WRF-Chem Version 3.8.1 User's Guide

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WRF-Chem Overview

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1.1 WRF-Chem 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://www2.mmm.ucar.edu/wrf/users/docs/user_guide_V3/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) as well as some additional unlisted capabilities:

- 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 3.14. 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
- Global emissions data from the one-half degree RETRO and ten-degree EDGAR data sets
- User-specified anthropogenic emissions such as those available from the U.S. EPA NEI-05 and NEI-11 data inventories. The user must provide the emissions data for their own domain in the proper WRF data file format.

- 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) are currently available for RADM2, RACM, RACM-MIM, SAPRC-99, MOZART and NMHC9 chemical mechanisms
- 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, also from Sasha Madronich, is faster than the previous Madronich scheme option.
- Five choices for aerosol schemes:
  - The Modal Aerosol Dynamics Model for Europe - MADE/SORGAM
  - The Modal Aerosol Dynamics Model for Europe with the Volitity Basis Set aerosols – MADE/VBS
  - The Modal Aerosol Module (MAM) 3 or 7 bin schemes closely coupled to the CAM5 physics
  - The Model for Simulating Aerosol Interactions and Chemistry (MOSAIC - 4 or 8 bins) sectional model aerosol parameterization
  - A bulk aerosol module from GOCART
- Aerosol direct effect through interaction with atmospheric radiation, photolysis, and microphysics routines. This is available for all aerosol options starting with version 3.5
- Aerosol indirect effect through interaction with atmospheric radiation, photolysis, and microphysics routines. This feature is available for modal and sectional aerosol options starting with version 3.5.
- An option for the passive tracer transport of greenhouse gases
- Two options for a 10-bin volcanic ash aerosol scheme based upon emissions from a single active volcano. One scheme includes SO_2 degassing from the volcano while the other ignores SO_2 degassing. Volcanic ash emissions can also be coupled to some aerosol modules (bulk and modal)
- 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

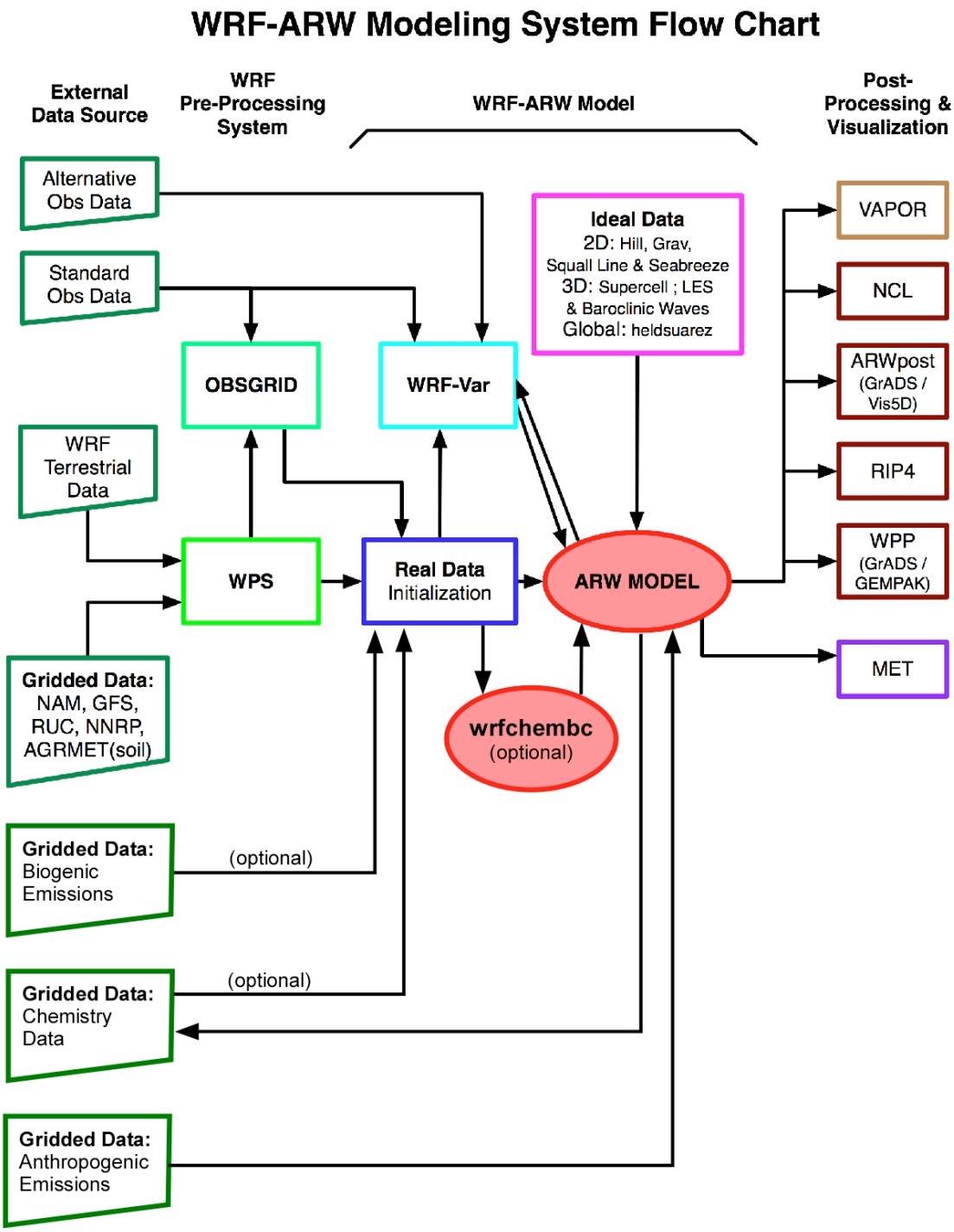
The chemistry model has been built to be consistent with the WRF model I/O Applications Program Interface (I/O API). That is, the chemistry model section has been built following the construction methodology used in the remainder of the WRF model. Therefore, the reader is referred to the WRF software 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. And while the chemistry model has been built with the intent to work within the WRF framework, *not all run time options (e.g., physical parameterizations) that are available for WRF will function properly with chemistry turned on*. Therefore, care must be taken in selecting the parameterizations used with the chemistry schemes.

1.3 Possible applications of the current modeling system

- Prediction and simulation of weather, or regional and 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 3.8.



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 core only) including chemistry
- Post-processing and visualization tools

The difference with regular WRF comes from the chemistry part of the model needing to be provided additional gridded input data related to emissions. This additional input data is provided either by the WPS (dust emission fields), or read in during the real.exe initialization (e.g., biomass burning, biogenic emissions, GOCART background fields, etc.), or read in during the execution of the WRF solver (e.g., anthropogenic emissions, boundary conditions, volcanic emissions, etc.). And while some programs are provided in an attempt to aid the user in generation of these external input data files, as stated earlier, not all emissions choices are set-up to function for all possible namelist options related to the WRF-Chem model. In other words, the generation of emissions input data for simulating the state of the atmosphere's chemistry can be incredibly complex. Some times the user will need to modify code, or the model configuration, to get it to function properly for their project. For more information regarding the input of emissions the reader is directed to the WRF-Chem Emissions Guide.

Chapter 2: WRF-Chem Software Installation

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2.1 Software Installation Introduction

The WRF modeling system software (including chemistry) installation is straight forward 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 for WRF 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 the pull-down tab Downloads, registration required, to find the netCDF link). Likewise, there is one exception as well, the fast lexical analyser (FLEX) library (libfl.a) will be needed if compiling the KPP chemistry code. This library is commonly included with GNU bison and is freely available for download at http://www.gnu.org/software/bison if it is not already installed on your unix systm.

