WRF-Chem Emissions Guide

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WRF-Chem Emissions Guide

WRF-Chem Overview

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1.1 Introduction

The WRF-Chem Emissions Guide is designed to provide the reader with information specific to the part of the WRF model related to generation of emissions input files. It will provide the user with limited description of the WRF-Chem model (Grell et al., 2005) and primarily focus on issues related to generating chemical input data files. For additional information regarding the WRF-Chem model, the reader is referred to the WRF-Chem User's Guide.

1.2 The WRF-Chem emissions utilties overview

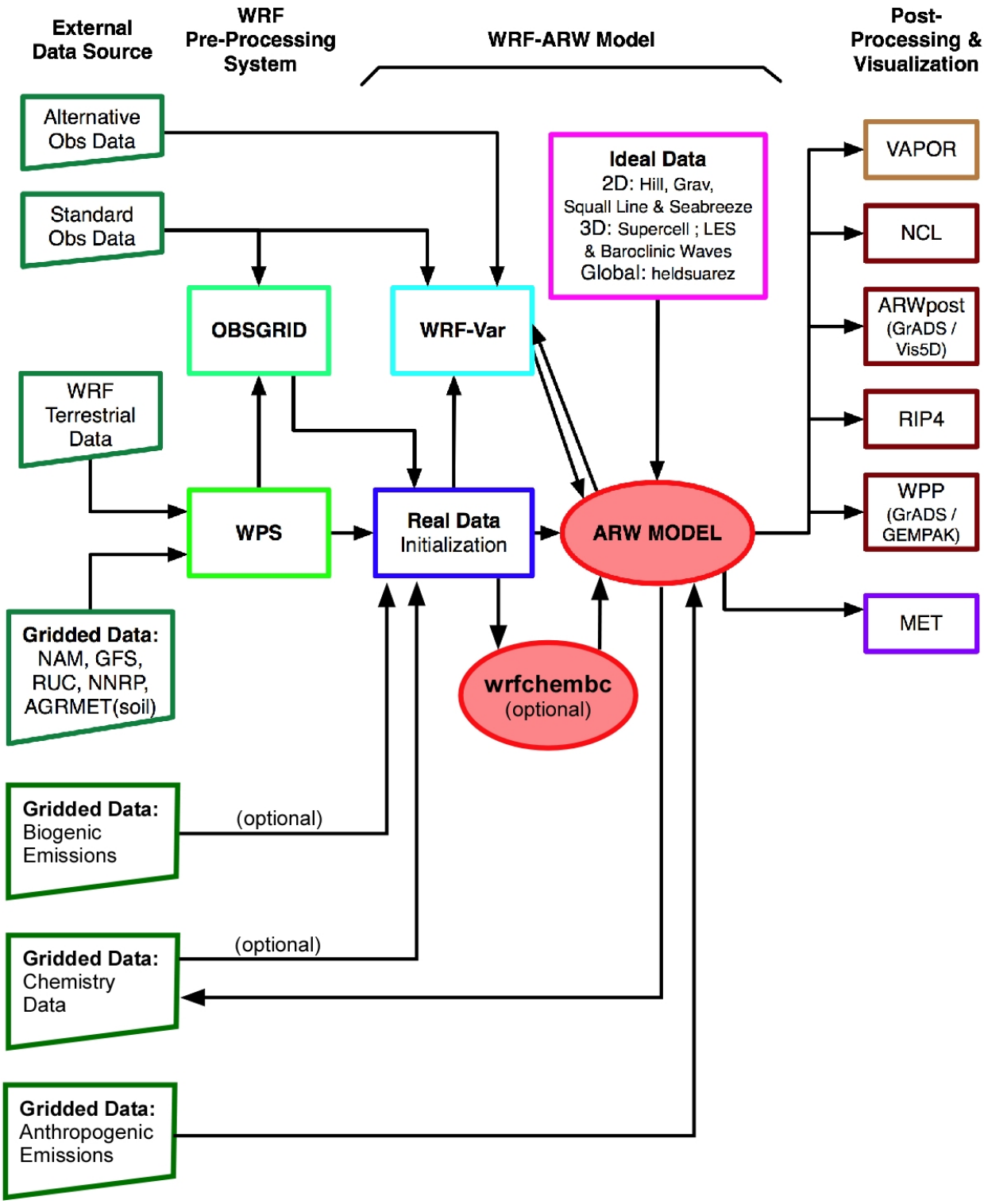
The following figure shows the flowchart for the WRF-Chem modeling system. In the WRF-Chem model there are several ways in which gridded chemicaldata can be introduced into the simulation. The static data (e.g., data based upon land useage, or vegetation) is introduced when running the real data initilization. Data that varies temporally (e.g., anthropogenic emissions) is read into the simulation when running the WRF model.

At this time there is no single tool that will construct the chemistry emissions input data sets for any domain and any chemical mechanism that is selected. **This places the requirement upon you, the WRF-Chem model user, to construct the emissions data set for your particular domain and desired chemistry.** However, several programs and data sets are provided by the WRF-Chem user community that can help to create the input data sets for your domain and your choice of chemical mechanism. These programs an their use are described in the following chapters. Note that it would be best to know the preferred domain location and chemistry options that will be used in the simulation before starting. In this way the choices regarding which utilities to be used will become clear.

1.3 Placement of chemical-emission input data files

The WRF-Chem emissions input data files need to be located in the WRFV3/test/em_real directory. Some users place the data in the WRFV3/run directory and link the file(s) the WRFV3/test/em_real directory, since they will be used over and over again. Others might leave the emissions input files in the various directories where

WRF-ARW Modeling System Flow Chart



they were constructed. It should not make any difference whether you use a link or copy the files to the WRFV3/test/em_real directory. The main point to take away is that, once the emission file construction is completed, the WRF-Chem code expects the emissions data files to be located in the WRFV3/test/em_real directory.

