Best Practices for Applying WRF-Chem 3.8.1

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As well as many other WRF-Chem developers

Overview

- General Considerations
- Highlight WRF-Chem Options
- Advise From Developers
  - NOAA/ESRL
  - NCAR/ACOM
  - PNNL
  - Others

General Considerations

Ask yourself

- **Am I following the WRF best practices for my domain?**
- **What chemistry option should I use for my project?**
  - Research or forecasting?
    - What is my computational power?
    - How quickly do I need a solution?
  - What horizontal and vertical resolution may be required to resolve important features?
    - Meteorology and chemistry might be different
  - Do I have appropriate emissions inventory (if necessary)?
    - Speciation for chemical mechanism correct?
    - Adequate spatial and temporal resolution?

General Considerations

- **What chemistry option should I use for my project?**
  - What process do I want to simulate?
    - Dispersion?
      - may include any tracer (dust, smoke, hazardous constituents,…), computing costs from a little more to about 2x plain WRF run
    - Air Quality?
      - usually requires gas-phase chemistry as well as aerosol modules, computing costs more than 5x plain WRF run with little upper limit
    - Fully interactive weather/climate and chemistry/aerosols?
      - Interaction of aerosols with radiation (direct and resulting semi-direct effect) could be anywhere between 2x to more than 100x plain WRF run;
      - indirect effect 10x to more than 100x plain WRF run.
  - Do I have appropriate initial and boundary conditions?
    - Spin-up time for chemistry (enough computational power)?

General Considerations

Special interest for air quality and weather forecasting: aerosols

- Aerosols may have a significant impact on weather forecasts through:
  - interaction with radiation (sometimes also called “direct effect”)
  - microphysics (sometimes also called “indirect effect”)

- Aerosols may also impact meteorological data assimilation

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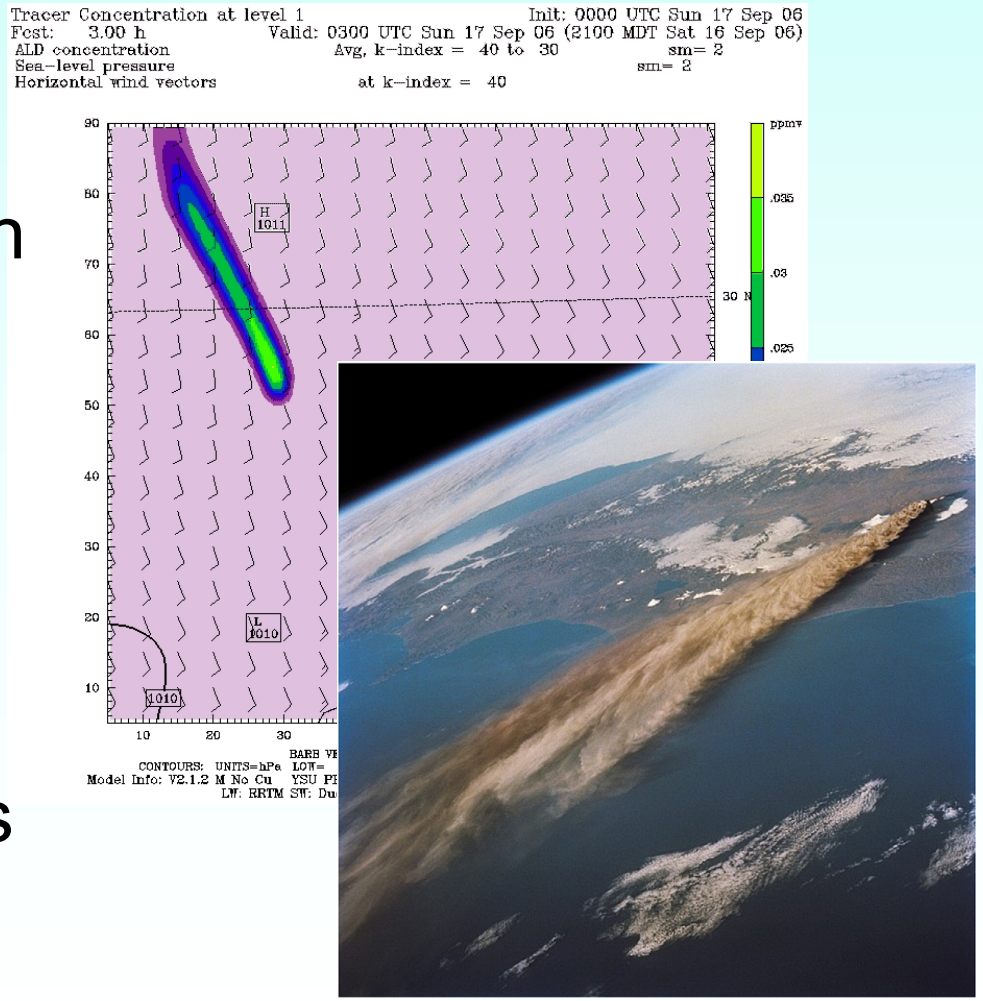
Available Aerosol Modules

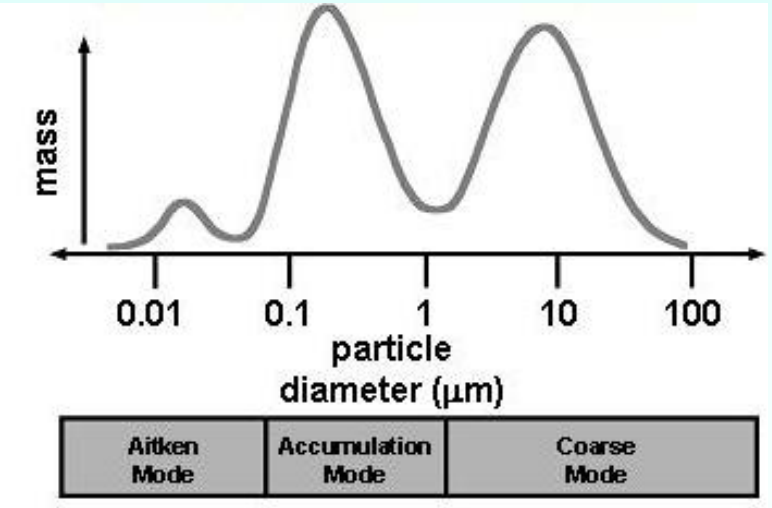
(1)Tracers: Dust, Smoke, Volcanic ash

(1) Bulk: Sections for dust and sea salt, otherwise total mass for a few species



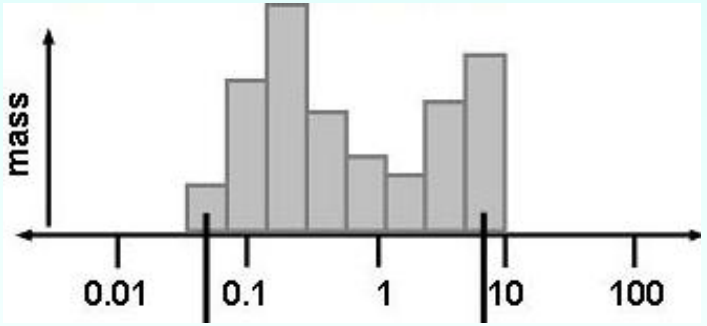
Available Aerosol Modules

(3) Modal



(4) Sectional

composition
sulfate
nitrate
ammonium
chloride
carbonate
sodium
calcium
other inorganics
organic carbon
elemental carbon