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 cannot 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 Preprocessing System, or WPS). Documentation for the WRF Model and its initialization package can be found at (http://www2.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

To obtain the WRF-Chem model one should follow these steps:

- 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://www2.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 by examining the WRF and WRF-Chem web pages

- Unzip and untar the file
  - > gzip –cd WRFV3-Chem-3.8.TAR | tar –xf –
  - Again, if there is a newer version of the code use it, 3.8 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://www2.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 EM_CORE 1
setenv NMM_CORE 0
```

and they explicitly define which model core to build. These are the default values that 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)** as these options 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

At this point all of the WRF-Chemistry model have been built. The model can be run and the run time messages should indicate that chemistry is included. But before one can use the WRF chemistry model to its full potential, the emissions input data needs to

be generated. The manufacturing of the emissions input data is the subject of the next chapter and the WRF-Chem Emissions Guide.

Chapter 3: Generation of WRF-Chem-Emissions Data

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3.1 Emissions Generation Overview

One of the main differences between running with and without chemistry is the inclusion of additional data sets describing the sources of chemical species. Ideally there would be single model, or utility code that would construct any and all emissions data sets for any domain and any chemistry option that a user selects. Unfortunately this is not the case and some of the emission files need to be prepared externally from the WRF-Chem simulation. **This places the requirement the WRF-Chem model user to construct the emissions data set for your particular domain and desired chemistry option from the wide variety of available data sources**. This also 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, a separate guide has been written that should help illustrate the methodology through which emissions data is generated for a forecast domain. In short, there are several utility programs and data sets provided by the WRF-Chem user community that may be used to create an emissions data set. There are some restrictions on the domain location and the choice of chemical mechanism that need to be considered when using these programs. See the separate WRF-Chem emissions document to learn more about these programs and their use.

3.2 Generating Dust Emissions

Adding dust aerosols to a WRF simulation is perhaps the easiest of all WRF-Chem options as the model generates the dust emissions fields during the actual run. The "online" dust emissions data is provided through land useage information produced by the WRF Preprocessing System (WPS) and the simulated meteorological fields. Hence, by compiling the WRF-Chem code, and following standard procedures of using the WPS to generate the WRF-Chem model input data, the user has added the option of including an aerosols scheme with minimal effort. Additional information about running with dust aerosols is available in Chapter 4 as well as under the tutorials link from the WRF-Chem web page at http://ruc.noaa.gov/wrf/WG11.

Chapter 4: Running the WRF-Chemistry Model

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4.1 Running WRF-Chem 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 name list 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 is described next. Some of these choices require other settings for other namelist options. The options that are printed with red lettering indicate those options 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	Additional Comments
	chem_opt = 0	no chemistry	
RADM2 /QSSA Chemistry	= 1	includes chemistry using the RADM2 chemical mechanism - no aerosols	
	= 2	includes chemistry using the RADM2 chemical mechanism and MADE/SORGAM aerosols.	
	= 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.	
	= 8	CBMZ chemical mechanism (chem_opt=6) and MOSAIC using 8 sectional aerosol bins.	
	= 9	CBMZ chemical mechanism (chem_opt=6) and MOSAIC using 4 sectional aerosol bins including some aqueous reactions	Due to errors, dust_opt=2, seas_opt=2 has been disabled.
	= 10	CBMZ chemical mechanism (chem_opt=6) and MOSAIC using 8 sectional aerosol bins including some aqueous reactions	Due to errors, dust_opt=2, seas_opt=2 has been disabled.
	= 11	RADM2 chemical mechanism and MADE/SORGAM aerosols including some aqueous reactions	Due to errors, dust_opt=2, seas_opt=2 has been disabled.
	= 12	RACM chemical mechanism and MADE/SORGAM aerosols including some aqueous reactions	Due to errors, dust_opt=2, seas_opt=2 has been disabled.
	= 13	Run with 5 tracers with emissions, currently set up for SO_2, CO, no, ald, hcho, ora2	Use of tracer_opt suggested instead of this option.
	= 14	Single tracer run using tracer_1 array	Use of tracer_opt suggested instead.
	= 15	Ensemble tracer option using 20 individual tracers and an ensemble tracer array	Use of tracer_opt suggested instead.
	= 16	Greenhouse Gas CO_2 only tracer	Use of tracer_opt might be a better

		choice in some cases
= 17	Greenhouse Gas tracer	
= 30	CBMZ chemical mechanism (chem_opt=6) and MADE/SORGAM modal aerosol	
= 31	CBMZ chemical mechanism (chem_opt=6) and MOSAIC using 4 sectional aerosol bin with dms	
= 32	CBMZ chemical mechanism with (chem_opt=6) and MOSAIC using 4 sectional aerosol bins with dms. Some aqueous reactions included	
= 33	CBMZ chemical mechanism (chem_opt=6) and MOSAIC using 8 sectional aerosol bin with dms. Some aqueous reactions included	
= 34	CBMZ chemical mechanism with (chem_opt=6) and MOSAIC using 8 sectional aerosol bins with dms. Some aqueous reactions included.	
= 35	CBMZ chemical mechanism (chem_opt=6) and MADE/SORGAM modal aerosol. Some aqueous reactions included	
= 41	RADM2/SORGAM with aqueous reactions included.	
= 42	RACM/SORGAM with aqueous reactions included (KPP)	Includes less complex aqueous reactions following CMAQ methodology, SO4 and NO3 wet deposition
= 43	NOAA/ESRL RACM Chemistry and MADE/VBS aerosols using KPP library. The volatility basis set (VBS) is used for Secondary Organic Aerosols	Includes less complex aqueous reactions following CMAQ methodology, SO4 and NO3 wet deposition
= 101	RADM2 Chemistry using KPP library	Includes less complex aqueous reactions following CMAQ methodology
= 102	RACM-MIM Chemistry using KPP library	Rosenbrock solver, can use larger time step
= 103	RACM Chemistry using KPP library	Rosenbrock solver, can use larger time step
= 104	RACM Chemistry and PM advection using KPP library	Rosenbrock solver, can use larger time step
= 105	RACM Chemistry and MADE/SORGAM aerosols using KPP library	PM total mass. This was originally implemented for wildfires
= 106	RADM2 Chemistry and	Rosenbrock solver, can use larger time

	MADE/SORGAM aerosols using KPP library	step
= 107	RACM Chemistry and MADE/SORGAM aerosols using KPP library using the ESRL chemical reaction table	Rosenbrock solver, can use larger time step
= 108	NOAA/ESRL RACM Chemistry and MADE/VBS aerosols using KPP library. The volatility basis set (VBS) is used for Secondary Organic Aerosols	Rosenbrock solver, can use larger time step
= 109	RACM Chemistry with MADE/VBS aerosols using KPP library along with the volatility basis set (VBS) used for Secondary Organic Aerosols	Includes less complex aqueous reactions following CMAQ methodology, SO4 and NO3 wet deposition
= 110	CB4 Chemistry using KPP library	Rosenbrock solver, can use larger time step
= 111	MOZART Chemistry using KPP library	Rosenbrock solver, can use larger time step
= 112	MOZART Chemistry and GOCART aerosols (MOZCART) using KPP library	Rosenbrock solver, can use larger time step. Use phot_opt=3
