WRF-Chem 3.6.1:
MOZART gas-phase chemistry with MOSAIC aerosols

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The extended MOZART gas-phase chemistry was coupled with MOSAIC 4-bin aerosol module to allow a more detailed calculation of aerosol composition and properties. This setup is particularly suitable for analysis of field project data and process studies focused on aerosol chemistry. Two options are available:

- chem_opt = 201 : mozart_mosaic_4bin
- chem_opt = 202 : mozart_mosaic_4bin_aq

Additional input files are needed to run this package for photolysis and dry deposition schemes and are available from http://www.acd.ucar.edu/wrf-chem/download.shtml.
The test case for the continental U.S. domain can be downloaded from the NCAR website.

Description of gas-phase mechanism MOZART:

The MOZART gas-phase chemistry (Emmons et al., 2010) was extended to include detailed treatment of monoterpenes (a-pinene, b-pinene, limonene) and MBO (Hodzic et al., in prep.), aromatics, HONO, C_2H_2, as well as an updated isoprene oxidation scheme (Knote et al., 2014a). This updated gas-phase mechanism is different from the gas-phase mechanism used in mozart (chem_opt=111) and mozcart (chem_opt=112).
With this package TUV and fTUV should be used for photolysis. The code was updated to account for aerosol feedbacks on photolysis.

Note:
Emissions used with the extended MOZART mechanism (chem_opt = 201, 202) differ from the other two MOZART options (chem_opt = 111, 112). Users need to provide emissions for speciated aromatic compounds (benzene, toluene, sum of xylenes). In chem_opts 111 and 112 “E_TOLUENE” is considered to be the sum of the emissions of toluene, benzene and xylenes, whereas it should contain only toluene in chem_opts 201 and 202. Additionally, “E_BENZENE” and “E_XYLENE” should be provided.
For biogenic emissions, online MEGAN is recommended as it will take care of speciating the biogenic VOCs.

Updates to the MOSAIC aerosol module

1) Updated secondary organic aerosols (SOA) formation mechanism

- **For chem_opt = 201,** the SOA scheme is based on Hodzic and Jimenez (GMD, 2011). The calculation of secondary organic aerosols has been replaced by a more computationally efficient scheme that uses ambient ageing measurements of organic aerosols, and that produces reasonable concentrations of SOA from anthropogenic and biomass burning precursors. Biogenic SOA is treated as a two product approach using updated yields.

- **For chem_opt = 202**, a volatility basis set (VBS) type description of SOA formation based on Lane et al. (2008) yields and updated by Knote et al. (2014b) is included. Oxidation of multiple biogenic and anthropogenic precursors forms compounds of varying volatility which then partition between the gas- and aerosol-phase depending on total organic aerosol load as well as temperature. Subsequent lowering of volatility through continuous oxidation in the gas-phase is considered, as well as removal of S/IVOCs (see point 3 below). Primary organic aerosols are considered as inert.

2) Glyoxal uptake into aqueous aerosols to form SOA (Knote et al., 2014a)

Currently, glyoxal SOA is turned on by default for mozart_mosaic_4bin (chem_opt = 201) or mozart_mosaic_4bin_aq (chem_opt = 202).

- with mozart_mosaic_4bin, a simple surface uptake is used ("simple" in Knote et al. 2014a).
- with mozart_mosaic_4bin_aq the complex version is used ("hybrid" in Knote et al. 2014a).

A new module was added called module_mosaic_gly.F which contains the glyoxal SOA formation and partitioning code.

- The glyoxal routine is called during ASTEM in module_mosaic_therm.F
- Available parameterizations are defined in module_data_mosaic_therm.F.
- The choice of glyoxal parametrization called for various chem_opts can be found in the mosaic_aerchem_driver routine in module_mosaic_driver.F If one would like to modify this choice set glysoa_param to a different option in module_mosaic_driver.F, and add additional tracers to the registry.chem.

3) Removal of S/IVOCS was therefore updated with new Henry's law coefficients

S/IVOCs compounds have been attributed new Henry's law constants (water solubility) calculated from explicit chemistry (Hodzic et al., GRL, 2014). These values have been included in the calculation of removal through convective and grid-scale precipitation, as well as dry deposition. They strongly affect the removal of SOA (as discussed in Knote et al., 2014b).