Chapter 2: Generation of Anthropogenic Emissions Data Files

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2.1 Preparation of anthropogenic emissions for use with WRF-Chem

Programs that can be used to generate anthropogenic emissions for a WRF-Chem simuation are described in the following subsections. It is assumed that the preferred domain location is knownalong with the chemistry options that will be used in the simulation. The "raw" anthropogenic-emissions data set described next can be used if the domain is (1) located either anywhere over the globe, or (2) over the 48 contiguous states of the United States. We will begin in the next section by showing the suggested methodology for constructing your own anthropogenic-emissions data set using the global anthropogenic emissions data sets.

2.2 Using the global-emissions data set

The use of a global-emissions data set with WRF-Chem is probably the most common choice of 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., CO_2, CH_4 and N_2O) 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 (Freitas et al., 2011). The program will map the global anthropogenic emissions data to a WRF-forecast domain using a Mercator, polar stereographic or Lambert conformal projection. This global anthropogenic emissions program and associated RETRO/EDGAR emissions is available from the WRF-Chem ftp site (ftp://aftp.fsl.noaa.gov/divisions/taq/global_emissions). After the emissions are

mapped to WRF domain, the data is output for RADM2 speciation into binary data file. The intermediate binary data file can then be converted into a WRF input data file using the convert utility program discussed in chapter 9.

2.2.1 Seting-up prep_chem_sources

In this section the set-up and running of the prep_chem_sources utiltity will be discussed. The code can be obtained from the WRF-Chem ftp site (ftp://aftp.fsl.noaa.gov/divisions/taq/global_emissions). After untaring the code it can be seen that the code exists in several subdirectories. These subdirectories are:

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

There are several libraries that are not normally needed to compile WRF that are needed to compile prep_chem_sources. These libraries are:

- 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.
- HDF5 1.8 (libmfhdf.a, libdf.a) or later distribution. You may download the software from http://www.hdfgroup.org/downloads/index.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

When compiling PREP-CHEM-SRC codes on a Linux system make sure the netCDF and HDF library has been installed using the same FORTRAN and C compilers that are used for WRF. For example, you will probably need to configure the HDF library build using command lines:

```
./configure --prefix=path_hdf5    \
--with-jpeg=path_jpeg \
                --with-zlib=path_zlib \
                --disable-netcdf
```

as these are what is often used with WRF. And then to compile the HDF library one uses the make command:

```
make && make install
```

2.2.2 Compiling the prep_chem_sources code

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

cd bin/build

and verify the compiler and library path settings in the include.opt.<your compiler> make option file. The user should set similar library paths and compile options (e.g., byte swapping) as used for the WRF-Chem code compilation otherwise the code might not compile or the binary intermediate output will be unreadable by the WRF-Chem convert program. Then, once the make option include file is configured for your computer system, the make command is issued with the compiler option (e.g., PGI) and the chemistry option (ie., RADM_WRF_FIM) listed in the command line

make OPT=opt.pgi CHEM=RADM_WRF_FIM

And with this command the code should compile and the prep_chem_sources.exe file being placed in the prep_chem_source/bin directory.

2.2.3 Running prep_chem_sources utility with WRF-Chem

To run the prep_chem_sources executable one must first edit the name list 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 name list one can run the PREP-CHEM-SRC 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). While a typical run configuration will produce all of these emissions files, the focus in this section will be on just the anthropogenic emissions. Once the prep_chem_sources executable has been run the binary intermediate files it produces for WRF-Chem will need to be converted to WRF input data files. The conversion code is discussed in more detail in

chapter 8 of this Guide so the running of the code for the anthropogenic emissions will be outlined next.

For each simulation 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
ln -sf WRF-2011-07-14-000000-g1-volc.bin     ../../WRFV3/test/em_real/volc_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_auxinput6          = 2
 io_form_auxinput7          = 2
 io_form_auxinput8          = 2
 io_form_auxinput12         = 2,
 io_form_auxinput13         = 0,
 auxinput6_inname           = 'wrfbiochemi_d01',
 auxinput7_inname           = 'wrffirechemi_d<domain>',
 auxinput8_inname           = 'wrfchemi_gocart_bg_d<domain>',
 auxinput12_inname          = 'wrf_chem_input',
 auxinput13_inname          = 'wrfchemv_d<domain>'
 auxinput5_interval_m       = 1440,1440
 auxinput7_interval_m       = 1440,1440
 auxinput8_interval_m       = 1440,1440
 auxinput13_interval_m      = 1440,1440
 frames_per_auxinput6       = 1,1
 frames_per_auxinput7       = 1,1
 frames_per_auxinput8       = 1,1
 frames_per_auxinput13      = 1,1
/

&chem
 kemit                      = 1,
 chem_opt                   = 301,    2,
 io_style_emissions         = 2,
 emiss_inpt_opt             = 1,      1,
```

```
emiss_opt              = 5,     5,
emiss_opt_vol          = 0,     1,
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 if so necessary. Otherwise, the global anthropogenic emissions file is ready to be used in a WRF-Chem simulation.

2.3 The 4-km resolution NEI 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 previous section as well as appendix B that describes the use of a global anthropogenic-emissions inventory for the WRF-Chem model. The methodology for transferring the NEI anthropogenic-emissions data set to the WRF model is discussed in the following section.

2.4 Anthropogenic-emissions construction methodology for WRF-Chem

The methodology for constructing an emissions data set using NEI data is the same as that when constructing an emissions data set using your own anthropogenic-emissions data set. For simplicity, this section will walk through the steps assuming one has the NEI emissions. The steps are as follows:

- 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. The main point is that the data is already mapped to a cartesian grid.
    - A 4-km emissions data set (area) and point source is available for the U.S. (ftp://aftp.fsl.noaa.gov/divisions/taq/emissions_data_2005). 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.

2.4.1 Construction of an anthropogenic-emissions-inventory conversion table

In this section some of the listed steps are expanded in greater detail. To generated the anthropogenic emissions data file, 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 2.1) 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 2.1. 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.