= 120	CBMZ Chemistry using KPP library	Rosenbrock solver, can use larger time step. Use phot_opt=3
= 131	CB05 Chemistry with MADE/SORGAM	Rosenbrock solver, can use larger time step.
= 132	CB05 Chemistry with MADE sectional aerosols and includes volatility basis set (VBS) for organic aerosol evolution	Rosenbrock solver, can use larger time step.
= 170	CBMZ Chemistry with MOSAIC aerosols using KPP library	Rosenbrock solver, can use larger time step
= 195	SAPRC99 Chemistry using KPP library	Rosenbrock solver, can use larger time step
= 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 time step
= 200	NMHC99 – disabled.	Incomplete installation of mechanism.
= 201	MOZART 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 time step
= 202	MOZART Chemistry with MOSAIC using KPP library. The MOSAIC aerosols uses 4 sectional aerosol bins and includes volatility basis set (VBS) for organic aerosol evolution. Also include aqueous	Rosenbrock solver, can use larger time step

	phase chemistry.	
= 203	SAPRC99 Chemistry with MOSAIC using KPP library. The MOSAIC aerosols uses 8 sectional aerosol bins and includes volatility basis set (VBS) for organic aerosol evolution. Also include aqueous phase chemistry.	Rosenbrock solver, can use larger time step
= 204	SAPRC99 Chemistry with MOSAIC using KPP library. The MOSAIC aerosols uses 8 sectional aerosol bins and includes volatility basis set (VBS) for organic aerosol evolution.	Rosenbrock solver, can use larger time step
= 300	GOCART simple aerosol scheme, no ozone chemistry	Only 18 variables. Optionally use dmsemis_opt=1, dust_opt=1 or 3, seas_opt=1
= 301	GOCART coupled with RACM-KPP	Only 18 variables Optionally use dmsemis_opt=1, dust_opt=1, seas_opt=1
= 303	RADM2 Chemistry and GOCART aerosols	Simple aerosol treatment. Optionally use dmsemis_opt=1, dust_opt=1 seas_opt=1
= 400	Volcanic ash fall and concentration only	Simple aerosol treatment. Optionally use dmsemis_opt=1 dust_opt=1, seas_opt=1
= 401	Dust concentration only	Simple ash treatment with 10 ash size bins
= 402	Volcanic ash fall and SO_2 concentration	Simple dust treatment with 5 size bins
= 403	Volcanic ash fall	Simple dust treatment with 4 size bins
= 501	CBMZ with CAM-MAM3	Simple ash treatment with 10 ash size bins and volcanic SO_2 gas emissions
= 502	CBMZ with CAM-MAM7	MAM chemistry with 3 mode aerosol species. Requires CAM5 Morrison and Gettleman scheme (mp_phys=11).
= 503	CBMZ with CAM-MAM3_AQ	MAM chemistry with 7 mode aerosol species. Requires CAM5 Morrison and Gettleman scheme (mp_phys=11).
= 504	CBMZ with CAM-MAM7_AQ	MAM chemistry with 3 mode aerosol species and aqueous chemistry. Requires CAM5 Morrison and Gettleman scheme (mp_phys=11). MAM chemistry with 7 mode aerosol species and aqueous chemistry. Requires CAM5 Morrison and Gettleman scheme (mp_phys=11).
= 600	CRIMECH chemical mechanism using	

		the KPP library
	= 601	CRIMECH chemical mechanism using the KPP library with MOSAIC aerosols. The MOSAIC aerosols uses 8 sectional aerosol bins.
	= 611	CRIMECH chemical mechanism using the KPP library with MOSAIC aerosols. The MOSAIC aerosols uses 4 sectional aerosol bins and includes aqueous phase chemistry.

4.3 Other chemistry namelist options

input_chem_inname <string>		name of chemistry input file
chem_in_opt	= 0	uses idealized profile to initialize chemistry
	=1	uses 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. Set as well if using a global model to provide chemical lateral BCs.
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. The aircraft emissions are read in through auxiliary input port 14
photdt	= 30	update time interval used by photolysis routine in minutes
phot_opt	= 0	no photolysis
	= 1	uses Madronich photolysis (TUV)
	= 2	uses Fast-J photolysis
	= 3	uses Madronich F-TUV photolysis (aerosol interaction is not hooked up with MOSAIC aerosols)
emiss_opt	= 0	no anthropogenic emissions
	= 2	uses radm2 anthropogenic emissions
	= 3	uses radm2/MADE/SORGAM anthropogenic emissions (recommended if using NEI emissions from emiss_v03.F)
	= 4	uses CBMZ/MOSAIC anthropogenic emissions
	= 5	GOCART RACM_KPP emissions (recommended if using RETRO/EDGAR emissions from prep_chem_sources)
	= 6	GOCART simple emissions
	= 7	MOZART emissions
	= 8	MOZCART (MOZART + GOCART aerosols) emissions
	= 9	Converts default RADM2 gas emissions to CBMZ. Aerosol

		emissions are speciated to MAM 3-mode aerosols
	= 10	MOZART (MOZART + aerosols) emissions
	= 13	SAPRC99 emissions
	= 14	CB05 emissions based on CBMZ speciation and to be used with emiss_inpt_opt=102
	= 15	CB05 emissions based on CB05 speciation and to be used with emiss_inpt_opt=101
	= 16	Greenhouse Gas CO_2 tracer emissions
	= 17	Greenhouse Gas tracer emissions
	= 19	CRIMECH emissions
	= 20	CRIMECH emissions including additional aerosol species
emiss_opt_vol	= 0	no volcanic ash emissions
	= 1	Include volcanic ash emissions for 10 size bins
	= 2	Include SO_2 as well as the volcanic ash emissions for 10 size bins
aircraft_emiss_opt	= 0	no aircraft emissions
	= 1	uses aircraft emissions
gas_drydep_opt	= 0	no dry deposition of gas species
	= 1	includes dry deposition of gas species
aer_drydep_opt	= 0	no dry deposition of aerosols
	= 1	includes dry deposition of aerosols
depo_fact	= 0.25	when using VBS for aerosols, the ratio between dry deposition velocities of organic condensable vapors and dry deposition of HNO_3 (default value = 0.25)
bio_emiss_opt	= 0	no biogenic emissions
	= 1	calculates biogenic emissions online using the Gunther scheme
	= 2	includes biogenic emissions reference fields in wrfinput data file and modify values online based upon the weather
	= 3	includes MEGAN biogenic emissions online based upon the weather, land use data. Need to include ne_area setting, the total number of chemical species, in the chemical namelist.
	= 16	Include CO_2 biomass emissions from the VPRM model. (Requires user to provide external files through auxiliary input port 15.)
	= 17	Include VPRM input fields, Kaplan wetland inventory input fields when chem_opt=17. (Requires user to provide external files through auxiliary input port 15.)
ne_area	= 41	Used by MEGAN biogenic emissions to provide a minimum total number of chemical species used by specified chemistry option. Best to set to a value larger than all chemical species (i.e., ne_area > 100).
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
	= 16	Used with chem_opt=16, or 17 only to add fluxes and emissions to

		passive tracers.
	= 101	RADM2 emission speciation adapted after reading the data file to follow the CBMZ/MOSAIC framework
	= 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 RADM2 data file
	= 104	Carbon Bond 4-emission speciation adapted after reading the RADM2 data file. Secondary Organic Aerosol (SOA) precursors computed from input data as well. Use for CAM5 micrphysics and MAM 3-mode aerosol
	= 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
	= 2	include biomass burning emissions and plume rise calculation for MOCART
	= 3	include biomass burning emissions and plume rise calculation for MOZART
	= 5	include biomass burning emissions and plume rise calculation for GHG tracers fo CO_2, CO and CH_4 (needs chem_opt=17)
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	Disabled due to errors in the scheme.
	=3	Include GOCART dust emissions with AFWA modifications
	=4	Include GOCART dust emissions with UOC modifications, set dust_schme option as well.
dust_schme	= 1	Dust emissions following Shao 2001, requires dust_opt=4.
	= 2	Dust emissions following Shao 2004, requires dust_opt=4.
	= 3	Dust emissions following Shao 2011, requires dust_opt=4.
dustwd_onoff	= 0	Dust wet deposition following Jung 2004 turned off.
	= 1	Dust wet deposition following Jung 2004 turned on, requires dust_opt=4.
seas_opt	= 0	no GOCART sea salt emissions
	= 1	include GOCART sea salt emissions
	= 2	Disabled due to errors in the scheme.
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