Modal and sectional schemes may be too expensive in operational NWP settings – but important in research and for air quality forecasting

Dust only: Consideration

- Dust emissions has a strong dependence on:
  - soil moisture
  - erodable fraction
  - Dust not included from other sources (e.g., roads, farms)

- dust_opt=3, or 4 are currently preferred to dust_opt=1, since they include more updated physics

Dust only: Consideration

- dust_opt=4 has not be as well tested
  - dust_schme = 1 Shao (2001)
  - dust_schme = 2 Shao (2004)
  - dust_schme = 3 Shao (2011)
    - simplification of dust_schme =2

Passive Tracers: Consideration

- Passive tracers can be run separately or along with chemistry
  - Tracer initialization and BCs: module_input_tracer.F
  - When using tracer_opt with WRF-Chem, tracers are advected (chem_adv_opt in namelist.input), vertically mixed (vertmix_onoff) and also mixed by cumulus parameterization (chem_conv_tr). Deposition and emission could be included with some code modification.

- Old tracer option (chem_opt=13 to 15) to be removed in future release

- Passive tracer options for greenhouse gases (chem_opt=16, 17)
  - no chemical reactions considered
  - Includes anthropogenic emissions, and biospheric fluxes of carbon dioxide CO_2 and methane (CH_4)

Options for Gas Phase Chemical Mechanism

- **Regional Acid Deposition Model, 2nd generation (RADM2)**
- **Regional Atmospheric Chemistry Mechanism (RACM)**
- **RACM - Mainz Isoprene Mechanism (RACM-MIM)**
- **RACM - Earth System Research Laboratory (RACM-ESRL), *updated RACM-MIM***
- **Carbon-Bond Mechanism version Z (CBM-Z)**
- **Carbon-Bond Mechanism (CB05)**
- **Model of Ozone and Related Chemical Tracers (MOZART)**
- **Statewide Air Pollution Research Center (SAPRC99)**
- **Common Reactive Intermediates gas-phase Mechanism (CRIMech)**

different implementations, coupled to different aerosol schemes and aqueous chemistry, suitable for different applications ranging from regional air quality to global atmospheric chemistry simulations

Comments About Chemistry Options in WRF-Chem

- **RADM2 based options:**
  - Most computationally efficient options for ozone chemistry
  - for air quality modeling, not all biogenic VOCs are included

- **RACM based options:**
  - more updated version of RADM, more biogenic VOCs are included, more coupling options
  - When coupled with modal aerosol and Secondary Organic Aerosol (SOA) module – is the top of the line setup for real-time air quality forecasting (at ESRL)

- **Carbon Bond based options:**
  - Widely used for research applications with sectional aerosol module
  - Studies using CAM5 physics and modal aerosols
  - Warning: CBM4 and NMHC9 are not yet fully functional in WRF-Chem

Comments About Chemistry Options in WRF-Chem

- **MOZART based options:**
  - Used in some of global atmospheric chemistry models (NCAR, GFDL)
  - Can run alone, or with GOCART for gas-phase experiments
  - Run with MOSAIC aerosols for global aerosol studies

- **SAPRC99 based options:**
  - Widely used for research applications with sectional aerosol module and VBS for organic aerosols

- **CRIMech based options:**
  - Very detailed chemistry mechanism based on Master Chemical Mechanism
  - Suitable for detailed chemistry analysis; If you have anthropogenic emissions and measurements to run and evaluate this scheme
  - Computationally very expensive!
  - Geosci. Model Dev. Discuss., 7, 871–929, 2014

Comments About Chemistry Options in WRF-Chem

KPP in WRF-Chem

Kinetic PreProcessor (KPP) reads chemical reactions and rate constants from ASCII input files and automatically generates code for chemistry integration using the Rosenbrok solver

Advantages:

No KPP for aerosols!

- less time consuming than manual coding
- less error prone
- numerically efficient
- flexibility in updating mechanism with additional species and equations
- suitable for adjoint code development

References:

• Damian, V., et al. (2002), The kinetic preprocessor KPP - a software environment for solving chemical kinetics, *Comput. Chem. Eng., 26(11), 1567-1579.*

• Sandu, A., and R. Sander (2006), Technical note: Simulating chemical systems in Fortran90 and Matlab with the Kinetic PreProcessor KPP-2.1, *Atmos. Chem. Phys., 6, 187-195.*

• Verwer, J., Spee, E., Blom, J. G., and Hunsdorfer, W. (1999), A second order Rosenbrock method applied to photochemical dispersion problems, *SIAM Journal on Scientific Computing, 20, 1456–1480*.

• www.mpch-mainz.mpg.de/~salzmann/my_home/sub/wkc.html

Chemistry Mechanisms

Chemical mechanisms	*Fixed versions*	*KPP*	*Coupled aerosol schemes*	*Indirect effect*
RADM2	Yes	Yes	MADE/SORGAM, GOCART	MADE/SORGAM with aqueous phase chemistry
RACM	-	Yes	MADE/SORGAM, GOCART	MADE/SORGAM with aqueous phase chemistry
RACM-MIM	-	Yes	-	-
RACM-ESRL	-	Yes	MADE/SORGAM, MADE/SOA_VBS	-
CBM-Z	Yes	Yes	MADE/SORGAM, MOSAIC, MAM	4bin/8bin with aqueous phase chemistry; CAM5 -MAM and aqueous phase chemistry
CB05	-	Yes	MADE/SORGAM	with aqueous phase chemistry
MOZART	-	Yes	GOCART, MOSAIC	-
SAPRC99	-	Yes	MOSAIC	8bin with aqueous phase chemistry
CRIMech	-	Yes	MOSAIC	4bin/8bin with with aqueous phase chemistry

Additional Considerations

- Photolysis: Madronich TUV photolysis is the only option that is aware of parameterized convection.
  - FAST-J and FTUV photolysis are not impacted by parameterized convection
- Direct effect: radiation is impacted by aerosol when using:
  - Goddard short wave,
  - RRTMG (both short and long wave)
  - CAM5
- Not all microphysics can be used with indirect effect.
  - Lin et al and Morrison are needed for indirect effect
    - Can use only the modal and sectional approaches.
  - Only double moment for resolved clouds (Qc) when used with WRF-Chem
    - These schemes in WRF (not WRF-Chem) have cloud droplet number (qndrop) as single moment.
  - Thompson aerosol aware microphysics (mp_phys=28) uses water and ice friendly aerosols (a simple option for aerosol indirect feedback)

Additional Considerations

- For now, indirect effect needs aqueous phase chemistry to be turned on at the same time

- Don’t use too many processors when running real.exe. Some systems prefer a smaller number of nodes.