A program is provided on the WRF-Chem ftp site (ftp://aftp.fsl.noaa.gov/divisions/taq/emissions_data_2005) 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 2.2.

For spatial partitioning, the emiss_v03.F program implicitly assumes the WRF-Chem grid has a horizontal grid spacing larger than 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.

Table 2.2. 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)

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.

The emissions units for both surface and elevated point sources are in *mole per square kilometer per hour* for gas phase species and in units of *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.

2.4.2 Additional details for running emiss_v03.F with the NEI-05 anthropogenic-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 System 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 obtain the average height of each vertical domain levels in meters.

Now that the program is built and runs, one should have produced one or more binary intermediate data files containing the anthropogenic emissions data for your WRF domain. The next step in the process is to convert the binary intermediate files to a WRF-Chem input file. The conversion code is discussed in chapter 8.

As the NEI emissions data is hourly and typically contains 12 hours of data, you need to run the convert_emissions program twice to generate a full day's worth of emission. This program will also need a wrfinput data file for the desired date and domain. This input file can be generated from a non-chemistry run of real.exe (e.g., chem_opt=0) as long as the start and end times match with the emissions start hour. That is, the 00 UTC emissions file needs a wrfinput file that begins at 00 UTC and likewise for 12 UTC. The emissions input file needs to be copied, or linked to the WRFV3/test_em_real directory. And it should be noted that the conversion program is capable of converting the other files from prep_chem_sources (less the anthropogenic emissions) during the same run. In this case, you might have linked the files with names as:

```
ln -sf wrfem_00to12Z                          ../../WRFV3/test/em_real/wrfem_00to12z_d01
ln -sf wrfem_12to24Z                          ../../WRFV3/test/em_real/wrfem_12to24z_d01

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-bb.bin        ../../WRFV3/test/em_real/emissfire_d01
ln -sf WRF-2011-07-14-000000-g1-volc.bin      ../../WRFV3/test/em_real/volc_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 (use chem_opt=2 and emiss_opt=3 for NEI emissions). 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_auxinput6          = 2
 io_form_auxinput7          = 2
 io_form_auxinput8          = 2
 io_form_auxinput12         = 2,
 io_form_auxinput13         = 0,
 auxinput6_inname           = 'wrfbiochemi_d01',
 auxinput7_inname           = 'wrffirechemi_d<domain>',
 auxinput8_inname           = 'wrfchemi_gocart_bg_d<domain>',
 auxinput12_inname          = 'wrf_chem_input',
 auxinput13_inname          = 'wrfchemv_d<domain>'
 auxinput5_interval_m       = 1440,1440
 auxinput7_interval_m       = 1440,1440
```

```
 auxinput8_interval_m              = 1440,1440
 auxinput13_interval_m             = 1440,1440
 frames_per_auxinput6              = 1,1
 frames_per_auxinput7              = 1,1
 frames_per_auxinput8              = 1,1
 frames_per_auxinput13             = 1,1
/

&chem
 kemit                             = 1,
 chem_opt                          =  2,    2,
 io_style_emissions                = 2,
 emiss_inpt_opt                    = 1,       1,
 emiss_opt                         = 2,       2,
 emiss_opt_vol                     = 0,       1,
 biomass_burn_opt                  = 1,       1,
 plumerisefire_frq                 = 120,     120
```

When complete and the data files are verified you can rename output to include the date if so necessary. Otherwise, the global anthropogenic emissions file is ready to be used in a WRF-Chem simulation.

2.5 The anthro-emiss utiltiy

In the fall of 2013 the NCAR/ACD group released a program called anthro_emis. This program is a FORTRAN based preprocessor to create WRF-Chem ready anthropogenic emissions files (wrfchemi_<domain>_<date> or wrfchemi_{00z,12z}_<domain>) from global inventories on a latitude/longitude projection.

The input latitude-longitude anthropogenic emission files must be netCDF conforming datasets and have the following structure:

- Each input dataset is for one input species,
    - Two one-dimensional variables named longitude and latitude containing the longitude and latitudes in degrees about which each input grid cell is centered. The longitude and latitude variables must be monotonically increasing.
- One of the following:
    - Date and datesec variables containing the date and seconds in day. The date is an integer encoding the date yyyymmdd,
    - A time variable representing the time since a given date. The base date must be contained in the time variable units attribute and be of the form yyyy-mm-dd.
- One or more three-dimensional variables containing the actual anthropogenic

emissions, designated as sub categories. The emissions data must be dimensioned as (longitude, latitude, time).

Additionally the input anthropogenic dataset may have the molecular weight of the input species in g per mole as either:

- a variable with the name molecular_weight,
- a global attribute with the name molecular_weigh,
- a sub category variable attribute with the name molecular_weight.

If the input dataset does not specify the species molecular weigh then the user may specify the input species molecular weight in the src_names namelist variable. If the molecular weight is specified via the src_names namelist variable then any molecular weight information in the input dataset is ignored.

Compilation of the anthro_emiss program is accomplished using the command "make_anthro" which will produce the anthro_emiss executable file. Before running the anthro-emiss program the input file(s) for the WRF domain(s) needs to have been constructed and the location known. In addition, there needs to be an input file (e.g., anthro_emiss.inp) constructed for the anthro_emiss program containing information such as the executable directory and the wrfinput file locations. With the anthro_emiss input file built, the code can be run using the redirecting command

anthro_emis < anthro_emis.inp.

If the user desires to capture the output going to screen to a data file (e.g., anthro_emiss.output) the command is instead:

anthro_emis < anthro_emis.inp >& anthro_emiss.output

Additional information regarding the anthro_emiss utility is provided in the README.txt file provided with the anthro_emiss utility program. To obtain this program or more information the user should go to the NCAR/ACD WRF-Chem web page at http://www.acd.ucar.edu/wrf-chem.