	= 16	sets values of CO_2, CO and CH_4 mixing ratios at boundaries to relevant constants. If a user wants to use boundary conditions from a global model, then the wrfbdy file should be modified and "have_bcs_chem" must be set to ".true."
	= 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
	= 16	sets initial values of CO_2, CO and CH_4 mixing ratios to relevant constants
	= 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)
conv_tr_wetscav = 0	subgrid convective wet scavenging turned off in the simulation (if no parameterization is used or for debugging)
= 1	subgrid convective wet scavenging turned on in the simulation (default)
conv_tr_aqchem = 0	subgrid convective aqueous chemistry turned off in the simulation (if no parameterization is used or for debugging)
= 1	subgrid convective aqueous chemistry turned on in the simulation (default). Currently connected to "MADE" modal aerosol options.
have_bcs_chem = .false.	gets lateral boundary data from idealized profile specified in chemistry routines (use caution when setting as the namelist variable is defined as a logical)
= .true.	gets lateral boundary data from wrfbdy data file (use caution when setting as the namelist variable is defined as a logical)
have_bcs_tracer = .false.	does not use tracer lateral boundary data from wrfbdy data file (use caution when setting as the namelist variable is defined as a logical)
= .true.	gets 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
cam_mam_mode = 3	Number of MAM aerosol modes
cam_mam_nspec = 74	Number of MAM 3-bin aerosol species
CAM_MP_MAM_cpled	Option to allow users to run Morrison-Gettleman micrphysics with prescribed aerosols (using &physics namelist options accum_mode, aitken_mode and coarse_mode) with the RRTMG radiation scheme. The RRTMG scheme will still use prognostic aerosols. Default value is set to .true. so that both the Morrison-Gettleman microphysics and the RRTMG radiation scheme use prognostic aerosols.

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 GF 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.
mp_physics	= 11	CAM5 Morrison-Gettleman scheme to be used with MAM chemistry
cu_physics	= 7	CAM5 Zhang-McFarlane scheme to be used with MAM chemistry
bl_pbl_physics	= 9	CAM5 UW PBL scheme to be used with CAM-MAM chemistry
shcu_physics	= 2	CAM5 UW shallow cumulus schemeto be used with CAM-MAM chemistry
accum_mode	= 1.e9	Background mass mixing ration for accumulation mode used with CAM_MP_MAM_cpled = .false.
aitken_mode	= 3.e8	Background mass mixing ration for Aitken mode used with CAM_MP_MAM_cpled = .false.
coarse_mode	= 2.e5	Background mass mixing ration for coarse mode used with CAM_MP_MAM_cpled = .false.

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
io_form_auxinput13 = 2	Volcanic ash emissions input (wrfchemv_d01) data format is WRF netCDF. Can be used if emiss_opt_vol > 1
= 11	parallel netCDF. Can be used if emiss_opt_vol > 1
io_form_auxinput14 = 2	aircraft emissions input data format is WRF netCDF.
= 11	parallel netCDF.
io_form_auxinput15 = 2	CO_2 or GHG emissions input data format is WRF netCDF. Can be used if chem_opt = 16 or 17.
= 11	parallel netCDF. Can be used if chem_opt = 16 or 17.

4.3.1 Running with only dust aerosols

The WRF-Chem code is able to predict dust transport along with the meteorology. To run with only dust, you should have obtained several input data files for the WRF Preprocessor System (WPS). These files are the dust related fields (erosion factor, clay fraction, sand fraction) that are included in the WPS GEOG directory and the GEOGRIB.TBL_ARW_CHEM table file. After downloading and comiling the WPS, one needs to link the GEOGRIB table to GEOGRIB.TBL_ARW_CHEM. The WRF WPS can then be run so that the dust erosion fields will be included the geogrib output and subsequently included in the meteorology input data files. With the dust erosion data now in the input files 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 and the dust_opt option is set to 1, 3, or 4.

4.3.2 Running with direct effect

Shortwave radiative feedbacks or what is known as the direct effect is included with the running of chemistry. To turn on the radiative feedbacks in your simulation you should select either the RRTMG radiation schemes, or the Goddard shortwave scheme and turn on aer_ra_feedback (aer_ra_feedback=1). With these options selected the aerosol shading will be active and one can select an aerosol compostition assumption for the Mie radiation calculation using aer_op_opt. Another namelist option related to radiation that is typically used in a simulation is cu_rad_feedback. When turned on (cu_rad_feedback = .true.) the shortwave and photolysis schemes will include the effects of unresolved clouds in the simulation. Otherwise, the simulation could have a grid cell containing a strong precipitating thunderstorm (parameterized instead of resolved precipitation) but the surface incident radiation and photolysis calculations will produce a result for an environment is totally cloud free.

4.3.3 Running with indirect effect

There are several chemistry options that include the indirect effect and each of these options contain aqueous phase chemistry (e.g., RADM2SORG_AQ, RACMSORG_AQ, CBMZ_MOSIAC_4BIN_AQ, CBMZ_MOSAIC_8BIN_AQ, etc.). It has been assumed by the developers that if a user chooses to run with includes aqeuous phase chemistry, then they also choose to be running with the indirect effect (chemistry-microphysics interactions). If you do not want to include the indirect effect then one must either include a prescribed climatological aerosol distribution (e.g., Gustafson et al., 2007) or choose a chemistry option that does not include aqueous phase chemistry.

To run with indirect effect on, one should turn on the aerosol direct effect (aer_rad_feedback = 1 and aer_op_opt > 0). Next the user needs to select a double microphysics scheme; either Lin et al. or the Morrison microphysics schemes are the current possible choices. Next turn on the prognostic number density option (progn=1) in the physics namelist to make the Lin et al. scheme double moment as well as communicate the desire to run indirect effect to other microphysics schemes. Finally, turn on the wet scavenging and cloud chemistry options (wetscav_onoff=1; cldchem_onoff=1).

4.3.4 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 name ist 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 E)
tracer_adv_opt	= 0	uses positive definite advection for tracers
	= 1	uses positive definite and monotonic advection for tracers. (Recommended)

The biomass-burning tracer (ppmv) obtains the 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.

4.3.5 Considerations when running with CAM-MAM chemistry

Starting with version 3.5 of the WRF-chem model, the CAM5 micrphysics and MAM aerosol schemes has been made available. The MAM aerosol scheme, short for Modal Aerosol Model, is either a 7-mode and 3-mode modal aerosol scheme (Liu et al., 2012) derived from the Community Atmosphere Model (CAM), a component of the CESM climate model. The MAM scheme provides internally mixed representations of number concentration and mass for Aitkin, accumulation, and coarse aerosol modes. At this time the MAM is coupled only with CBM-Z photochemistry within WRF-Chem. In addition to MAM, the microphysics scheme from CAM has been ported to the WRF model. This scheme represents stratiform microphysical processes through a prognostic, two-moment formulation following the original parameterization of Morrison and Gettelman (2008). It should be noted that the CAM-MAM scheme (chem_opt=503) was extensively tested with the CAM physics inside WRF (CAMMGMP, CAMUWPBL, CAMZM, CAMUWSHCU, and RRTMG). The CAM physics options as well as the MAM chemistry could run with different combinations of the pre-existing physics and chemistry parameterizations in WRF, however, it is not recommended due to the lack of evaluation. Runs not using the full CAM-MAM package options should be examined by the user to ensure accuracy or whether the results contain numerical artifacts. In addition, the user could encounter warning and error messages when running MAM chemistry