Below is the brief reminder how this is handled in the model:

- Washout of gases and aerosols by convective precipitation is considered using Grell and Dévényi (2002), which we modified to use Henry's law constants in gas-droplet partitioning.

- Grid-scale precipitation removes aerosols through the scheme implemented in MOSAIC (Easter et al., 2004; Chapman et al., 2009), while washout of trace gases is performed as described in Neu and Prather (2012). The Neu and Prather (2012) scheme also employs an equilibrium approach based on Henry's law constants to consider transfer into cloud droplets and subsequent conversion into rain droplets, as well as collection of gases by falling rain droplets. Both, washout through grid-scale and convective precipitation considers the same gas species with an identical set of Henry's law constants.

- Dry deposition of gases is parameterized in WRF-chem based on Wesely (1978), modeling deposition as a series of resistors consisting of an atmospheric, a laminar sublayer, and a bulk

surface resistance. The latter is a function of the Henry's law constant of a gas to describe partitioning into plants and other wet surfaces.

Recommended setup:

We recommend that the following options be used with these two packages, as they have been tested.

Our recommended microphysics is the Morrison double moment scheme (mp_physics = 10) as it is the only scheme that is hooked up with cloud chemistry, washout of trace gases (Neu and Prather) as well as the explicit aerosol aqueous-phase. Note that precipitation has to be prognostic for this to work (progn = 1). All major PBL schemes should work, but we only tested the MYNN scheme with the 2.5th-order turbulence closure (bl_pbl_physics = 5). We recommend to use the urban physics parameterization (e.g. sf_urban_physics = 2). The Grell 3D cumulus convection scheme is the only scheme hooked up with cloud chemistry and tracer transport (cu_physics = 5). Both fTUV and TUV work, but we recommend the use of the full TUV (phot_opt = 1) as the additional runtime is acceptable. The direct aerosol feedback (aer_ra_feedback = 1) is hooked up with both chem_opt 201 and 202. The indirect aerosol feedback (i.e. activation as cloud droplets) only works with chem_opt = 202. We also recommend using the heterogeneous uptake of N2O5 onto aerosol particles (n2o5_hetchem=1). Dust, sea salt and fire plume rise options were not tested, and we used dust_opt=3, seas_opt=2 and no plume rise.

Example for the Namelist.input file for chem_opt=201

```
&chem
 kemit                 = 8,
 chem_opt              = 201,
 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                  = 0,
 vertmix_onoff                  = 1,
 chem_conv_tr                   = 1,
 conv_tr_wetscav                = 1,
 conv_tr_aqchem                 = 0,
 seas_opt                       = 2,
 dust_opt                       = 3,
 dmsemis_opt                    = 1,
 biomass_burn_opt               = 0,
 aer_ra_feedback                = 1,
 n2o5_hetchem                    = 1,
 ne_area                        = 140,
 opt_pars_out                   = 1,
 have_bcs_chem                  = .true.,
 have_bcs_upper                 = .true.,
 /
```

Example namelist.input for chem_opt=202: similar to the namelist.input for chem_opt = 201 above, except:

```
 chem_opt                       = 202,
 cldchem_onoff                  = 1,
 conv_tr_aqchem                 = 1,
```