Chapter 3: Generation of Biogenic Emissions Data Files

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3.1 Preparation of biogenic emissions for use with WRF-Chem

The WRF-chemistry model does have four options to compute the biogenic-emissions data. These options are: None, Guenther, BEIS and MEGAN biogenic emissions. Each of these options will be discussed in the following sections.

3.2 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. For example, the prep_chem_sources program has the option to include estimated biogenic emissions with the anthropogenic emissions. Be sure to include biogenic emissions for every update time in the anthropogenic emissions input data. The biogenic emissions information is not static and it will be lost whenever there is an update to the anthropogenic emissions data.

3.3 Guenther biogenic emissions

For the second option (bio_emi_opt=1), the model calculates the biogenic emissions online using the USGS land-use 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. Therefore, this option is the easies to use. However, the overall simulation might not compare well with observations due to the limited vegetation types in the simulation resulting in several key chemical species (e.g., isoprene) having relatively low emisison rates.

3.4 BEIS 3.14 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 3.14. The land use for this emissions inventory is obtained from the Biogenic-Emissions Land-use Database version 3 (BELD3). The reference fields

need to be provided as an additional input data file (wrfbiochemi_d01) for the real.exe program. At this time the data files containing the reference fields have not been made available to the general public.

The BEIS3.14 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_beis314.F of WRF-Chem. Reference emission files (30°C, 1000 PAR) from BEIS3.14 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 website. As part of the reference emission pre-processing, BEIS3.14 contains season-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_beis314.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 3.1. 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

When using this option the WRF-Chem code will expect a data file called wrfbiochemi_d01 (for domain 1) and a setting of bio_emiss_opt = 2 in your namelist.input file. One will need to run real.exe (with bio_emi_opt=2 in the namelist) when creating the wrfinput data file to load the static biogenic emissions variables should now be included in the wrfinput data file.

3.5 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) web site http://www.acd.ucar.edu/wrf-chem/. 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.

The University Corporation for Atmospheric Research (UCAR) provides Fortran source code files to create MEGAN 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.

3.5.1 Compiling MEGAN preprocessor

The MEGAN preprocessor Fortran source code and data set have been made available for download from NCAR/ACD at the web site http://www.acd.ucar.edu/wrf-chem/. This site will for each visitor to register by providing some contact details. After registering just click on the "bio-emiss" button on the user registration page to go to the biogenic emissoin page. At this page one can download the MEGAN Fortran source code, makefile and MEGAN data input files. The files can be downloaded to a directory of your choice. Keep in mind that the MEGAN code needs to access the WRF run directory and the wrfinput_d01 file during MEGAN data preprocessing.

Next the downloaded files need to be extracted usign the tar command. One can 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
```

After extracting the file be sure that the correct environment variables for your FORTRAN compiler and netCDF libraries are set correctly by editing the make_util script file if necessary. At this point the MEGAN source code in the MEGAN directory can be compiled by issuing the command:

```
> make_util megan_bio_emiss
```

And once the code is compiled the executable file megan_bio_emiss will be created in the MEGAN directory.

3.5.2 Preprocessing MEGAN data files

With the MEGAN executable constructed one needs to have a WRF input file available for the desired domain (2). If a wrfinput file is not available, then run real.exe for a meteorology only case to produce the input files. While this step will create a file named wrfinput_d01 examination of the file will show that it does not contain any input data arrays for MEGAN. The next step using MEGAN pre-processing tool will examine the wrfinput_d01 for geographical and temporal parameters for the production of biogenic emissions and use them in the construction of the WRF biogenic emission files.

Edit the MEGAN preprocessor input file (megan_bio_emiss.inp) and set the values in the test file for:

1. domains – the number of domains used in your WRF model simulation

2. start_lai_month - the month before the month in which your WRF run is set to start. Typically this will be set to 1.
3. end_lai_month –the month in which your WRF run is set to end. Typically this will be set to 12.
4. wrf_dir – the directory where the associated wrfinput_d01 for your WRF-Chem simulation resides, and
5. megan_dir – the directory in which the downloaded MEGAN data files reside.

Keep in mind that the leaf area index (lai) parameter data files are provided in the MEGAN preprocessing download. There will be twelve of these files as one file exists for each month.

With the input file constructed the MEGAN bioegenic-emissions data can be created for the WRF-Chem domain(s) and time frame by running the MEGAN utility. The utility us executed by issuing the command:

```
> megan_bio_emiss < megan_bio_emiss.inp > megan_bio_emiss.log
```

Here the execution command uses redirection to supply the executable with the input file and saves all of the screen output to a log file called megan_bio_emiss.log. Whereas the reading and writing of data files is a serial process, the running of this program can take a relatively long time depending on a range of factors such as computer power and available memory. Once the execution of the program is finished is the always best to examine the log file and the output for any possible errors or issues. 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. The MEGAN data elements in the WRF-Chem biogenic emission data 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})

With the successful running of the MEGAN preprocessor, the created WRF-Chem biogenic input files (wrfbiochemi_d0x files) should be copied (or linked) into the WRF-Chem directory WRFV3/test/em_real.

3.5.3 Running WRF-Chem with MEGAN

At this point a normal WRF-Chem simulation can be made. This includes the running of real.exe to create the input and boundary files as well as combine any static

emission fields to the appropriate input file. When running the WRF-Chem code with MEGAN biogenic emissions data be sure to set the appropriate namelist values. In this case one will use bio_emiss_opt=3 and will need to set the parameter "ne_area" to a value equal to or greater than the total chemical species used. See chapter 4 of the WRF-Chem User's Guide for more inforamtion about the ne_area parameter.

Keep in mind that after running real.exe the wrfbiochemi_d01 and wrfinput_d01 files could also include variables for running BEIS3.14, but the values for BEIS variables will all be all zero. If one is wanting to use BEIS biogenic emisisons, then the user will need to create a different wrfbiochemi_d01 file using a different source for the biogenic emisisons input data.

With the static MEGAN biogenic emissions data loaded into the wrfinput file and the WRF biogenic emissions data file availble for reading during the run, the WRF executable can be run. During execution of the WRF code the MEGAN emissions will be calculated online using the simulated meteorological conditions along with the biogenic emissions.

Chapter 4: Generation of Biomass Burning Emissions Data Files

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4.1 Preparation of biomass burning emissions

The WRF-Chem model contains an online plume calculation capable of computing the plume rise and release of biomass burning emissions based upon the simulated meteorology. The input data for this scheme requires the user to specify the location of the fire and the amount of emitted species. To aid in this process there are several utilities that read satellite fire location data and map the required information to the user's WRF domain. These biomass burning emission utilities will be discussed in the following sections.

4.2 Using prep_chem_sources for biomass burning emissions

The prep_chem_sources program is capable of providing biomass burning emissions or wildfire emissions to the WRF-Chem retrospective simulation or real time forecast. The prep_chem_sources program is capable of using the Wildfire Automated Biomass Burning Algorithm (WF_ABBA), or the Moderate Resolution Imaging Spectroradiometer (MODIS) fire location data. The WF_ABBA data comes from the geostationary NOAA weather satellite (GOES) that provides half-hourly fire data for the Western Hemisphere. Specifically, GOES-East provides coverage for North and South America while GOES-West covers North America only. Data files containing the WF_ABBA fire location are distributed by the University of Wisconsin-Madison (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 wildfire location data is available from MODIS at the NASA web site: http://earthdata.nasa.gov/data/near-real-time-data/firms. The prep_chem_sources reads this data, the WF_ABBA 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 (e.g., Grell et al, 2011). Other sources for wildfire emissions can be added to the fire emissions as well using the extra fire emissions option in the program.

Once the prep_chem_sources executable has been run the binary intermediate files it produces for WRF-Chem will need to be converted to WRF input data files. The conversion code is discussed in more detail in chapter 8 of this Guide so the running of the code for the biomass burning emissions will be discussed next.

For each simulation that you are going to use biomass burning data, you need to run the prep_chem_sources and convert_emissions programs. 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
ln -sf WRF-2011-07-14-000000-g1-volc.bin     ../../WRFV3/test/em_real/volc_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, biomass_burn_opt = 1). 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_auxinput6          = 2
 io_form_auxinput7          = 2
 io_form_auxinput8          = 2
 io_form_auxinput12         = 2,
 io_form_auxinput13         = 0,
 auxinput6_inname           = 'wrfbiochemi_d01',
 auxinput7_inname           = 'wrffirechemi_d<domain>',
 auxinput8_inname           = 'wrfchemi_gocart_bg_d<domain>',
 auxinput12_inname          = 'wrf_chem_input',
 auxinput13_inname          = 'wrfchemv_d<domain>'
 auxinput5_interval_m       = 1440,1440
 auxinput7_interval_m       = 1440,1440
 auxinput8_interval_m       = 1440,1440
 auxinput13_interval_m      = 1440,1440
 frames_per_auxinput6       = 1,1
 frames_per_auxinput7       = 1,1
 frames_per_auxinput8       = 1,1
 frames_per_auxinput13      = 1,1
/

&chem
 kemit                      = 1,
 chem_opt                   = 301,   2,
 io_style_emissions         = 2,
 emiss_inpt_opt             = 1,     1,
 emiss_opt                  = 5,     5,
 emiss_opt_vol              = 0,     1,
```

```
biomass_burn_opt          = 1,     1,
plumerisefire_frq         = 120,   120
```

And when complete and the converted biomass burning files is verified you can rename output, or just right away use the biomass burning emissions file (wrffirechemi_d01) in a WRF-Chem simulation.

In the WRF-Chem model, the wildfire-emissions data is obtained 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.

4.3 Using FINN biomass burning emissions

The Fire INventory from NCAR (FINN) program (Wiedinmyer et al., 2011) can be used to provide fire emissions data for a WRF-Chem simulation. FINN uses daily, one kilometer resolution, global estimates of the trace gas and particle emissions from open burning of biomass, which includes wildfire, agricultural fires, and prescribed burning, but does not include biofuel use and trash burning. Emission factors used in the calculations have been updated with recent data, particularly for the non-methane organic compounds (NMOC). The resulting global annual NMOC emission estimates are as much as a factor of 5 greater than some prior estimates. Chemical speciation profiles, necessary to allocate the total NMOC emission estimates to lumped species for use by chemical transport models, are provided for three widely used chemical mechanisms: SAPRC99, GEOS-CHEM, and MOZART-4. Using these profiles, FINN also provides global estimates of key organic compounds, including formaldehyde and methanol.

Any uncertainties in the emissions estimates arise from several of the method steps. The use of fire hot spots, assumed burned area, land cover maps, biomass consumption estimates, and emission factors all introduce error into the model estimates. The uncertainty in the FINN emission estimates are about a factor of two; but, the global estimates agree reasonably well with other global inventories of biomass burning emissions for CO, CO_2, and other species with less variable emission factors.

FINN emission estimates have been developed specifically for modeling atmospheric chemistry and air quality in a consistent framework at scales from local to global. The product is unique because of the high temporal and spatial resolution, global coverage, and the number of species estimated. FINN can be used for both hindcast and forecast or near-real time model applications and the results are being critically evaluated with models and observations whenever possible.

Near-real-time fire emissions from the FINN, based on MODIS Rapid Response fire count (FIRMS) are made available at the NCAR/ACD web site http://www.acd.ucar.edu/acresp/dc3/AMADEUS/finn/emis and the FINN fire emissions for previous years are available from http://bai.acd.ucar.edu/Data/fire.

Chapter 5: Generation of Volcanic Emissions Data Files

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5.1 Preparation of volcanic emissions for use with WRF-Chem

In this section the ash and SO_2 emissions from prescribed volcanic activities is described. The volcanic ash emissions can either be for a single volcano producing just ash, or for a single volcano emitting ash and sulfurdioxide. Both methods use the prep_chem_sources utility program for specifying the location of the volcano on the WRF-Chem domain and the type of emissions from the volcano. For additional information on volcanic emissions that are produced when running prep_chem_sources the reader is referred to Freitas et al. (2011).