independent of CAM microphysics as this is not fully tested and the model could be running in an unsupported configuration.

When running without chemistry, the CAM microphysics scheme (Morrison and Gettelman microphysics; Morrison and Gettelman, 2008) requires TKE to be computed in oder for the scheme to function properly, so it must be used with PBL a scheme that produces TKE (e.g., UW PBL or MYJ). This scheme also uses outputs from Zhang-McFarlane cumulus scheme and the UW shallow cumulus schemes as sources of input data (Zhang and McFarlane, 1995). Care must be taken as these fields are set to zero when Zhang-McFarlane cumulus scheme and the UW shallow cumulus scheme are not in use and could result in run time errors. It is recommend that one use the CAM microphysics with the complete CAM physics suite (the UW shallow cumulus, Zhang-MacFarlane deep cumulus the UW PBL) when running the model to avoid encountering a run-time error.

When running the CAM physics suite (Morrison and Gettelman microphysics, UW shallow cumulus, Zhang-MacFarlane deep cumulus and UW PBL) with chemistry, it is recommended that the user can select from the four MAM aerosol packages. The CAM microphysics suite has not been tested with the other chemisry packages and could result in run error. If however, one wanted to test the UW PBL scheme with other chemistry options, this PBL scheme should not produce run time errors as it is an independent package. It should also be noted that the CAM microphysics in WRF does not include the full CAM5 macrophysics treatments. For this model implementation a simplified version of CAM5 macrophysics is incorporated in the CAM microphysics driver which aids in computing the CAM fractional clouds as opposed to pre-existing WRF cloud fractions (values between 0 and 1). The simplified cloud fraction inside WRF's CAM scheme uses the same formulation to calculate convective cloud fraction, and liquid and ice cloud fraction for stratiform clouds.

4.4 Typical choices for namelist options

The addition of chemistry to WRF is making the choice of runtime configuration 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:

chem_adv_opt = 2
moist_adv_opt=2
scalar_adv_opt=2
tke_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 desired. 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 is used by cu_phys=5 (G3 scheme) and should be set 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 surface layer and PBL physics is perhaps the most contested decision in the modeling community and at times highly dependent on the users experiences and preferences. The user must keep in mind that results can differ significantly depending on their choice of PBL and land surface schemes. The YSU scheme could lead to the deepest boundary layers when using the above choices (1-2-1). The user may also elect to instead set the input parameters to 2-2-2, using the MYJ scheme. There is no aprior way of telling which options will work better for a particular simulation. Sometimes a user might choose the RUC soil parameterization (2-3-2) in

combination with either YSU or MYJ scheme. These settings may work fine when the input conditions come from the Rapid Update Cycle (RUC) or Rapid Refresh (RAP; Benjamin et al., 2015) configuration of the WRF model. The question of what modeling system the input and boundary conditions come from (such as GFS, NAM, ECMWF, etc.) and what physical parameterizations used in that modeling system could also play a role too in determining the most suitable choice of PBL physics. For example, the user may want to try to be consistent with the larger scale model, or choose 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 from operational models (e.g., RAP) that could be essential in reducing model forecast 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

When running WRF-chem, it is advised that the user always select 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 using chem_opt=1 or 2, it is advised that the chemistry timestep is the same as that 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. A user can opt to use a 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 a NOAA-Aeronomy Laboratory Regional Oxidation Model (NALROM). 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 SO_2. The first reference index for the idealized profile, iref(1), is set to the number 12, indicating that SO_2 is taken from the 12th species in the input data table. Not all chemical species match up so cleanly. For example, the NALROM 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 NALROM:

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 VPRM and Greenhouse Gas tracer namelist options

There are several chemistry namelist options that are used only by the CO_2 tracer and Greenhouse Gas tracer chemistry options. These namelist options are:

vprm_opt	This option allows a user to select a parameter set for the VPRM model. There are three sets of parameters - “VPRM_TABLE_US”, “VPRM_TABLE_EUROPE” and “VPRM_TABLE_TROPICS” (included in chem/chemics_init.F) used for different regions. Users may need to build own parameter sets for the domain and time period of interest. (default is “VPRM_param_US”)
wpeat	Used to specify the scaling factor for the CH_4 wetland emissions from peatlands. It indicates the fraction of heterotrophic respiration that is considered to be CH_4 emissions. (default is 0.05)
wflood	Used to specify the scaling factor for the CH_4 wetland emissions from floodplains. Weighting between peat and floodplain wetlands depends on the mean annual temperature. Users may need to calibrate the Kaplan wetland inventory with observations first and then adjust both scaling factors. (default is 0.19)
term_opt	user to select the parameter set for the calculation of the termite emissions. Two sets of parameters are included: "CH4_termite_NW" to be used for the American continent and Australia and "CH4_termite_OW" for Europe, Asia, and Africa. Both are included in chem/chemics_init.F. (default is "CH4_termite_NW")

4.7 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 conditions, 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://www2.mmm.ucar.edu/wrf/users/workshops/WS2011/WorkshopPapers.php.

4.8 Making a nested domain WRF-Chem simulation

To make a nested domain run one should first 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 start by making a nested domain weather forecast (Chapter 4 of WRF Users Guide). After the nested meteorology only simulation is functioning correctly, then move on to running with chemistry included in the simulation.

Once the input files are produced the user can generate the emissions files for both domains using their program of choice (e.g., the emiss_v03.F program discussed in section 9 of the WRF-Chem Emissions Guide). File anthropogenic emissions file names will be differentiated by the domain (ie., 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. That is, for each domain you will run convert_emiss.exe using settings for a single domain in your namelist.input file. More specifically, follow the description in section 3 to generate wrfchemi_d01 for the coarse domain, and move it to a safe place by changing its name. Change the namelist.input file, moving the nested information to the mother domain column. Move the 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,
emiss_opt_vol           = 0, 0,
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,
depo_fact               = 0.25, 0.25,
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,
conv_tr_wetscav         = 1, 1,
conv_tr_aqchem          = 1, 1,
biomass_burn_opt        = 1, 0,
plumerisefire_frq       = 30, 0,
aer_ra_feedback         = 0, 0,
aer_op_opt              = 0, 0,
have_bcs_chem           = .false., .false.,
```

