found in the tar file above). Adjust the text file exo_coldens.inp for:
   1. domains – the number of domains used in your WRF model,
   2. exo_flnm – exo_coldens.nc,
   3. wrf_dir – the directory where the associated wrfinput_d<nn> resides, and
   4. exo_dir – the directory in which the MOZART data file exists.

8) To create the exo_coldens data files for MOZART, issue the command:
   >exo_coldens < exo_coldens.inp > exo_coldens.out

   This creates a file for each domain exo_coldens_d<nn> which should be copied to the WRF run directory for use in WRF-Chem MOZART/MOZCART model runs.

Running WRF-Chem with MOZART (MOZCART)

9) Selecting the MOZART/MOZCART settings in the namelist.input of the WRF-Chem run directory (chem_opt and emiss_opt) will switch on the ingestion of the files noted above into WRF-Chem.

Appendix F: Using the Lightning-NOx Parameterization

Instructions for using the Lightning-NOx paramterization

The WRF/Chem model is has a parameterization able to provide an estimate of the nitrogen oxides production from lightning (LNOx). The code for this production is called from the emissions_driver.F routine and model code files related LNOx are module_lightning_driver.F and module_ltng_crm.F. The LNOx parameterization is **appropriate only for cloud resolving scales** (and not parameterized convection). There are several options for running the LNOx parameterization that can be designated in the namelist.input file under the chemistry namelist. These options are as follows:

Variable Names	**Default Value**	**Description and Options**
lightning (max_dom)	= 0, 0, 0,	Denotes LNOx parameterization; 0 = no lightning; 1 = DeCaria scheme; 2 = Barthe scheme (not available yet). Set to 1 to turn on LNOx parameterization.
lightning_time_step (max_dom)	= 0, 0, 0,	Time interval (seconds) for calling LNOx parameterization. Usually set to 60 seconds.
lightning_start_seconds (max_dom)	= 0, 0, 0,	Start time (seconds) for calling LNOx parameterization. Allow 10 minutes or so for model to spin up before calling LNOx.
temp_upper (max_dom)	= -45., -45., -45.,	Temperature (degC) of upper peak of LNOx source for the vertical distribution of NO.
temp_lower (max_dom)	= -15., -15., -15.,	Temperature (degC) of lower peak of LNOx source for the vertical distribution of NO.
N_IC (max_dom)	= 0, 0, 0,	Moles of NO produced per intracloud (IC) lightning flash. Recommendations are 300-500 moles NO / flash.
N_CG (max_dom)	= 0, 0, 0,	Moles of NO produced per intracloud (IC) lightning flash. Recommendations are 300-500 moles NO / flash.
passive_ltng (max_dom)	= 1, 1, 1,	Switch to include a passive NO tracer. The amount of NO

		produced is equal to the source from LNOx. The tracer is transported but does not undergo chemical reactions. The chem._tracer_opt (in the &dynamics section) must be set to 3 to allow this option to work.
flashrate_factor (max_dom)	= 1.0, 1.0, 1.0,	Factor to adjust the number of flashes. This factor is used for multiple nests (that include LNOx production) and allows similar values to be predicted in the inner and outer nests. One can estimate a flashrate_factor based on the ratio of the nests' horizontal resolution: flashrate_factor = dx_inner / dx_outer. For example, if dx_inner = 1 km and dx_outer = 3 km, then flashrate_factor = 0.33 for the inner domain and 1.0 for the outer domain.
flashrate_method (max_dom)	= 1, 1, 1,	Method for predicting the number of flash rates. Method 1 = maximum vertical velocity (Price and Rind, 1992); Method 2 = updraft volume for w>5m/s (Deierling and Petersen, 2008).
iccg_method (max_dom)	= 1, 1, 1,	Method for partitioning between intracloud and cloud-to-ground lightning flashes. Method 1= prescribe CG/IC ratio to 0.1; Method 2 = a rough assignment to the climatology of Boccippio et al (2001).
cellcount_method (max_dom)	= 1, 1, 1,	Method for counting storm cells. Method 1 = model determines either method 2 or 3; Method 2 = cell count is tile-wide = good for big domains where multiple storms will occur; Method 3 = cell count is domain-wide = good for small domains (<150 km) where only one storm is occurring.