5.2 Volcanic ash emissions

To determine ash emission field during volcanic eruption events, prep_chem_sources follows the database developed by Mastin et al. (2009). This database provides a set of parameters to model volcanic ash cloud transport and dispersion during eruptions. There is information on 1535 volcanoes around the world comprising location (latitude, longitude and height) and the corresponding parameters plume height, mass eruption rate, volume rate, duration of eruption and the mass fraction of erupted debris finer than about 63 μm are provided. The emissions preprocessing tool provides the place of the volcano in the nearest model grid box and the corresponding emission parameters (mass eruption rate, plume height and duration). Then this information is used within WRF-Chem to determine the vertical distribution of the erupted mass. Within the modeling transport system, 75% of the erupted mass is detrained in the umbrella cloud and 25% beneath. The base of the umbrella cloud is roughly located at 73% of the plume height. The total erupted mass is calculated using the correspondent erupted volume times the ash mass density, which is defined as being 2,500 kg m^{-3}.

The total ash mass is distributed between 10 bins of aerosol particles with diameter size range starting from 2 mm down to less than 3.9 μm, using the correspondent percentage of mass described by the Mount Saint Helens eruption of 1980 (Carey and Sigurdsson, 1982). For each bin, the aerodynamic radius, needed by the setting velocity calculation, is defined as half of the arithmetic mean between the limits of the diameters of each bin size. The algorithm to calculate the settling velocity was originally developed for the GOCART model (Chin et al., 2002). This calculation is based on the Stokes law corrected by the Cunningham slip factor (Pruppacher and Klett, 1997). The time interval which the ash mass is released in the domain of the model simulation is given by the 'duration' parameter specified in the volc_emissions.f90.

5.3 Volcanic SO_2 degassing emissions

The data provided by the AEROCOM program (http://www-lscedods.cea.fr/aerocom/AEROCOM_HC/volc, Diehl, 2009, Diehl et al., 2011) contains volcanic SO_2 emissions and other variables for all days from 1 January 1979 to 31 December 2007 for all volcanoes with historic eruptions listed in the Global Volcanism Program database provided by the Smithsonian Institution. There is one file for each year that contains the number of events for each day of that year over the entire world. For each event, the volcano name, date, height above the mean sea level, cloud column height, longitude, latitude and daily emission rate of SO_2 are provided. There is also a separation between eruptive and non-eruptive volcanic emissions.

In similar fashion to the volcanic ash, the emissions processing code prep_chem_sources places the SO_2 emissions from each volcano in the grid box which surrounds its geographical location. The total emission is calculated by summing the emissions of all volcanoes within the grid cell. Next, the total emission and the minimum and maximum column heights of the set of volcanoes within the grid cell are provided. The units are kg $[SO_2]$ m^{-2} dy^{-1}.

Chapter 6: Generation of Tracer Emissions Data Files

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6.1 Preparation of tracer emissions for use with WRF-Chem

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 simplest way to produce tracer emissions is to modify the sample program provided in chapter 8.2 to suit your needs. Upon examination of the sample program one will see that it can be modified to ignore the reading, or setting of anthropogenic emissions data sets and instead simply fill the EMISS3D array. The three-dimensional emissions array (EMISS3D) 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 (e.g., chem_opt=13). Then use the array "ename" in the sample program to get the name and order of the emitted species. Knowing the chemical species index in ename, one can set the emissions for the chemical index, N, in the output array. For example, if the tracer emissions is to be defined for CO at the surface for grid point (18,23), then the read and setting section of the SAMPLE program would be:

```
! Zero all emissions
EMISS3D(1:IX, 1:KX, 1:JX, 1:NRADM, 1:IHOUR) = 0.

N=11
DO IHR=1,12  ! file contains 12 hours of data (00 to 11 UTC)
  EMISS3D(18,1,23,N, IHR) = 1.E-06
ENDDO
```

Once the SAMPLE program has been modified, compiled and run, a binary intermediate file containing the tracer emissions will be produced. This binary file containing will need to be converted as a NEI emissions data set to a WRF netCDF input file using the convert_emiss.F program discussed in the previous section. Another example routine using this methodology has been made available on the WRF-Chem ftp server at: ftp://aftp.fsl.noaa.gov/divisions/taq/emissions_data_2005/emiss_v03_tracer.F

If using the sample programs is not functional for the user's problem another methodology can be used. It has ben assumed that an option that allows users to use pre-existing data and code with only small modifications needed to produce input or output files for their needs would be the best way for students to begin using the model.

6.2 The CO_2 tracer option

The CO_2 tracer option allows a user to simulate biospheric CO_2 fluxes using Vegetation Photosynthesis and Respiration Model (VPRM) coupled to WRF-Chem. The VPRM model uses satellite data and WRF meteorology to derive biospheric CO_2 fluxes from different biomes. All the chemistry species such as CO_2 and CO in this option are treated as passive tracers. No chemistry and removal processes are considered for this option. The option simulates transport and mixing of several CO_2 and CO tracers from different sources such as background, anthropogenic and biospheric. More information regarding VPRM is provided by Pillai et al. (2011) and Ahmadov et al. (2009).

6.3 The Greenhouse Gas tracer option

The Greenhouse Gas tracer option allows a user to perform simulations of CO_2, CO, and CH_4 within WRF-Chem. All chemistry species are treated as passive tracers. The option includes all tracers from the CO_2 tracer option but also includes CH_4 tracers (biogenic, anthropogenic, background) and biomass burning tracers for CO_2, CO, and CH_4 as well. Biogenic CH_4 fluxes are simulated with the Kaplan wetland inventory, the soil uptake model from Ridgwell, and the termite database of Sanderson coupled to WRF-CHEM. The flux models use WRF meteorology and soil characteristics to calculate the CH_4 fluxes. The wetland inventory additionally relies on an external wetland inundation map and carbon pool. Similar to chem_opt=16 no chemistry and removal processes are considered. Detailed information is found in Beck et al. (2011).