Chapter 5: Visualizing WRF-Chem Data files

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5.1 Visualizing WRF-Chem 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 supports four 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://www2.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 that 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

NCL is among the many post-processing utilities to visualize WRF output. This section briefly describes 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).

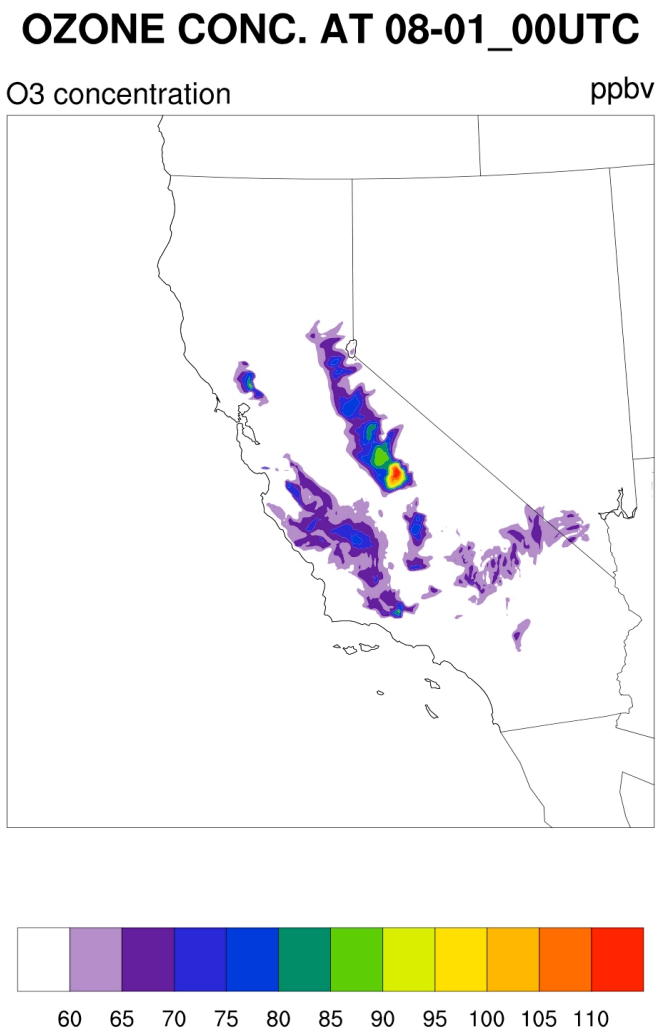

Fig. 5.1 A sample of a color-filled contour plot generated using the NCL script. The colored regions represent locations in which the surface ozone concentration (ppbv) is in the range indicated by the color bar shown at the bottom of the figure.

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.

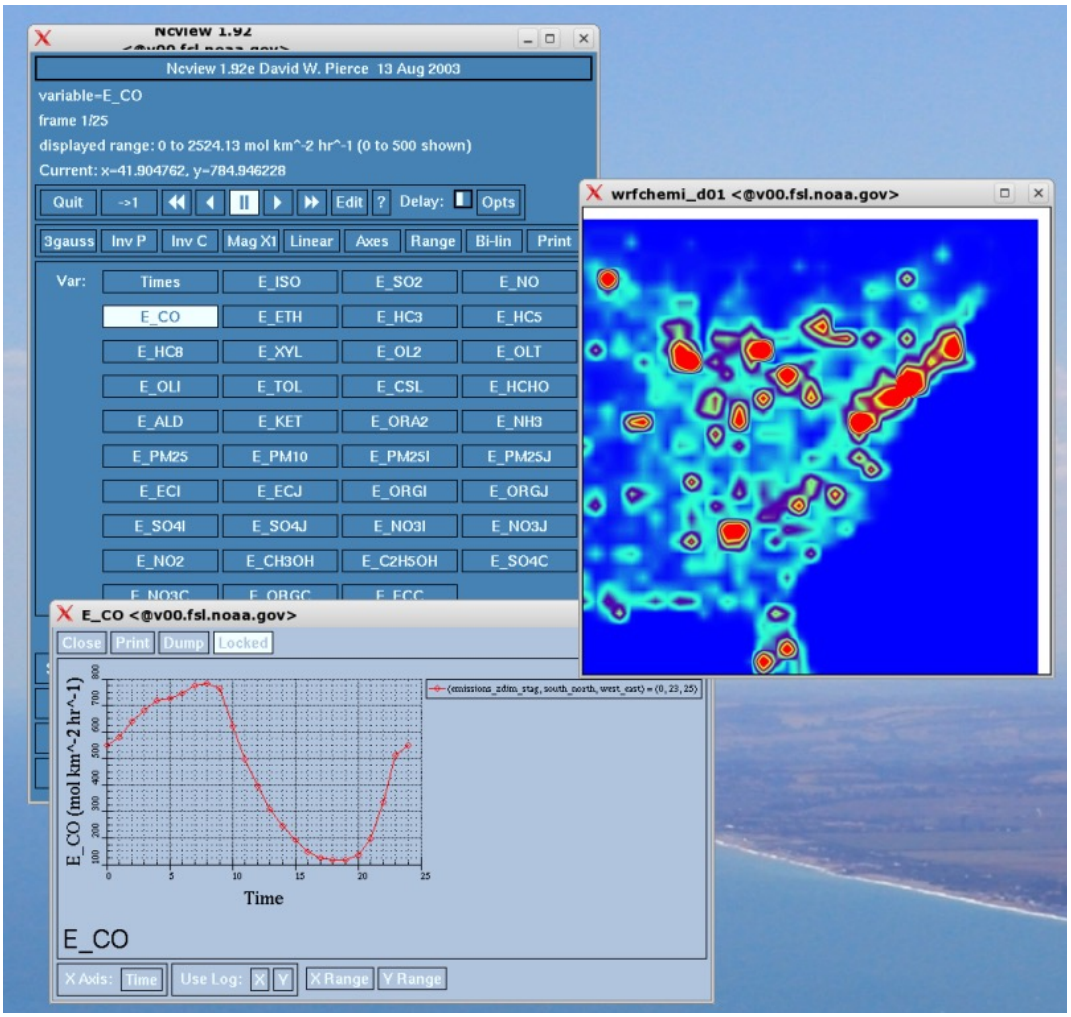

Fig. 5.2 A screen-capture image showing how the Ncview user interface allows the user to examine the WRF-Chem emissions-input data file. The color image shows the surface emissions for carbon monoxide and the plot shows the temporal evolution of the surface CO emissions at a single point.

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://www2.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 two namelists: the userin namelist that holds the general input specifications and the trajcalc namelist that controls the creation of trajectory 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.