- Check for consistency between the netCDF file attributes with all input data files
  - e.g., mminlu should be the same for: wrfinput, wrfbdy, wrffdda, wrfchemi, wrffirechemi, wrfbiochemi, exo_coldens, and wrf_seasons)

Anthropogenic Emissions

- One can generate anthropogenic emissions input data using any desired methodology
  - Most familiar tools work with RETRO/EDGAR or NEI emissions data sets
    - PREP_CHEM_SRC (Freitas et al., 2011) V1.5 includes HTAP emissions
    - Emiss_v03
  - Tools available from NCAR/ACOM
    - anthro_emiss
      - works with data on lat/lon grid
    - Aircraft emissions
  - Some groups use Sparse Matrix Operator Kernel Emissions (SMOKE) model to generate input emissions

Attributes in a wrfchemi netcdf file

```
:GRID_ID = 1 ;
:PARENT_ID = 0 ;
:I_PARENT_START = 1 ;
:J_PARENT_START = 1 ;
:PARENT_GRID_RATIO = 1 ;
:DT = 45.f ;
:CEN_LAT = 40.00001f ;
:CEN_LON = -97.f ;
:TRUELAT1 = 33.f ;
:TRUELAT2 = 45.f ;
:MOAD_CEN_LAT = 40.00001f ;
:STAND_LON = -97.f ;
:POLE_LAT = 90.f ;
:POLE_LON = 0.f ;
:GMT = 0.f ;
:JULYR = 2013 ;
:JULDAY = 154 ;
:MAP_PROJ = 1 ;
:MAP_PROJ_CHAR = "Lambert Conformal" ;
:MMINLU = "MODIFIED_IGBP_MODIS_NOAH" ;
:NUM_LAND_CAT = 20 ;
:ISWATER = 17 ;
:ISLAKE = -1 ;
:ISICE = 15 ;
:ISURBAN = 13 ;
:ISOILWATER = 14 ;
```

You can use the NCO tools to do many different operations with netcdf files

e.g. Change attributes – integers:

ncatted -a NUM_LAND_CAT,global,o,i,20 “file”

To rename dimensions, variables, and attributes in a netCDF file use **ncrename**

For the manual check http://nco.sourceforge.net/

Biogenic Emissions

- Generate emissions input data using any desired methodology
  - Preprocessor tools available
    - PREP_CHEM_SRC (Freitas et al., 2011)
    - MEGAN (Guenther et al., 2012)

- Model has several options once static data is produced
  - Gunther,
  - BEIS,
  - MEGAN

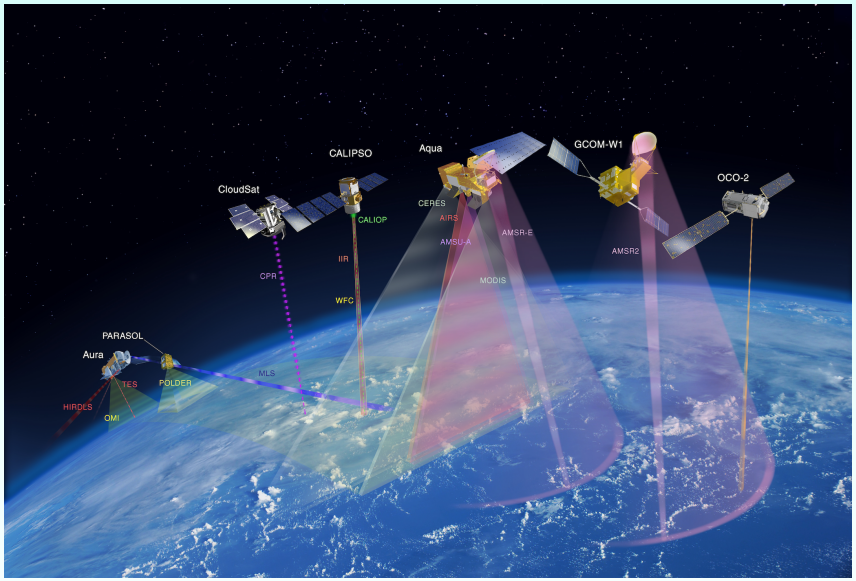
- Recommend MEGAN (Model of Emissions of Gases and Aerosols from Nature)
  - Estimate emission of VOCs, NOx and CO from vegetation
    - Driving variables include land cover, Leaf Area Index, weather and atmospheric chemical composition
    - The land cover differs between MEGAN and WRF at this time.

Fire Emissions

- Biomass burning – use any tool available
  - Two choices available from developers:
    - PREP_CHEM_SRC (Freitas et al. 2011)
    - FINN (Wiedinmyer et al., GMD, 2011)
  - Fire location based upon satellite observations
    - MODIS
    - WF-ABBA

Wildfire Satellite Data

- Moderate-Resolution Imaging Spectroradiometer (MODIS) instruments on NASA's Aqua and Terra satellites.
  - Daily global 1km fire data
  - Available in real-time
    - https://earthdata.nasa.gov/data/near-real-time-data/firms
  - Data archives can be found online
  - Reads text (.txt) data files



- GOES, MET, MTSAT
  - Automated Biomass Burning Algorithm (ABBA) fire products

    (http://wfabba.ssec.wisc.edu)
  - Derived from radiances from bands 1 (visible), 2 (3.9 micron), and 4 (11 micron)
  - Available in real time (GOES: North & South America domain, MET-9: Africa, MTSAT: Austrailia)

Fire Emissions

- PREP_CHEM_SRC
  - Needs user provided satellite data files
  - Can be used in real time based upon user download ability
  - Can be used with archived observation data
  - Speciates emissions for RADM/RACM chemical mechanism
  - Provides binary intermediate file that needs to be converted to WRF input

- FINN
  - Products are available in near real-time (~ 1 day delay)
  - Smoldering emissions are expected as input (follows PREP_CHEM_SRC). Thus one needs to set:
    - **scale_fire_emiss** controls separation between smoldering and flaming emissions (Set to .true.)
      - Assumes the total emission strength is provided
    - **biomass_burn_opt** must be >= 2
  - Archived for previous years (2002 – 2013)
  - Speciate emissions for MOZART, SAPRC99 and GEOS-Chem
  - Utility program needed to convert data for use with WRF-Chem
  - http://www.acd.ucar.edu/acresp/forecast/fire-emissions.shtml

- You can bypass all the emission tools (emiss_v04, convert_emiss, prep_chem etc.) and create your emission files (anthropogenic or any other) by using Matlab, IDL, Python or other tools;

- The emissions files have to follow the common format (e.g. netcdf) that can be read by WRF! Check wrfinput* file e.g.;

- The WRF code (take a look at share/input_wrf.F) has some checks to make sure users read correct input data into the model. As long as you have correct attributes in your emission file in netcdf format, the model can read it.

