WRF-Chem/MOZART and WRF-Chem/MOZCART

(updated July 2017)

The MOZART gas phase chemistry has been included in WRF-Chem V3.2 through KPP:

chem_opt = 111 MOZART gas phase chemistry, no aerosols
chem_opt = 112 MOZART gas phase chemistry and GOCART aerosols (MOZCART)

For details about the MOZART chemical mechanism see:
Emmons, L.K., S. Walters, P. G. Hess et al., Description and evaluation of the Model for Ozone and Related chemical Tracers, version 4 (MOZART-4), Geosci. Model Dev., 3, 43–67, 2010.

Emissions:

Anthropogenic Emissions: emiss_opt= 7 (MOZART) or emiss_opt=8 (MOZCART)
For users who use the EPA NEI emissions provided by Stu McKeen on the WRF-Chem ftp server, Table 1 gives a suggested mapping of MOZART species to EPA SAPRC/NEI speciation.

The MEGAN online biogenic emission option (bio_emiss_opt=3) has been updated to accommodate the MOZART/MOZCART speciation.

MOZART and MOZCART are linked to the fire plumerise module (biomass_burn_opt=2). Fire emissions are assumed to be provided in separate input files (wrffirechemi_d<nn>_<yyyy>-<mm>-<dd>_<hh>:<mm>:<ss>) and to include the total emissions strength.

WRFV3.4 update: The scale_fire_emiss namelist variable controls whether or not the total emission strength is split into a "smoldering" and a "flaming" part within the plumerise module. The scale_fire_emiss variable defaults to .false. and is only valid for the MOZART or MOZCART chem options. If wrffire_chemi files are created with the Fire_Emis preprocessor using FINN input (http://bai.acom.ucar.edu/Data/fire/) then the total emission strength is provided and scale_fire_emiss has to be set to .true..

Special considerations when using the MOZART or MOZCART options:

(1) MOZART and MOZCART only work with photolysis option photo_opt=3 (FTUV). The FTUV code has been updated to read in climatological O3 and O2 overhead columns instead of using a fixed value. This requires an additional input file for each domain named exo_coldens_d<nn>. A fortan based code for creating this additional input file together with instructions can be downloaded from:
http://www.acom.ucar.edu/wrf-chem/download.shtml

(2) The Wesely dry deposition routine has been updated to allow for seasonal changes in the dry deposition (gas_drydep_opt=1). This requires an additional input file for each domain named wrf_season_wes_usgs_d<nn>. A fortan based code for

creating this additional input file together with instructions can be downloaded from: http://www.acom.ucar.edu/wrf-chem/download.shtml

(3) CH4, H2, and N2O concentrations are held constant at values specified in the initial conditions.

(4) Wet deposition of gas species is not included in the V3.2 release.

WRFV3.4 Updates:

(1) Wet scavenging of 31 gas species is included in V3.4 for the MOZART and MOZCART chem options. The namelist chem group variable wetscav_onoff must be set to 1 to activate wet scavenging. The default value for wetscav_onoff is 0, which turns wet scavenging off.
For more information about the wet scavenging scheme see the presentation 8A.6 by Pfister et al. given at the WRF User Workshop 2011 (http://www.mmm.ucar.edu/wrf/users/workshops/WS2011/WorkshopPapers.php).

(2) Upper boundary conditions (UBC) for selected gas species may be specified via the chem group namelist variable have_bcs_upper. The variable have_bcs_upper defaults to .false. wherein no species concentrations are specified near the upper boundary. If have_bcs_upper is set to .true. then the following species will have concentrations from the model top down to the tropopause overwritten: o3, no, no2, hno3, ch4, co, n2o, and n2o5

The namelist variable fixed_ubc_press, default = 50.(units are hPa), controls the pressure level down to which upper boundary concentrations are overwritten. From the level fixed_ubc_press down to the tropopause concentrations are relaxed with a 10 day time constant to fixed values. The UBC implementation requires two input data files:

- the file clim_p_trop.nc which includes a climatology for tropopause levels
- an input file with upper boundary conditions for gas species. The filename is controlled via the namelist variable fixed_ubc_inname. Climatologies for 4 different time periods derived from WACCM RCP simulations are available:
  ubvals_b40.20th.track1_1950-1959.nc
  ubvals_b40.20th.track1_1980-1989.nc
  ubvals_b40.20th.track1_1996-2005.nc
  ubvals_rcp4_5.2deg_2020-2029.nc

The needed inputs can be downloaded from the ACD WRF-Chem Website (https://www2.acom.ucar.edu/wrf-chem/wrf-chem-tools-community)
Additional output of tropopause diagnostics is enabled (TROPO_P, TROPO_Z, TROPO_LEV).

For more information about the UBC scheme see the presentation 8A.2 by Barth et al. given at the WRF User Workshop 2011 (http://www.mmm.ucar.edu/wrf/users/workshops/WS2011/WorkshopPapers.php).

(3) "Tracking" output: vertical profiles of prescribed meteorological and chemical species at a set of prescribed times and horizontal coordinates are written to a special output file, wrfout_track_d<nn>. The namelist variable track_loc_in is a count of the track locations and must be set to a positive value otherwise the default setting of zero will result in no track output of any variables. Times and locations must be specified in the file wrfinput_track.txt(see example below). Meterological variables z, p, t, u, v, w, alt, qcloud, qrain, qice, qsnow, qgraup, and qvapor are output if track_loc_in is non-zero. Chemical species concentrations may also be output if both namelist variables track_chem_num and track_chem_name are set. The total number of chemical species to output must be <= 100.

As an example the following namelist settings will output the default meterological variables and co and o3 species concentrations at the two times and locations specified in the wrfinput_track.txt file :

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

The following two lines comprise the contents of the ascii input file wrfinput_track.txt :

```
2010-08-10_00:12:00 41.450 -87.300
2010-08-10_00:36:00 41.510 -87.390
```

This will result in the indicated variables being output to wrfout_track_d01 at the times 00:12:00 UTC and 00:36:00 UTC on August 10, 2010 at the grid points nearest to the points (41.450,-87.300) and (41.510,-87.390). Note that the tracking tool does not interpolate in time. The indicated output times need to be given in multiples of model time steps else no output is produced.
The exact Fortran format for the lines in the file wrfinput_track.txt is (A19,1X,F7.3,1X,F7.3) and the horizontal coordinates are ordered for latitude, longitude with standard WRF conventions wherein south latitudes and west longitudes are negative.

(4) Aircraft emissions: emissions of so2, no, co, and ch4 from aircraft may be included for the MOZART, MOZCART chemistry options. The namelist chem group variable aircraft_emiss_opt controls whether or not aircraft emissions are used. The default value , 0, turns aircraft emissions off. The value 1 enables aircraft

emissions. Another chem group namelist variable, kemit_aircraft, controls the vertical extent of the aircraft emissions and defaults to a value of 1. The default value means that aircraft emissions will only be applied to the lowest vertical level. If active, aircraft emissions will be applied at every time step.

(5) Lightning: NO (nitrogen oxide) production from lightning may be included in MOZART, MOZCART chemistry options using a scheme that has been included in WRF-Chem by J. Wong (U. of Colorado). The namelist chem group variable lightning_opt controls whether or not lightning no production is active. For the default setting, 0, no lightning production is off. For MOZART, MOZCART the setting 101 turns on the lightning no production scheme. The namelist chem group variables lightning_start_seconds and lightning_time_step control lightning NO production timing. The variable lightning_start_seconds specifies, in seconds, the time in a simulation at which no production starts. The default value of 0 means that lightning is active for the entire time span of a simulation. The variable lightning_time_step specifies the period in seconds at which no production from lightning is active. The default value of 0 should be replaced by a multiple of the simulation time step. Finally the namelist chem group variable flashrate_factor is a multiplier in the range (0.,1.] determining the actual lightning no production applied. The default value is 1. This factor is dependent on the grid resolution and has to be tuned to to a given grid size.