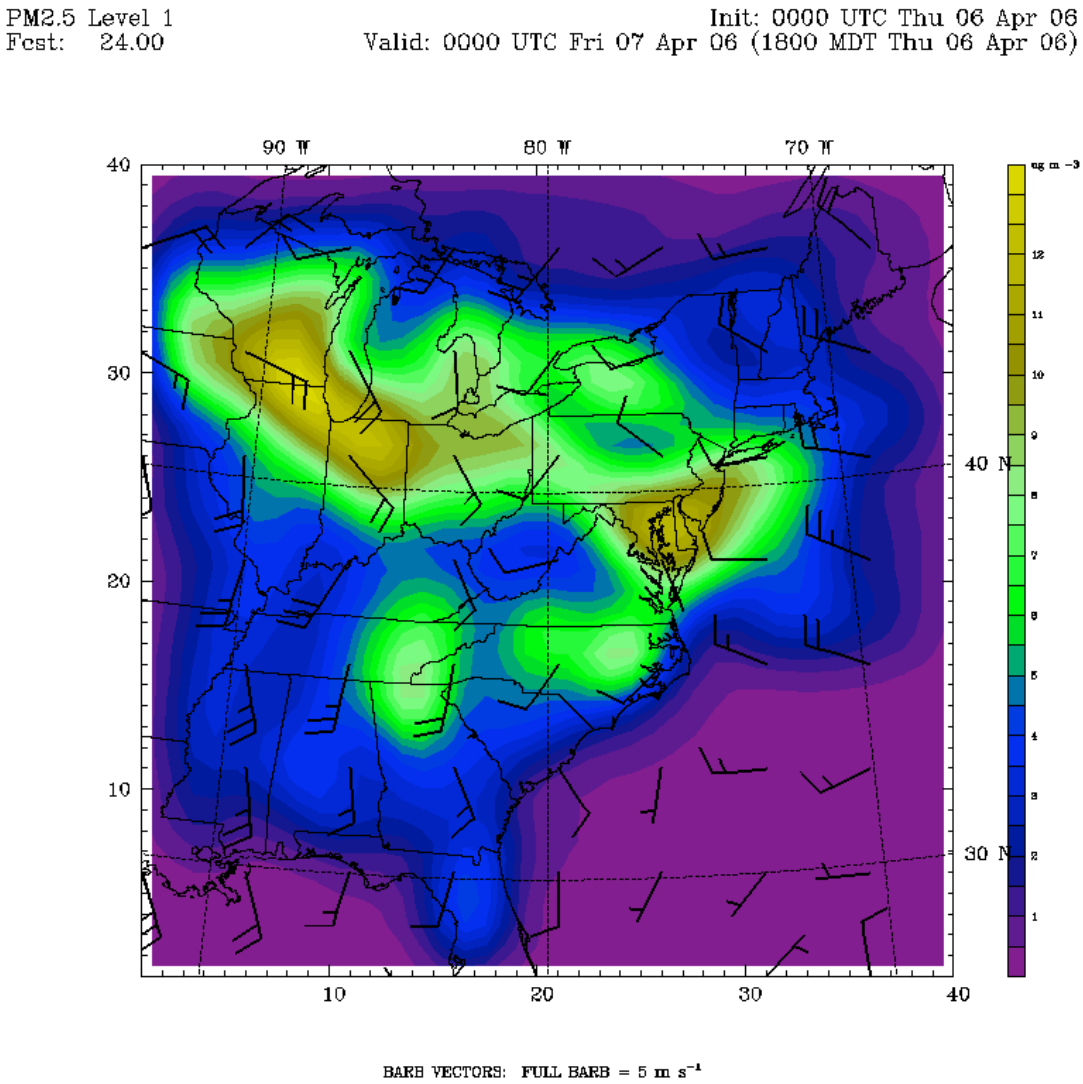

Fig. 5.3. An NCAR GKS figure produced using by the RIP visualization tool. The image shows the surface fine particulate matter (PM2.5) concentration (micrograms per cubic meter) and the horizontal surface winds (barbs).

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 WRF-Chem KPP 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 UNIX 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 that 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 part 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); and
- 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 that is located in the util/wkc directory.

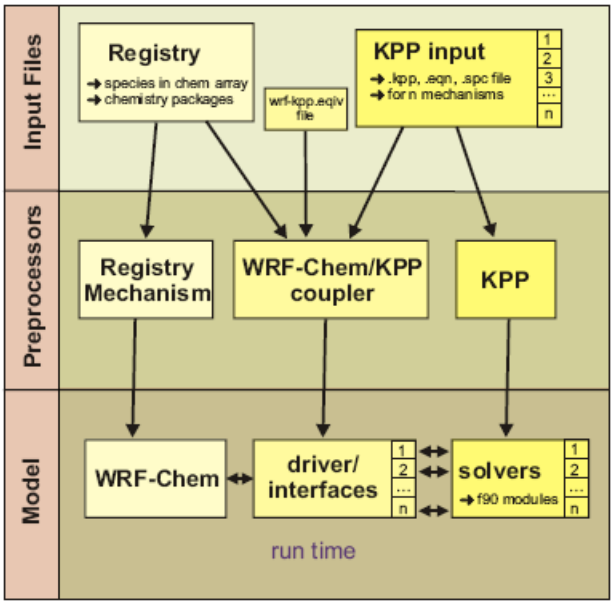

Fig. 6.1. Schematic showing the flow structure of KPP in the WRF-Chem model. Flowing down from the top, the Registry and KPP input data files (ASCII) are preprocessed into Fortran 90 and C code which is coupled to the WRF-Chem solvers.

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.

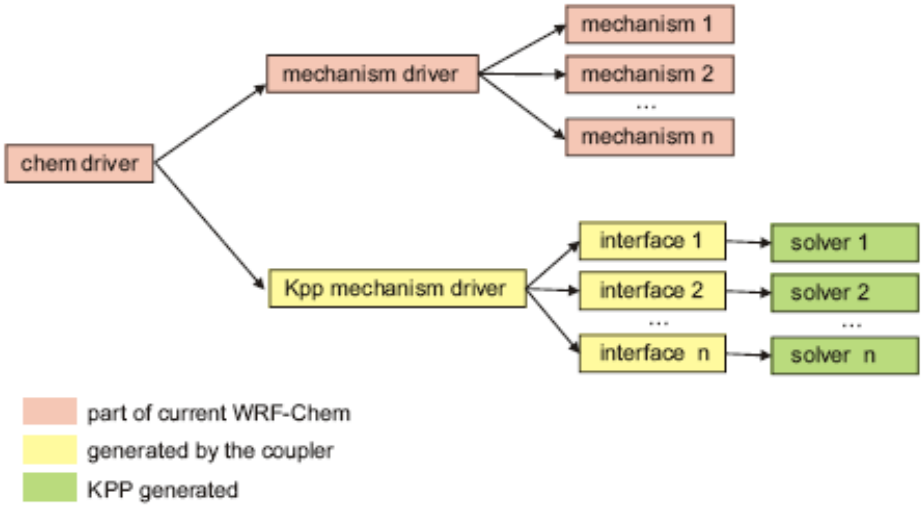

Figure 6.2: Schematic of the KPP call tree. Here the chem_driver routine in WRF-Chem calls a separate mechanism driver for each chemical mechanism implemented with KPP. This model configuration requires only one additional subroutine to be added to WRF-Chem so that the user can switch between the different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

6.7 Available integrators

References for the chosen integrator after compiling WRF-Chem with KPP can 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. More on the methodology to add additional integrators to the WKC will be discussed in a later section.

6.8 Adding 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 a mechanism:

- edit the registry file Registry.EM_CHEM to
    - add species to the chem array structure (if necessary), and
    - 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); and
- 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 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 NO_2 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 N_2O_5 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 are used. Instead pass down the data in the subroutine statements. And 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 3.8 of the WRF-Chem model. This guide is not intended to be an exhaustive report about all that is needed to set up and use the WRF-Chem model. While it does attempt to provide the latest and most accurate information about the configuration and running of the WRF-Chem model, errors or incomplete information may have been unintentionally 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. 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 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.

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.

7.2 WRF-Chem publications

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Appendix A: WRF-Chem Quick Start Guide

1. Compiling WRF-Chem

a. Download the WRF and then the WRF-Chem from the NCAR web site http://www2.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

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 global RETRO/EDGAR emissions data set and prep_chem_sources**

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

   b. Compile prep_chem_sources following the instructions in the README file

   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
      iv. ln –sf ../../../Prep_sources_chem_cptec_wrf/WRF-2008-07-15-000000-g1-volc.bin volc_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). In addition, the RETRO/EDGAR emissions are for just a few emitted species and the emiss_opt=5 is most often used for this data set.

   g. Run the convert_emiss program. It is acceptable if the program was compiled with the distributed memory (dmpar only) as it will run with one or multiple processors. The WRF input files that should be generated are: wrfinput_d01 (2a), the files from set (e.) above, and your WRF namelist.input.

h. Check whether the program successfully produced the emissions input (wrfchemi_d01 or wrfchemv_d01, wrffirechemi_d01 and wrfchemi_gocart_bg_d01). These should all be netcdf files if you specified that I/O form in your namelist.input file and so you can check the data with utilities like 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's 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/or 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. Visualizing the output can be done 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 NEI data set for domains located over the USA

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_2011

b. Modify the emiss_v03.F program file to correspond to your domain setup (see also chapter of the WRF-Chem Emissions Guide).

c. Compile emiss_v03.F
   i. There are examples provided at the beginning of the program like for the case when 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 binary 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 for anthropogenic emissions.) for each auxiliary input. Default output time interval from emiss_v03 is 3600 seconds. You should also set the correct emission input option (emiss_opt=3 for NEI emissions, or emiss_opt=5 for RETRO/EDGAR) for the anthropogenic emissions and your choice of chem_opt (see chapter 2 of the WRF-Chem Emissions Guide). In addition, the NEI emissions include smoke stack emissions so the input data will have a vertical dimension set with the kemit option.