Chapter 7: Other WRF-Chem Utilties

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7.1 Boundary conditions with WRF-Chem

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. But like the meteorological model, the lateral boundaries of the limited domain mesh need to provided information about the environment outside the domain. If no lateral boundary data is provided for the chemistry the model will default to the idealized chemical profile (section 4.5 of the WRF-Chem User's Guide). This idealized chemical profile resembles the chemical environment observed over North America during the summer and is probably not the best suited for most WRF-Chem simulations. Therefore, it is a best practice to provide chemical data from a larger domain simuation, or global chemical model, to the lateral boundaries of the WRF-Chem simualtion. To aid with this process several tools have been provided to update the WRF boundary condition file and will be discussed in the next sections.

7.2 The wrfchembc utility

One utility program to produce chemical lateral boundary conditions, 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/Boundary/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..

7.3 The mozbc utility

The MOZBC utility program 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; and
- 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 interest 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.

7.4 Including an upper boundary bounary condition for chemical species

An upper boundary condition for select gas species may be specified by setting the have_bcs_upper in the chemistry namelist. The namelist variable have_bcs_upper defaults to .false. meaning that no chemical species concentrations are specified near the upper boundary. By setting have_bcs_upper to ".true." the model will specify the o3, no, no2, hno3, ch4, co, n2o, and n2o5 concentrations at the top of the model. These values will override the original values as defined in the idealized chemical profile (section 4.5).

When have_bcs_upper = ".true." the chemistry namelist variable "fixed_upper_bc" is activated. This namelist variable controls the lowest pressure level where the upper boundary concentrations are overwritten (default value of 50 mb). From the pressure level defined by "fixed_upper_bc" down to the tropopause the concentrations are relaxed, using a 10 day time constant, to fixed values.

To use the upper boundary contisions, the user is required to provide two additional input data files:

- the file clim_p_trop.nc that includes a climatology for tropopause levels,
- an input file with upper boundary conditions for gas species. The filename for the boundary conditions is provided to the WRF model via the chemistry namelist variable "fixed_ubc_inname".

Climatologies for 4 different time periods derived from WACCM RCP simulations have been made available to users from the NCAR/ACD website (www.acd.ucar.edu/wrf-chem). These files are named: ubvals_b40.20th.track1_1950-1959.nc, ubvals_b40.20th.track1_1980-1989.nc, ubvals_b40.20th.track1_1996-2005.nc, and ubvals_rcp4_5.2deg_2020-2029.nc where the years used to produce the climatology are specified in the file names. Additional output variables are included in the model when using the upper boundary conditions. These tropopause diagnostics (TROPO_P, TROPO_Z, TROPO_LEV) are listed in the registry and a user should verify that they will included in the output file before running the model. Additional information about the upper boundary condition scheme was provided in presentation 8A.2 (Barth et al.) given at the 2011 WRF User Workshop. The presentation can be accessed online at http://www.mmm.ucar.edu/wrf/users/workshops/WS2011/WorkshopPapers.php.

Chapter 8: WRF-Chem Conversion Utility

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8.1 Converting binary intermediate file to a WRF-Chem data file

The final step in the process for some of the utility programs is to produce a WRF-Chem netCDF 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 input file would be generated by the emissions mapping step. However, if not provided by the user, the WRF input data file (e.g., wrfinput_d01) can be read and the metdata information extracted and added to the anthropogenic-emissions input data file.

When selecting a file name for the WRF chemical emissions, it was decided to use the prefix of wrfchemi for anthropogenic emission. Using this prefix, the name of the final netcdf data file(s) can either include the hour of the day wrfchemi_<hour>_d<domain_id> or the full date and time wrfchemi_d<domain_id>_<date/time> depending upon the user's intent. The chemistry namelist variable io_style_emissions allows the model run to switch between the two naming conventions. The nameing option including the date and time stamp is designed for daily varying emissions (io_style_emissions=2). When selecting this option the date/time specified in the WRF-Chem emissions data file must match the simulation date/time or no emissions data will be read potentially resulting in a run-time error. The emissions file name option that includes just the hour (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>. Each of these files contain hourly emissions data with hours ranging from 00:00 to 11:00 UTC for the wrfchemi_00z_d<domain_id> file, or from 12:00 to 23:00 UTC for the other. This latter naming convention is used by convert_emiss.F when using the provided NEI-05 emissions inventory.

The NEI-05 emissions inventory is representative of a "typical ozone season day" for the United States and is often used for any day of the year. Hence, when running a multiday WRF-Chem forecast only two emissions files are needed for the entire model run. A user could also select to use the two netcdf 4-D emissions file style when using RETRO/EDGAR emissions even though the anthropogenic emissions are updated monthly. The key to use the Global emissions is to recognize the update interval of the emissions and that simulation only needs to read the emissions one time at the start of the simulation and not again until the end of the month. Therefore, with the gobal data the wrfchemi_00z_d01 or the wrfchemi_12z_d01 emissions input file would contain only the anthropogenic emissions for the start of the simulation and the update interval would be defined as a time period greater than the simulation time.