Boundary Conditions

Below is a typical mozmapper.inp script species mapping for the conversion of global MOZART data to the new mechanisms MZ-MOSAIC4BINS:

```
spc_map = 'o3 -> O3', 'no -> NO',
        'no2 -> NO2', 'no3 -> NO3', 'nh3 -> NH3', 'hno3 -> HNO3', 'hno4 -> HO2NO2',
        'n2o5 -> N2O5', 'ho -> OH', 'ho2 -> HO2', 'h2o2 -> H2O2',
        'ch4 -> CH4', 'co -> CO', 'ch3o2 -> CH3O2', 'ch3ooh -> CH3OOH',
        'hcho -> CH2O', 'ch3oh -> CH3OH', 'c2h4 -> C2H4',
        'ald -> CH3CHO', 'ch3cooh -> CH3COOH', 'acet -> CH3COCH3', 'mgly -> CH3COCHO',
        'paa -> CH3COOOH',
        'pan -> PAN', 'mpan -> MPAN', 'macr -> MACR',
        'mvk -> MVK', 'c2h6 -> C2H6', 'c3h6 -> C3H6', 'c3h8 -> C3H8',
        'c2h5oh -> C2H5OH',
        'onit -> ONIT', 'onitr -> ONITR', 'isopr -> ISOP',
        'isopn -> ISOPNO3', 'acetol -> HYAC', 'glyald -> GLYALD',
        'hydrald -> HYDRALD', 'mek -> MEK',
        'bigene -> BIGENE', 'open -> BIGALD', 'bigalk -> BIGALK',
        'tol -> TOLUENE',
        'cres -> CRESOL', 'dms -> DMS', 'so2 -> SO2', 'sulf -> SO4',
```

```
        'oc_a01->9.60024e-2*OC1+9.60024e-2*OC2+1.152026*SOA;1.e9'
        'oc_a02->.254356*OC1+.254356*OC2+3.05226*SOA;1.e9',
        'oc_a03->6.00723e-2*OC1+6.00723e-2*OC2+.720865*SOA;1.e9',
        'oc_a04->.00104*OC1+.00104*OC2+.012481*SOA;1.e9',
        'bc_a01->6.5325E-01*CB1+6.5325E-01*CB2;0.413793103e9',
        'bc_a02->2.5458E-01*CB1+2.5458E-01*CB2;0.413793103e9',
        'bc_a03->4.0521E-03*CB1+4.0521E-03*CB2;0.413793103e9',
        'bc_a04->1.6794E-06*CB1+1.6794E-06*CB2;0.413793103e9',
        'so4_a01->2.4433e-2*SO4;3.31423e9',
        'so4_a02->.47111*SO4;3.31423e9',
        'so4_a03->.47857*SO4;3.31423e9',
        'so4_a04->2.5727e-2*SO4;3.31423e9',
        'no3_a01->2.4433e-2*NH4NO3;2.76186e9',
        'no3_a02->.47111*NH4NO3;2.76186e9',
        'no3_a03->.47857*NH4NO3;2.76186e9',
        'no3_a04->2.5727e-2*NH4NO3;2.76186e9',
        'nh4_a01->2.4433e-2*NH4;6.22876e8',
        'nh4_a02->.47111*NH4;6.22876e8',
        'nh4_a03->.47857*NH4;6.22876e8',
        'nh4_a04->2.5727e-2*NH4;6.22876e8',
        'na_a01->.2*SA1;1.e9',
        'na_a02->.4*SA1;1.e9',
        'na_a03->.2*SA1+.8*SA2;1.e9',
        'na_a04->.8*SA3;1.e9',
        'cl_a01->.3*SA1;1.e9',
        'cl_a02->.6*SA1;1.e9',
        'cl_a03->.3*SA1+1.2*SA2;1.e9',
        'cl_a04->1.2*SA3;1.e9',
        'oin_a01->0.5*[DUST1];1.e9',
        'oin_a02->0.5*[DUST1]+0.24*[DUST2];1.e9',
        'oin_a03->0.76*[DUST2]+1.0*[DUST3];1.e9',
        'oin_a04->1.0*[DUST4];1.e9',
        'num_a01-
>1.73e17*OC1+1.73e17*OC2+1.73e17*SOA+5.64e17*CB1+5.64e17*CB2+7.67e16*SO4+6.39
e16*NH4NO3+1.44e16*NH4+3.22e17*SA1+4.83e17*SA1+0.5*3.93e17*[DUST1];1.0',
        'num_a02-
>1.71e16*OC1+1.71e16*OC2+1.71e16*SOA+9.91e15*CB1+9.91e15*CB2+6.06e16*SO4+5.05
e16*NH4NO3+1.14e16*NH4+2.90e16*SA1+4.36e16*SA1+0.5*1.17e16*[DUST1]+0.24*1.17e16
*[DUST2];1.0',
        'num_a03-
>1.13e14*OC1+1.13e14*OC2+1.13e14*SOA+1.80e12*CB1+1.80e12*CB2+2.44e15*SO4+2.03
e15*NH4NO3+4.69e14*NH4+4.12e14*SA1+1.64e15*SA2+0.76*9.55e13*[DUST2]+9.55e13*[D
UST3];1.0',
```

'num_a04-
>4.09e10*OC1+4.09e10*OC2+4.09e10*SOA+3.42e07*CB1+3.42e07*CB2+3.25e12*SO4+2.71e12*NH4NO3+6.12e11*NH4+7.60e13*SA3+1.49e12*[DUST4];1.0',