- To learn more how the emission files are read by WRF-Chem, check also share/mediation_integrate.F

Chemical Boundary Conditions

- Default BCs not recommended due to poor upper troposphere/stratosphere representation
- Can use any method to modify the lateral boundary conditions and initial fields
  - User needs to consider the chemistry moving from GCM to their particular WRF simulation
- Available lateral boundary condition modifying routines:
  - wrfchembc
  - mozbc (Recommended), MOZART data available for download
  - Set have_bcs_chem = .true.
- Available ways to modify chemical Initial conditions
  - Recycle chemistry from previous simulation (auxinput12)
  - mozbc
    - Uses MOZART, or MACC data
  - Set chem_in_opt= 1
- Upper boundary condition
  - Initial profile does not adequately describe stratosphere

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Advise from NOAA/ESRL

- Chemical data assimilation – Not yet officially released
  - NCEP's Grid Point Statistical Interpolation (GSI, 3DVAR)
  - Shows significant improvement in forecast
- Ensemble Kalman Filter (enKF) has also been used, adjoint in development
- Email WRF-Chem help if:
  - You want to get in contact with developers
  - Find out the do's and do not's

Advise from NOAA/ESRL

- Focus: Research and real time forecasts; Collaboration inside ESRL
- In practice:
  - Large domain – much bigger than location, or area of interest
  - Use more detailed MEGAN biogenics
  - Use Global Chemical Model data for boundary conditions (RAQMS, MACC, etc.)
  - Use RADM/RACM chemistry with MADE/VBS
  - Use Grell-Freitas Cumulus parameterization
  - Use RRTMG radiation
  - Cycle chemistry rather than restart

- When building a nested domain
  - Use NDOWN first
    - computationally significantly cheaper
    - Build emissions an debug each domain individually
  - Using restart may require some debugging for each chemistry option
    - All fields are not in the restart files. Need to add/remove on a case by case basis

Advise From NCAR/ACOM

- Focus: Research MOZART chemistry, lightning and several other emission sources

- MOZART User's Guide
  - Describes options related to using MOZART in WRF-Chem
  - http://www.acd.ucar.edu/wrf-chem/MOZART_UsersGuide.pdf

- Also provide several tools for users
  - Biogenic emissions: MEGAN
  - Anthropogenic emissions: anthro_emiss, aircraft
  - FINN fire emissions

Advise from PNNL: Best Practices for MOSAIC

Chem_opt=8 (CBM-Z coupled with MOSAIC) is the most used and tested version of MOSAIC, but users need to be aware of its limitations that depend on the application

- Interstitial aerosols using 8 size bins, but no cloud-aerosol interactions or wet removal
  - *No wet removal is an important sink that is neglected, so this version should be used only for cases with little precipitation*
- Other MOSAIC options include more detailed chemistry and species (Ca, CO_3, DMS, MSA) that will only be imporant for certain applications and locales
  - *Ca and CO_3 used for heteorgeneous reactions associated with dust and HNO_3.*
  - *DMS (biological emission) and MSA (aerosol product) useful for more complete representations of SO_4 for marine applications.*

  ] users need to define emissions
- Does not include SOA, so simulations will likely underpredict total organic matter

Chem_opt=10 is more complete and more appropriate for more applications

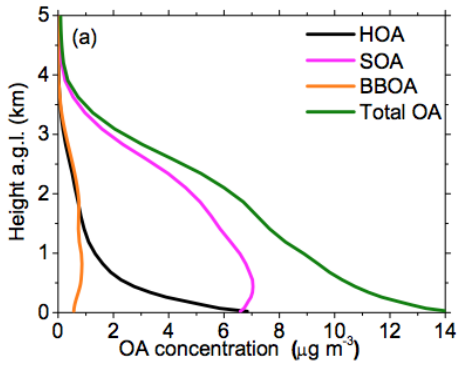
- Includes both interstitial and cloud-borne aerosols using 8 size bins, cloud aerosol interactions, aqueous chemistry, and wet removal, but still lacks SOA

4 size bin versions of these 2 options are available that reduce computational cost. If users are interested in only PM mass they may be viable options. But there may be differences in behavior of 4 and 8 size bins when computing effects of aerosols on radiation and clouds that are not fully tested.

Advise from PNNL: “Best” version of MOSAIC

Chem_opt=198 (SAPRC99 coupled with MOSAIC) is the most complete version available in the repository.

- Interstitial aerosols using 4 size bins, but no cloud-aerosol interactions or wet removal
- Volatility Basis Set (VBS) approach for SOA
- Includes Ca and CO_3 for heteorgeneous reactions associated with dust and HNO_3



Shrivastava et al., ACP, 2011

But the best / more complete versions are not yet in the public version of WRF-Chem:

- With 8 size bins

+ ⇦ *Fast et al., ACPD, 2014*

- With cloud-borne aerosols, cloud-aerosol interactions, aqueous chemistry, wet removal (shrivastava et al.,)

+ ⇦ *Shrivastava et al., JGR, 2013*

- With cloud-borne aerosols, cloud-aerosol interactions, aqueous chemistry, wet removal for both resolved clouds and parameterized shallow and deep convective clouds

+ ⇦ *Berg et al., GMDD, 2014*

- VBS that treats SOA as non-volatile, non-absorbing semi-solid and includes first-order gas-phase fragmentation reactions

⇦ *Shrivastava et al., JGR, 2013*

Contact PNNL investigators for packages not in public version

Considerations for Cloud-Aerosol Interactions

- PNNL's implementation of cloud-aerosol interactions have been done in either the Lin microphysics (it was modified to a 2-moment approach) or the Morrison microphysics
  - *Recommend Morrison scheme*
- Care must be taken in drawing conclusions regarding impact of cloud-aerosol interactions on other quantities (e.g. precipitation, cloud properties) based on the domain size
  - *For "large" grid spacings ($\Delta x > 10$ km) parameterized convection becomes relatively more important (depending on the region), so those simulations will be "incomplete"*
  - *If the user wants to focus on cloud-aerosol interactions, suggest $\Delta x < 5$ km or less*
- **Most common mistake** is taking the differenece of WRF (no chemistry) and a simulation using MOSAIC or MADE/SORGAM with cloud-aerosol interactions, and calling that the "indirect effect". That is not the case in the strict sense of the definition.
  - *Both microphysics schemes are only double moment for Qc when using WRF-Chem*
  - *In that case, could run the same cloud-aerosol interaction configuration with lower aerosol concentrations (either prescribing, lowering emissions, or lowering background values)*
  - *Contact WRF-Chem help, or PNNL developers for assistance*
- **Another common mistake** is that users are not aware that the autoconversion scheme changes between progn=0 & 1 when using Lin microphysics, so there is another factor affecting the results besides changing the inclusion of aerosols

CAM5 Physics Package: Recommended Settings

To run CAM5 physics in WRF that is **closest to the global CAM5 model**, use mp_physics=11, cu_physics=7, shcu_physics=2, bl_pbl_physics=9, chem_opt=503 (CBMZ_CAM5_MAM3)

- Morrison-Gettleman (M&G) microphysics, Zhang-McFarlane deep convection, UW shallow convection, UW boundary layer, and Modal Aerosol Module (MAM)
- Recommend using RRTMG radiation options, which are also used in global CAM5
- Most WRF surface layer schemes work with CAM5. **Note:** the Community Land Model (CLM, sf_surface_physics=5) has been ported to WRF, but this version is not the same as in CAM5 and has not been tested when coupled to CAM5 physics in WRF-Chem.
- CBM-Z photochemistry is used to couple with MAM. **Note:** the global CAM5 model either uses prescribe oxidants or MOZART. PNNL has coupled MAM with MOZART, but this version is not in repository.
- For emissions use, emiss_opt=9, emiss_input_opt=102 or 104.
  - *102 uses RADM/SORGAM type of emissions then converts them to what CBM-Z and MAM needs. On-line sea-salt and dust emissions can be used in this case.*
  - *For 104, the user will have to create CBM-Z and MAM specific emission species that include prescribed sea-salt and dust emissions.*

Do not switch CAM5 options with other WRF options. The M&G microphysics assumes prognostic aeorsols from MAM when computing cloud-aerosol interactions.