8.2 Binary data file format

Perhaps the best way to explain the format of the intermediate binary data file is to provide a sample FORTRAN program that demonstrates how it is written. The arrays are defined in the program as cell center data on an Arakawa C grid. Next the names of the emitted species are defined and the 3D emissions array is filled. Once this is accomplished all of the 3D emissions data is written to file with a header defining the number of emissions fields and their names.

```
PROGRAM SAMPLE

!  IX          x-dimension of output  data (ix= e_we-1 for WRF domain)
!  JX          y-dimension of output  data (jx= e_ns-1 for WRF domain)
!  KX          z-dimension of output  data (kx =kemit for WRF domain)

PARAMETER(IX=39,JX=39,KX=19)
PARAMETER(NRADM=30, IHOUR=12)
CHARACTER (len= 9), DIMENSION(NRADM)     ::  ENAME
REAL, DIMENSION(IX2,KX,JX2,NRADM,IHOUR)   :: EMISS3D
! Temporary array used for output of data
REAL, DIMENSION(IX2,KX,JX2)   :: TMP

! Names of emission variables and the order they are written to file
DATA ENAME /    &
     'e_so2 ','e_no  ','e_ald ','e_hcho','e_ora2',                    &
     'e_nh3 ','e_hc3 ','e_hc5 ','e_hc8 ',                            &
     'e_eth ','e_co  ','e_ol2 ','e_olt ','e_oli ','e_tol ','e_xyl ',   &
     'e_ket ','e_csl ','e_iso ','e_pm25i','e_pm25j',                  &
     'e_so4i','e_so4j','e_no3i','e_no3j','e_orgi','e_orgj','e_eci',    &
     'e_ecj','e_pm10'/

! < Read and set all emissions here and place data in EMISS3D array>

OPEN(19,FILE='wrfem_00to12Z',FORM='UNFORMATTED')
WRITE(19)NRADM
WRITE(19)ename

DO IHR=1,12  ! file contains 12 hours of data (00 to 11 UTC)
     WRITE(19)IHR
      DO N=1,NRADM
         TMP(1:IX,1:KX,1:JX) =  EMISS3D(1:IX,1:KX,1:JX,N, IHR)
         WRITE(19) TMP
      ENDDO
ENDDO

END PROGRAM SAMPLE
```

8.3 Building the WRF-Chemistry emissions conversion code

The convert_emiss program is used to convert the binary intermediate files produced from prep_chem_soruces, emiss_v03 or similar programs into WRF-Chemistry emissions input files. To compile the conversion code, it is assumed that the user has already built the WRF-Chemistry model. In the WRFV3 directory, set the environmental variables to compile the chemistry code and then type the command "compile emi_conv". This command will use the WRF-Chemistry compiled libraries along with the convert_emiss.F program in the chemistry code to produce a new WRF-Chem executable program called convert_emiss.exe. The convert_emiss.exe executable file resides in the chemistry directory as it is not actually part of the WRF code, but rather a hybrid program that uses many of the WRF subroutines and libraries. You can find the code exectuables if you issue the commands:

> 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.

At this point all of the WRF-Chemistry conversion utility has been built and the emissions input data can to be generated.

8.4 Namelist settings for running convert_emiss

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>',
 auxinput12_inname           = 'wrf_chem_input',
 auxinput13_inname           = 'wrfchemv_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,
 io_form_auxinput13          = 2,
io_form_auxinput14           = 0,
io_form_auxinput15           = 0,
/

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

Since version 3.3, the name list 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).

When running the emissions utility programs and converting the input data into a WRF-Chem input data files, there are several items to keep in mind. First, it is assumed that one has already configured and compiled the WRF-Chem model. This needs to be accomplished before building the emissions conversion program with the command "compile emi_conv" in WRFV3 directory. If the WRF-Chem code is not constructed then several required modules will not be found and a compile error will result.

Second, the user should run convert_emiss.exe for a 24 hour period starting at 0000 UTC and ending at 0000 UTC. The netCDF output files named wrfchemi_d01 will

need to be saved under a file with a different name such as wrfchemi_d01_2008-07-14_00:00:00. The filename(s) need to match the name of the input data file as specified in the WRF module 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 so that they can be read in during the WRF-Chem simulation.

Finally, 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.

Chapter 9: Summary

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9.1 Summary

Presented in this WRF-Chem Emissions are the descriptons and directions for setting-up and using the utilities associated with the WRF-Chem model. This guide is not intended to be an exhaustive report about all that is available to aid in the set up and use the WRF-Chem model emissions utilities. While it does attempt to provide the latest and most accurate information about the configuration and running of the various emission utiltities, errors or incomplete information may have been unintentionally presented. Also, due to the complexity of the each utility and the WRF-Chem model along with the diverse needs of each user, there may be insufficient information for your particular research or operational application. If a user has questions regarding the model that this document fails to answer, the one should contact the WRF-Chem help desk at wrfchemhelp.gsd@noaa.gov, or explore the WRF community forum and see if the user community can povide an answer.

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 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.

All WRF-Chem users are also advised to link their 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 the most up to date list of relevant publications regarding the WRF-Chem model. When presenting, or publishing results from studies using 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). And likewise, when using other significant features in the WRF-Chem model, the user should examine the reference list on the WRF-Chem web page and cite the developer's paper(s) (http://ruc.noaa.gov/wrf/WG11/References/WRF-Chem.references.htm). 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.

9.2 WRF-Chem and utility program related publications

Ahmadov, R., et al., 2012: A volatility basis set model for summertime secondary organic aerosols over the eastern United States in 2006, *J. Geophys. Res.*, **117,** D06301, doi:10.1029/2011JD016831

Barnard, J.C., J.D. Fast, G.L. Paredes-Miranda, and P.W. Arnott, 2008: Closure on the single scattering albedo in the WRF-Chem framework using data from the MILAGRO campaign. *Atmos. Chem. Phys. Discuss.,* **9,** 5009-5054.

Barnard, J., J. Fast, G. Paredes-Miranda, W. Arnott, and A. Laskin, 2010: Technical Note: Evaluation of the WRF-Chem "Aerosol Chemical to Aerosol Optical Properties" Module using data from the MILAGRO campaign. *Atmos. Chem. Phys*., **10,** 7325-7340.

Barth, M., C., J. Lee, A., Hodzic, G. Pfister, W. C. Skamarock, J. Worden, J. Wong, and D. Noone, 2012: Thunderstorms and upper troposphere chemistry during the early stages of the 2006 North American Monsoon, *Atmos. Chem. Phys. Discuss.,* **12,** 16407-16455, doi:10.5194/acpd-12-16407-2012.

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