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.

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 land-use 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 3.14. 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 (Chapter 3 of the WRF-Chem Emissions 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 Emissions 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 overwritten

   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 than 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.

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

Another tool for generating chemica lateral boundary conditions is available from NCAR/ACD and is called mozbc. The mozbc utility and is provided to the community at the NCAR/ACD website http://www.acd.ucar.edu/wrf-chem and along with the code the user can obtain MOZART model data for the dates and location of interest. The user is directed to the NCAR/ACD web site for the latest information regarding this utility.

Appendix B: 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 that 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

4) 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

5) 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.

6) 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:
   A. domains – the number of domains used in your WRF model
   B. exo_flnm – exo_coldens.nc
   C. wrf_dir – the directory where the associated wrfinput_d<nn> resides, and
   D. exo_dir – the directory in which the MOZART data file exists

7) 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)

8) 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 C: Using the Lightning-NOx Parameterization in WRF-Chem

The WRF-Chem model has a parameterization able to provide an estimate of the lightning-generated nitrogen oxides production (LNOx). The LNOx parameterization is based on the Price and Rind (1992, hereafter PR92) schemes with modifications based on Barth et al. (2012) and Wong et al. (2013). To determine LNOx, the lightning flash rate, the location (both horizontally and vertically), and the amount of NO produced per flash must be estimated. The lightning flash rate parameterization is located in the physics directory using module_lightning_driver.F, which is called from dyn_em/solve_em.F. The location and production of NO per flash parameterization is located in the chem directory using module_lightning_nox_driver.F, which is called from emissions_driver.F. The parameterization of lightning-generated NOx is valid for both parameterized convection and resolved convection, but different parameters may be used. Details on the parameters used in the namelist.input file are explained next.

Physics section:

To turn on the lightning flash rate parameterization in WRF, set the *physics* namelist option lightning option to one of the following values:

lightning_option	**Description**
1	PR92 based on maximum *w*; distributes flashes within dBZ > 20 For convection-resolved resolutions with microphysics turned on for reflectivity calculations.
2	PR92 based on 20 dBZ cloud top; distributes flashes within dBZ > 20 For convection-resolved resolutions with microphysics turned on for reflectivity calculations.
11	PR92 based on level of neutral buoyancy obtained from convective parameterization For convection-parameterized resolution using either GD or G3 cu physics options. Adjusted by areal ratio relative to dx=36 km (Wong et al., 2013), intended for use at 10 < dx < 50 km.

Setting the lightning option will produce four new 2D arrays: ic_flashrate, cg_flashrate both with units number per second, and ic_flashcount, cg_flashcount with units number of flashes, where ic and cg represent intra-cloud and cloud-to-ground, respectively. The ic_flashrate and cg_flashrate arrays are instantaneous output that can be used to diagnose the lightning flashrate and LNOx parameterizations. The arrays ic_flashcount, cg_flashcount accumulate the number of flashes during the simulation. To find the number of flashes between output times, simply subtract the flashcount array from the previous output time from the current output time to get number of flashes per dt (where

dt = time between output files).

Set the *physics* namelist option iccg_method to control the IC:CG ratio:

iccg_method	Description
0	Default method depending on lightning_option, currently all options use iccg_method=2 by default.
1	Constant everywhere, set with namelist options iccg_prescribed_num (numerator) and iccg_prescribed_den (denominator).
2	Coarsely prescribed 1995–1999 NLDN/OTD climatology based on Boccippio et al. (2001).
3	Parameterization by Price and Rind (1993) based on cold-cloud depth.
4	Gridded input via arrays iccg_in_num (numerator) and iccg_in_den (denominator) from wrfinput for monthly mapped ratios.

Additional namelist settings in the *physics* section are available for more detailed control of the parameterization:

Namelist Option	Description
iccg_prescribed_num	Prescribes numerator of IC:CG ratio. Used by iccg method=1,4 Default = 0
iccg_prescribed_den	Prescribes denominator of IC:CG ratio. Used by iccg method=1,4 Default = 1
iccg_in_num	Gridded array from the wrfinput file for monthly mapped IC:CG ratios. iccg_in_num is the numerator of the ratio. Gridpoints with iccg_in_num=0 and iccg_in_den=0 values use ratio defined by iccg_prescribed_num and iccg_prescribed_den. See more information below.
iccg_in_den	Gridded array from the wrfinput file for monthly mapped IC:CG ratios. iccg_in_den is the denominator of the ratio. Gridpoints with iccg_in_num=0 and iccg_in_den=0 values use ratio defined by iccg_prescribed_num and iccg_prescribed_den. See more information below.
lightning dt	Time interval (seconds) for calling lightning parameterization. Default uses model time step.
lightning start seconds	Start time for calling lightning parameterization. Recommend at least 10 minutes for spin-up.

flashrate factor	Factor to adjust the predicted number of flashes. Recommend 1.0 for lightning option=11 between dx=10 and 50 km. Manual tuning recommended for all other options independent for each nest.
cellcount method	Method for counting storm cells. Used by CRM options (lightning options=1,2). 0 = model determines method used. 1 = tile-wide, appropriate for large domains 2 = domain-wide, appropriate for single-storm domains
cldtop_adjustment	Adjustment from LNB in km. Used by lightning option =11. Default is 0, but recommends 2 km.

Gridded data of the IC:CG ratios written in the form of a ratio numerator and denominator (iccg_in_num and iccg_in_den) can be read from the wrfinput file to prescribe the IC to CG flash ratio. To get the gridded data into the wrfinput file, the user needs to interpolate the IC:CG ratio dataset to the WRF grid as a pre-processing step. The user also needs to provide his/her own dataset.

Chemistry section:

To emit LNOx, in the form of nitrogen oxide (NO), set the *chem* namelist option lnox_opt to one of the following values:

lnox_option	Description
1	Combined IC+CG single-mode vertical distributions (Ott et al., 2010). Outputs passive tracer array in addition to the NO source.
2	Separate IC, CG vertical distributions following DeCaria et al. (2000). In addition to providing a source to NO, outputs two passive tracer arrays lnox_ic and lnox_cg.

Additional *chem* namelist settings are available for more detailed control of the parameterizations:

Namelist Option	Description
N_IC	Moles of NO emitted per IC flash. For lnox opt=1, the total number of moles NO per flash is the weighted average based on the calculated IC:CG ratio of N_IC and N_CG. Default is 500 moles.
N_CG	Moles of NO emitted per CG flash. For lnox opt=1, the total

	number of moles NO per flash is the weighted average based on the calculated IC:CG ratio of N_IC and N_CG. Default is 500 moles.
lnox_passive	Set to .true. to emit passive tracers only. Set to .false. to emit both NO and passive tracer. Default = .false.
ltng_temp_upper	Temperature (C) of upper peak of LNOx vertical distribution for IC lightning (used by lnox opt=2).
ltng_temp_lower	Temperatures (C) of lower peak of LNOx vertical distribution for both IC and CG lightning (used by lnox opt=2).

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