CAM5 Physics Package: Alternative

Depending on the application, one can use CBMZ_CAM5_MAM (chem_opt = 501):

- This version does not include cloud-aerosol interactions and wet scavenging, and runs somewhat faster since cloud-borne aerosols are not included
- In this case, prescribed aerosols are used in the Morrison & Gettleman microphysics
- This also gives users more freedom to mix and match WRF and CAM5 physics, for example:
  - *One could use Zhang-McFarlane deep convection scheme with WRF options for all other parameterizations. This is useful to compare performance of parameterizations in a series of sensitivity simulations.*
  - *Morrison & Gettleman microphysics should only be coupled to a TKE-based boundary layer scheme*

Depending on the application, one can use no chemistry (chem_opt = 0):

- In this case, users can use the meteorological CAM5 physics options without chemistry or aerosols

Note: The 7-mode aerosol model MAM7 does not work in WRF-Chem – it is a placeholder for now. Only the 3-mode version has been tested.

Note: gaschem_onoff, aerchem_onoff, wetscav_onoff, cldchem_onoff, vertmix_onoff switches have not been tested with CAM5 physics options, so use with caution to verify output

Advise For CRIMech

- Be careful about when switching to CRIMech!
  - Need to get the non-methane volatile organic compounds (NMVOC) gas-phase emissions right
  - Added the "ecrimech" and "ecrimechtno" namelist options
    - provide the right emitted species, but the emission files were generated using our own tool rather than the emissions tool provided with WRF-Chem.
  - Table 5 in their publication provides the VOC fractionation
    - Also a map for emissions to CBM-Z
    - S. Archer-Nicholls, D. Lowe, S. Utembe et al. , GMD, 2014
  - Contact Univ. of Manchester for more information/help

- MEGAN recommended for biogenic emissions
  - the older Guenther scheme to work for CRIMech too, but the speciation in MEGAN species is better.

Advise For CRIMech

- Getting the chemical boundary conditions right is important.
  - MOZART provides the quickest solution
  - The speciation is listed in Table 6.
    - S. Archer-Nicholls, D. Lowe, S. Utembe et al. , GMD, 2014
- Otherwise the standard settings for radiation schemes, etc., should work
- A word of warning about methane
  - We have included methane as a reactive species in our scheme, but haven't included it in our emitted species
    - With a large domain there's enough at the boundaries, depositional losses are relatively small
    - For smaller sized domains is would be wise to either include emissions of methane or to modify the deposition routines (and chemical mechanisms) to stop the loss terms.

Final Words of Advise

- Contact WRF-Chem help, or the developers directly if you want specifics regarding any particular feature in WRF-Chem

- Appendix

Other Resources/Information

Publication list online: https://ruc.noaa.gov/wrf/wrf-chem/References/WRF-Chem.references.htm

Please use this list to find papers to read and cite.

- Please send us your publications too!
- Inter-journal special issue on WRF-Chem; Geoscientific Model Development (GMD) and Atmospheric Chemistry and Physics (ACP)
  - GMD is restricted to WRF-Chem community version,
  - ACP open to all WRF-Chem applications
- Add any older GMD and ACP WRF-Chem articles to special issue as well, can be done even if already in other special issues

- WRF-Chem tutorials and presentations
- WRF repository additions
  - Please make it easy for us If you plan to provide development work back to the community, (provide documentation, follow coding standards)
- Check WRF-Chem web page for model information

  https://ruc.noaa.gov/wrf/wrf-chem/

- Definitions
  - DMS = Dimethyl sulfide $(CH_3)_2$
  - MSA = Methanesulfonic Acid
    - forms from oxidation of DMS
  - Ca = Calcium and Carbonate particles (CO_3) are both found in mineral dust.
  - HNO_3 = Nitric Acid
  - SOA = Secondary Organic Aerosols
  - CAM5 = NCAR Community Atmosphere Model version 5

Running WRF-Chem with the MOZART chemistry options

MOZART

MOZART-GOCART

MOZART-MOSAIC

Thanks to those who contributed their namelist options and advice:

Rajesh Kumar, Christoph Knote, Megan Bela, Gabriele Pfister, Alma Hodzic, Mary Barth

Introduction

MOZART User's Guide

http://www.acd.ucar.edu/wrf-chem/MOZCART_UsersGuide.pdf

Describes options to select when running with the MOZART-GOCART chemical option, chem_opt = 112

Is being updated to describe MOZART-MOSAIC chemical option

MOZART appropriate for

simulations of pure gas-phase

MOZART-GOCART appropriate for

simulations of months-years,

simulations focused on trace gas chemistry

MOZART-MOSAIC appropriate for

short-term simulations or aerosol-climate studies

detailed analysis of trace gas and aerosol processes

Emissions

- Anthropogenic Emissions:
  - **emiss_opt = 7/8/10**

    for gases only/gases & GOCART/gases & MOSAIC
  - Maps hydrocarbons to MOZART mechanism
- Biogenic Emissions: **bio_emiss_opt = 3**
  - MEGAN biogenic emissions with speciation to MOZART
- Fire Emissions
  - Can use the fire plumerise module
  - **scale_fire_emiss** controls whether the total fire emission strength is split into smoldering and flaming parts
  - If FINN is used for fire emissions, then the total emission strength is provided and **scale_fire_emiss** should be **.true**.
  - **biomass_burn_opt** must be >= 2

Emissions

- Aircraft Emissions: **aircraft_emiss_opt = 1**
  - SO_2, NO, CO and CH_4 only; applied every time step
  - **kemit_aircraft** = number of model levels to apply aircraft emissions
  - Need wrfaircraftchemi_* input files for each domain

Lightning-NOx Emissions

- Lightning NO Emissions
  - Namelist variables in both *phys* and *chem* sections

phys section

  - **lightning_option** sets what method to use and will produce 4 new 2D arrays: ic_flashrate, cg_flashrate, ic_flashcount, cg_flashcount
  - **iccg_method** sets how to get IC to CG ratio (more details in User's Guide: http://ruc.noaa.gov/wrf/WG11/Users_guide.pdf)
  - **lightning_dt** = time interval for calling lightning parameterization, should be a multiple of model time step
  - **lightning_start_seconds** = start time for calling lightning parameterization (recommend at least 10 minutes)
  - **flashrate_factor** = factor to multiply predicted number of flashes (recommend set to 1, then adjust to improve result)