(6) Variable renaming: In V3.4 the variable *so4* has been renamed to *sulf* in both MOZART and MOZCART chemistry options. Please consider this change also when setting initial and boundary conditions.

(7) Convective wet scavenging: In V3.4 convective wet scavenging may be done in the Grell convection routine grelldrvct(chem/module_ctrans_grell.F). This wet scavenging is in addition to the resolved scale wet scavenging in item (**1**) above. The namelist chem group variable conv_tr_wetscav determines whether or not convective wet scavenging is applied. The default value is 1 which enables convective wet scavenging. If you do **not** want convective wet scavenging you must set conv_tr_wetscav to 0. Please note that this feature has not yet been tested for MOZART and MOZCART options.

Table: Mapping of MOZART emissions species to EPA/NEI species

MOZART	EPA NEI
E_CO	CO
E_NO	0.9*NOx
E_NO2	0.1*NOx
E_SO2	SO2
E_NH3	NH3
E_C2H5OH	scale to CO: 0.00396 * CO
E_BIGALK	HC04 + HC05 + HC06 + HC20 + HC34 + HC35
E_BIGENE	HC08 + HC09 + HC16 + HC39 + HC40
E_C2H4	HC07
E_C2H6	HC02
E_C3H6	HC31
E_C3H8	HC38 + HC32
E_CH2O	HC14
E_CH3CHO	HC15 + HC24
E_CH3COCH3	HC18
E_CH3OH	HC21
E_MEK	HC19
E_TOLUENE	HC12 + HC13 + HC17 + HC33 + HC36 + HC37 + HC22 + HC23 + HC25 + HC26
E_ISOP	HC10 + HC27 + HC28 + HC29
E_C10H16	HC11
GOCART Aerosols:	
E_sulf	PM02
E_PM_25	PM01
E_BC	PM05
E_OC	PM04
E_PM_10	PM10-PRI

HC01) Methane
HC02) Alkane1 ;k(OH) < 500 /ppm/min; (primarily Ethane)
HC03) Alkane2 ;500 < k(OH) < 2500 /ppm/min (excluding C3H8,C2H2,organic acids)
HC04) Alkane3 ;2500 < k(OH) < 5000 /ppm/min (excluding butanes)
HC05) Alkane4 ;5000 < k(OH) < 10000 /ppm/min (excluding pentanes)
HC06) Alkane5 ; k(OH) > 10000 /ppm/min
HC07) Ethylene
HC08) Olefin1 ; k(OH) < 70000 /ppm/min (excluding propylene)
HC09) Olefin2 ; k(OH) > 70000 /ppm/min (excluding dienes and styrene)
HC10) Isoprene
HC11) Sum of Terpenes
HC12) Aromatic 1 ; k(OH) < 20000 /ppm/min (excluding benzene and toluene)
HC13) Aromatic 2 ; k(OH) > 20000 /ppm/min (excluding xylenes)
HC14) Formaldehyde
HC15) Acetaldehyde
HC16) Higher Aldehydes
HC17) Benzaldehyde
HC18) Acetone
HC19) Methyl-Ethyl ketone
HC20) PRD2 (see SAPRAC-99)
HC21) Methanol
HC22) Glyoxal
HC23) Methylglyoxal
HC24) Biacetyl
HC25) Phenols
HC26) Cresols
HC27) Methacrolein
HC28) Methylvinyl ketone
HC29) IPRD (see SAPRAC-99)
HC30) Unreactive
HC31) Propylene
HC32) Acetylene
HC33) Benzene
HC34) Butanes
HC35) Pentanes
HC36) Toluene
HC37) Xylenes
HC38) Propane
HC39) Dienes
HC40) Styrene
HC41) Organic Acids
PM01) PMFINE - unspeciated primary PM2.5
PM02) PSO4 - PM2.5 sulfate
PM03) PNO3 - PM2.5 nitrate
PM04) POA - PM2.5 organic aerosol
PM05) PEC - PM2.5 elemental carbon

For questions and comments please refer to the NCAR WRF-Chem User Forum (https://www2.acom.ucar.edu/wrf-chem/discussion-forum)