Emissions

- Lightning NO Emissions (cont'd)
  - Namelist variables in both *phys* and *chem* sections

  chem section

  - **lnox_option** sets what method to vertically distribute NO emissions (see User's guide)
  - **N_IC, N_CG** sets number of moles of NO emitted per IC or CG flash
  - **lnox_passive = .true.** Emits only passive tracers. Chemistry will not be affected. (set to false to emit to NO mixing ratio)
  - **ltng_temp_upper, ltng_temp_lower** sets vertical location of maximum NO emissions for IC and CG flashes in the cloud-resolving lightning-NOx scheme
  - http://ruc.noaa.gov/wrf/WG11/Users_guide.pdf

Photolysis, Dry Deposition, etc

- Photolysis Rates: **photo_opt = 3**
  - Fast TUV code, which reads in climatological O3 and O2 overhead columns instead of using a fixed value
  - Need additional input file that can be downloaded from NCAR: http://www.acd.ucar.edu/wrf-chem/download.shtml
- Dry Deposition: **gas_drydep_opt = 1**
  - Wesely scheme requires additional input files for seasonal changes. Fortran code to make these files can be downloaded from NCAR.
- CH_4, H_2, and N_2O mixing ratios are held constant at values specified in initial conditions

Upper Boundary Condition

- Upper boundary conditions for selected trace gases
  have_bcs_upper = .true.
  - O_3, NO, NO_2, HNO_3, CH_4, CO, N_2O, N_2O_5 mixing ratios from model top to tropopause overwritten
  - **fixed_upper_bc** controls pressure level of where trace gases are set to a climatological fixed value (between model top and **fixed_upper_bc** pressure level, default = 50 hPa)
  - Between **fixed_upper_bc** pressure level and tropopause values are relaxed between WRF-Chem and climatology
  - Two input data files needed:
  - clim_p_trop.nc is a climatology of tropopause levels
  - File containing the stratosphere mixing ratios. Name is set by **fixed_ubc_inname** Climatologies from WACCM are available
  - Additional output of tropopause model level, pressure, height: tropo_lev, tropo_p, tropo_z

http://www.acd.ucar.edu/wrf-chem/processors.shtml

Aerosols

- GOCART: Bulk aerosol scheme
- MOSAIC 4-bin: Sectional scheme
  - with simple SOA parameterization
  - with SOA volatility basis set parameterization and explicit aqueous-phase

Wet Scavenging

- Wet scavenging for resolved precipitation that is determined by the cloud physics schemes

  MOZART uses Neu and Prather (2012) scheme for trace gases: **wetscav_onoff = 1**
- works with only 3 cloud physics schemes: Morrison, Thompson, and CAM scheme.WRF-Chem V3.8.1 will also have WSM6 double-moment

- second bullet point: scavenging parameters for individual gases (Henry's Law coefficients, fractional retention in mixed-phase precipitation, ice deposition) can be set in chem/module_mozcart_wetscav.F
- convective:
- WRF-Chem V3.8.1 has aqueous chemistry, set conv_tr_aqchem = 1

- Convective wet scavenging **conv_tr_wetscav = 1**
  - Use with Grell convection scheme
  - WRF-Chem V3.8.1 will also have aqueous chemistry, set **conv_tr_aqchem** = 1

Special Output

- By setting up “tracking output” can get vertical profiles of meteorological and chemical species at prescribed times and lat/lons written to a special output file: **wrfout_track_d<nn>**
  - **track_loc_in** = number of track locations in input file
  - **wrfinput_track.txt** is input file containing time, latitude, longitude points
  - For **track_loc_in > 0**, get z, p, t, u, v, w, alt, qcloud, qrain, qice, qsnow, qgraup, and qvapor
  - **track_chem_num** and **track_chem_name** need to be set. Total number of chemical species must be <= 100.
  - Example on next page

Tracking Output Example

```
&domains
track_loc_in = 2,
/
&chem
track_chem_num = 2
track_chem_name = ‘co’, ‘o3’,
/
```

wrfinput_track.txt contains, for example:
201008-10_00:12:00 41.450 -87.300
201008-10_00:36:00 41.510 -87.390

The indicated output times need to be given in multiples of model time steps or else no output is produced.

Fortran format for the lines in the wrfinput_track.txt file is
(A19,1X,F7.3,1X,F7.3)
Latitudes and longitudes use WRF conventions as shown above.

MOZART/GOCART namelist example

```
&dynamics
rk_ord                  = 3,
w_damping               = 1,
diff_opt                = 1,
km_opt                  = 4,
base_temp               = 290.
damp_opt                = 0,
zdamp                   = 5000.,  5000.,  5000.,
dampcoef                = 0.01,   0.01,   0.01
diff_6th_opt            = 0,
diff_6th_factor         = 0.12,
khdif                   = 0,    0,    0,
kvdif                   = 0,    0,    0,
non_hydrostatic         = .true., .true., .true.,
moist_adv_opt           = 2,    0,    0,
scalar_adv_opt          = 2,    0,    0,
chem_adv_opt            = 2,    0,    0,
tke_adv_opt             = 2,    0,    0,
time_step_sound         = 4,    4,    4,
h_mom_adv_order         = 5,    5,    5,
v_mom_adv_order         = 3,    3,    3,
h_sca_adv_order         = 5,    5,    5,
v_sca_adv_order         = 3,    3,    3,
/

&physics
mp_physics              = 8,    3,    3,
progn                   = 0,
ra_lw_physics           = 4,    1,    1,
ra_sw_physics           = 4,    1,    1,
radt                    = 30,   30,   30,
sf_sfclay_physics       = 1,    1,    1,
sf_surface_physics      = 2,    2,    2,
bl_pbl_physics          = 1,    1,    1,
bldt                    = 0,    0,    0,
cu_physics              = 1,    1,    0,
cudt                    = 0,    5,    5,
surface_input_source    = 1,
num_soil_layers         = 4,
sf_urban_physics        = 0,    0,    0,
mp_zero_out             = 2,
mp_zero_out_thresh      = 1.e-8,
maxiens                 = 1,
maxens                  = 3,
maxens2                 = 3,
maxens3                 = 16,
ensdim                  = 144,
cu_rad_feedback         = .false.,
/
```

```
&chem
kemit                   = 1,
kemit_aircraft          = 0,
chem_opt                = 112,
bioemdt                 = 3.00,
photdt                  = 30,
chemdt                  = 3.00,
io_style_emissions      = 2,
emiss_opt               = 8,        3,
emiss_inpt_opt          = 111,
aircraft_emiss_opt      = 0,
chem_in_opt             = 0,        0,
phot_opt                = 3,        0,
gas_drydep_opt          = 1,        1,
aer_drydep_opt          = 1,
bio_emiss_opt           = 3,        0,
gas_bc_opt              = 1,        0,
gas_ic_opt              = 1,        0,
aer_bc_opt              = 1,        0,
aer_ic_opt              = 1,        0,
gaschem_onoff           = 1,        0,
wetscav_onoff           = 1,        0,
cldchem_onoff           = 0,        0,
vertmix_onoff           = 1,        0,
biomass_burn_opt        = 2,        0,
plumerisefire_frq       = 30,       0,
dust_opt                = 1,
seas_opt                = 1,
aer_op_opt              = 1,
opt_pars_out            = 1,
aer_ra_feedback         = 1,
scale_fire_emiss        = .true.
have_bcs_chem           = .true., .false., .false.,
chemdiag                = 0,
chem_conv_tr            = 1,        0,
ne_area                 = 81,
/
```

MOZART/GOCART LNOx-aircraft namelist example

```
&time_control
…
…
io_form_auxinput5               = 2,
frames_per_auxinput5              = 1, 1, 1,
auxinput5_inname                = 'wrfchemi_d<domain>_<date>',
auxinput5_interval_m              = 60, 60, 60,
io_form_auxinput6               = 2,
frames_per_auxinput6              = 1, 1, 1,
auxinput6_inname                = 'wrfbiochemi_d<domain>',
io_form_auxinput7               = 2,
frames_per_auxinput7              = 1, 1, 1,
auxinput7_inname                = 'wrffirechemi_d<domain>_<date>',
auxinput7_interval_m              = 60, 60, 60,
io_form_auxinput14               = 2,
frames_per_auxinput14               = 1, 1, 1,
auxinput14_inname                = 'wrfaircraftchemi_d<domain>_<date>',
auxinput14_interval_m               = 60, 60, 60,
iofields_filename             = "output.txt","output_10min.txt",
ignore_iofields_warning           = .true.,
debug_level                   = 0
/


&physics
mp_physics                    = 10, 10,
do_radar_ref                   = 1,
ra_lw_physics                  = 4, 4,
ra_sw_physics                  = 4, 4,
radt                          = 10,10,
sf_sfclay_physics                = 1, 1,
sf_surface_physics                 = 2, 2,
bl_pbl_physics                 = 1, 1,
bldt                          = 0, 0,
cu_physics                       = 5, 5,
cudt                           = 0, 0,
cugd_avedx                                        = 1,
cu_rad_feedback                           = .true.,.true.,
cu_diag                                   = 1,
isfflx                        = 1,
ifsnow                          = 0,
icloud                         = 1,
surface_input_source                = 1,
num_soil_layers                  = 4,
mp_zero_out                     = 2,
num_land_cat                                      = 20,
lightning_option                          = 11,1,
iccg_method                                       = 2,2,
lightning_dt                                      = 75,75,
cellcount_method                          = 0,1,
lightning_start_seconds                   = 600,600,
flashrate_factor                          = 5.0,1.0,
cldtop_adjustment                         = 0,0,
/
```

```
&chem
kemit                         = 11,
chem_opt                        = 112,   112,
bioemdt                        = 0,     0,
photdt                         = 15,    15,
chemdt                         = 0.,    0.,
io_style_emissions                 = 2,
emiss_inpt_opt                   = 111,   111,
emiss_opt                       = 8,      8,
emiss_opt_vol                     = 0,
chem_in_opt                      = 0,     0,
phot_opt                       = 3,      3,
gas_drydep_opt                     = 1,      1,
aer_drydep_opt                     = 1,      1,
bio_emiss_opt                    = 3,      3,
ne_area                       = 118,
gas_bc_opt                       = 112,   112,
gas_ic_opt                      = 112,   112,
aer_bc_opt                       = 112,   112,
aer_ic_opt                      = 112,   112,
gaschem_onoff                      = 1,      1,
aerchem_onoff                      = 1,      1,
wetscav_onoff                     = 1,      1,
cldchem_onoff                      = 0,      0,
vertmix_onoff                     = 1,      1,
chem_conv_tr                       = 1,      1,
conv_tr_wetscav                    = 1,      1,
conv_tr_aqchem                     = 1,      1,
seas_opt                      = 1,
dust_opt                      = 1,
dmsemis_opt                       = 1,
biomass_burn_opt                   = 2,      2,
plumerisefire_frq                 = 30,     30,
have_bcs_chem                      = .true., .true.,
aer_ra_feedback                    = 1,      1,
aer_op_opt                      = 1,
opt_pars_out                       = 1,
diagnostic_chem                    = 1,
track_chem_name                    =
"co","o3","no","no2","so2","hcho","hno3","h2o2","isopr","tol","bigalk","bc1","bc2","oc1","oc2","p
25","p10","dust_1","dust_2","dust_3","dust_4","seas_1","seas_2","seas_3","seas_4","dms",
track_chem_num                     = 26,
kemit_aircraft                   = 40,
aircraft_emiss_opt                 = 1,1,
lnox_opt                       = 1,2,
N_IC                          = 500., 500.,
N_CG                           = 500., 500.,
/
have_bcs_upper                     = .false.,  .false.,
fixed_ubc_press                   = 50.,    50.,
fixed_ubc_inname                    = 'ubvals_b40.20th.track1_1996-2005.nc',
```

MOZART/GOCART LNOx-aircraft namelist example

```
&time_control
…
…
io_form_auxinput5               = 2,
frames_per_auxinput5              = 1, 1, 1,
auxinput5_inname                = 'wrfchemi_d<domain>_<date>',
auxinput5_interval_m              = 60, 60, 60,
io_form_auxinput6               = 2,
frames_per_auxinput6              = 1, 1, 1,
auxinput6_inname                = 'wrfbiochemi_d<domain>',
io_form_auxinput7               = 2,
frames_per_auxinput7              = 1, 1, 1,
auxinput7_inname                = 'wrffirechemi_d<domain>_<date>',
auxinput7_interval_m              = 60, 60, 60,
io_form_auxinput14               = 2,
frames_per_auxinput14               = 1, 1, 1,
auxinput14_inname                = 'wrfaircraftchemi_d<domain>_<date>',
auxinput14_interval_m               = 60, 60, 60,
iofields_filename             = "output.txt","output_10min.txt",
ignore_iofields_warning           = .true.,
debug_level                   = 0
/


&physics
mp_physics                    = 10, 10,
do_radar_ref                   = 1,
ra_lw_physics                  = 4, 4,
ra_sw_physics                  = 4, 4,
radt                          = 10,10,
sf_sfclay_physics                = 1, 1,
sf_surface_physics                 = 2, 2,
bl_pbl_physics                 = 1, 1,
bldt                          = 0, 0,
cu_physics                       = 5, 5,
cudt                           = 0, 0,
cugd_avedx                                        = 1,
cu_rad_feedback                           = .true.,.true.,
cu_diag                                   = 1,
isfflx                        = 1,
ifsnow                          = 0,
icloud                         = 1,
surface_input_source                = 1,
num_soil_layers                  = 4,
mp_zero_out                     = 2,
num_land_cat                                      = 20,
lightning_option                          = 11,1,
iccg_method                                       = 2,2,
lightning_dt                                      = 75,75,
cellcount_method                          = 0,1,
lightning_start_seconds                   = 600,600,
flashrate_factor                          = 5.0,1.0,
cldtop_adjustment                         = 0,0,
/
```

```
&chem
kemit                         = 11,
chem_opt                        = 112,   112,
bioemdt                        = 0,     0,
photdt                         = 15,    15,
chemdt                         = 0.,    0.,
io_style_emissions                 = 2,
emiss_inpt_opt                   = 111,   111,
emiss_opt                       = 8,      8,
emiss_opt_vol                     = 0,
chem_in_opt                      = 0,     0,
phot_opt                       = 3,      3,
gas_drydep_opt                     = 1,      1,
aer_drydep_opt                     = 1,      1,
bio_emiss_opt                    = 3,      3,
ne_area                       = 118,
gas_bc_opt                       = 112,   112,
gas_ic_opt                      = 112,   112,
aer_bc_opt                       = 112,   112,
aer_ic_opt                      = 112,   112,
gaschem_onoff                      = 1,      1,
aerchem_onoff                      = 1,      1,
wetscav_onoff                     = 1,      1,
cldchem_onoff                      = 0,      0,
vertmix_onoff                     = 1,      1,
chem_conv_tr                       = 1,      1,
conv_tr_wetscav                    = 1,      1,
conv_tr_aqchem                     = 1,      1,
seas_opt                      = 1,
dust_opt                      = 1,
dmsemis_opt                       = 1,
biomass_burn_opt                   = 2,      2,
plumerisefire_frq                 = 30,     30,
have_bcs_chem                      = .true., .true.,
aer_ra_feedback                    = 1,      1,
aer_op_opt                      = 1,
opt_pars_out                       = 1,
diagnostic_chem                    = 1,
track_chem_name                    =
"co","o3","no","no2","so2","hcho","hno3","h2o2","isopr","tol","bigalk","bc1","bc2","oc1","oc2","p
25","p10","dust_1","dust_2","dust_3","dust_4","seas_1","seas_2","seas_3","seas_4","dms",
track_chem_num                     = 26,
kemit_aircraft                   = 40,
aircraft_emiss_opt                 = 1,1,
lnox_opt                       = 1,2,
N_IC                          = 500., 500.,
N_CG                           = 500., 500.,
/
have_bcs_upper                     = .false.,  .false.,
fixed_ubc_press                   = 50.,    50.,
fixed_ubc_inname                    = 'ubvals_b40.20th.track1_1996-2005.nc',
```

MOZART/MOSAIC namelist example

```
&physics
 mp_physics                 = 10,
 progn                      = 1,
 ra_lw_physics              = 4,
 ra_sw_physics              = 4,
 radt                       = 30,
 sf_sfclay_physics          = 5, ! Ravans suggestion
 sf_surface_physics         = 2, ! NOAH
 bl_pbl_physics             = 5, ! MYNN 2.5
 bldt                       = 0,
 cu_physics                 = 5, ! Grell 3D
 cudt                       = 0,
 cugd_avedx                 = 1, ! set to 3 for 4km run, 1 for
36km
 isfflx                     = 1,
 ifsnow                     = 1,
 icloud                     = 1,
 surface_input_source       = 1,
 num_soil_layers            = 4,
 sf_urban_physics           = 1,
 sst_update                 = 1,
 mp_zero_out                = 2,
 mp_zero_out_thresh         = 1.e-8,
 cu_rad_feedback            = .true.,
 cu_diag                    = 1,
 slope_rad                  = 0,
 topo_shading               = 0,
 /
```

```
&chem
kemit                       = 8,
chem_opt                    = 999,
bioemdt                     = 30,
photdt                      = 30.,
chemdt                      = 6.0,
io_style_emissions          = 2,
emiss_inpt_opt              = 102,
emiss_opt                   = 10,
chem_in_opt                 = 1,
phot_opt                    = 3,
gas_drydep_opt              = 1,
aer_drydep_opt              = 1,
bio_emiss_opt               = 3,
gas_bc_opt                  = 1,
gas_ic_opt                  = 1,
aer_bc_opt                  = 1,
aer_ic_opt                  = 1,
gaschem_onoff               = 1,
aerchem_onoff               = 1,
wetscav_onoff               = 1,
cldchem_onoff               = 1,
vertmix_onoff               = 1,
chem_conv_tr                = 1,
conv_tr_wetscav             = 1,
conv_tr_aqchem              = 1,
seas_opt                    = 2,
dust_opt                    = 3,
dmsemis_opt                 = 1,
biomass_burn_opt            = 0,
aer_ra_feedback             = 1,
ne_area                     = 140,
opt_pars_out                = 1,
have_bcs_chem               = .true.,
have_bcs_upper              = .false.,
/
```

CRIMech namelist example

```
&physics
mp_physics                          = 2,
progn                               = 1,
ra_lw_physics                       = 4,
ra_sw_physics                       = 2,
radt                                = 5,
sf_sfclay_physics                   = 2,
sf_surface_physics                  = 2,
bl_pbl_physics                      = 2,
bldt                                = 0,
cu_physics                          = 5,
cu_diag                             = 1,
cugd_avedx                          = 1,
cudt                                = 0,
isfflx                              = 1,
ifsnow                              = 1,
icloud                              = 1,
surface_input_source                = 1,
num_soil_layers                     = 4,
sf_urban_physics                    = 1,
mp_zero_out                         = 2,
mp_zero_out_thresh                  = 1.e-12
maxiens                             = 1,
maxens                              = 3,
maxens2                             = 3,
maxens3                             = 16,
ensdim                              = 144,
cu_rad_feedback                     = .true.,
sst_update                          = 1,
sst_skin                            = 1,
usemonalb                           = .true.,
tmn_update                          = 1,
/
```

```
&chem
kemit                               = 5,
chem_opt                            = 601,
bioemdt                             = 30,
photdt                              = 30,
chemdt                              = 1,
io_style_emissions                  = 2,
emiss_inpt_opt                      = 121,
emiss_opt                           = 20,
emiss_opt_vol                       = 0,
chem_in_opt                         = 0,
phot_opt                            = 2,
gas_drydep_opt                      = 1,
aer_drydep_opt                      = 1,
bio_emiss_opt                       = 3,
gas_bc_opt                          = 0,
gas_ic_opt                          = 0,
aer_bc_opt                          = 0,
aer_ic_opt                          = 0,
gaschem_onoff                       = 1,
aerchem_onoff                       = 1,
wetscav_onoff                       = 1,
cldchem_onoff                       = 1,
vertmix_onoff                       = 1,
chem_conv_tr                        = 1,
seas_opt                            = 3,
dust_opt                            = 0,
dmsemis_opt                         = 2,
biomass_burn_opt                    = 0,
have_bcs_chem                       = .true.,
aer_ra_feedback                     = 1,
chemdiag                            = 1,
n2o5_hetchem                        = 2,
ne_area                             = 250,
/
```