This is an example for the mapping from the CESM data

spc_map = 'o3 -> O3', 'no -> NO', 'no2 -> NO2', 'hno3 -> HNO3', 'hno4 -> HO2NO2', 'ho -> OH', 'h2o2 -> H2O2', 'ch4 -> CH4', 'hcho -> CH2O', 'co -> CO', 'c2h6 -> C2H6', 'ald -> CH3CHO', 'pan -> PAN', 'bigene -> BIGENE', 'bigalk -> BIGALK', 'isopr -> ISOP', 'tol -> 0.3*TOLUENE', 'benzene -> 0.7*TOLUENE', 'so2 -> SO2', 'bc_a02->0.2*BC;1.0', 'bc_a03->0.8*BC;1.0', 'so4_a02->0.4*SO4;1.0', 'so4_a03->0.5*SO4;1.0', 'so4_a04->0.1*SO4;1.0', 'oc_a02->0.4*OC;1.0', 'oc_a03->0.5*OC;1.0', 'oc_a04->0.1*OC;1.0', 'oin_a02->0.05*DU01+0.05*DU02+0.05*DU03;1.0', 'oin_a03->0.85*DU01+0.85*DU02+0.85*DU03;1.0', 'oin_a04->0.10*DU01+0.10*DU02+0.10*DU03;1.0', 'num_a02->1.25e07*BC + 1.47e07*SO4 + 1.39e07*OC + 1.18e06*DU01 + 1.18e06*DU02 + 1.18e06*DU03;1.0', 'num_a03->7.82e05*BC + 2.88e05*SO4 + 2.72e05*OC + 3.14e05*DU01 + 3.14e05*DU02 + 3.14e05*DU03;1.0', 'num_a04-> 8.99e02*SO4 + 8.49e02*OC + 5.77e02*DU01 + 5.77e02*DU02 + 5.77e02*DU03;1.0'

Emissions

The emission options in the namelist need to be set to:

emiss_inpt_opt = 102,
emiss_opt = 10,

Additional tracers for antropogenic CO (e_co_a) and biomass burning CO (e_co_bb) are needed with chem_opt = 201, 202. If they are not available in the inventory the anthropogenic SOA won't be simulated.

Conversion from CB05-speciated emissions (as provided by U.S. EPA in the NEI model-ready files) is done as follows (excerpt from the supplement of the upcoming revised version of Knote et al., 2014b):

- Table Gases: *Mapping of emitted species as provided in the emissions input (AQMEII phase 2 data, Carbon Bond Mechanism Version 5 (CB05) speciation) onto the MOZART mechanism. Lumped structure species PAR, OLE and IOLE are converted into MOZART lumped molecules species assuming a (mole-wise) fractional contribution of 0.14, 0.02, and 0.84 of C3H6, BIGENE and BIGALK (based on measurements by Borbon et al., 2013) and the identities given in the table below.*

MOZART species	**CB05 Emissions input species**
E_MACR	ACROLEIN + BUTADIENE13
E_CH3CHO	ALD2 + ALDX

E_BENZENE	BENZENE
E_CH4	CH4
E_CO	CO
E_C2H6	ETHA
E_C2H4	ETH
E_C2H5OH	ETOH
E_CH2O	FORM
E_ISOP	ISOP
E_CH3OH	MEOH
E_NH3	NH3
E_NO2	NO2
E_NO	NO
E_HONO	HONO
E_SO2	SO2
E_SULF	SULF
E_C10H16	TERP
E_TOLUENE	TOL
E_XYLENE	XYL
E_C3H6	OLE + PAR
E_BIGENE	OLE + 2 × PAR, IOLE + 2 × PAR
E_BIGALK	5 × PAR
E_C3H8	1.12×10^{-2} × CO (Borbon et al., 2013)
E_CH3COCH3	1.18×10^{-2} × CO (Borbon et al., 2013)
E_MVK	2.40×10^{-4} × CO (Borbon et al., 2013)
E_C2H2	5.87×10^{-3} × CO (Borbon et al., 2013)

- Table Aerosols: *Emissions mapping for aerosol species. Each WRF-chem species listed below is actually 2 variables, for emissions into the Aitken and the accumulation size mode respectively. This is based on a modal aerosol description like e.g. in MADE (Ackermann et al., 1998). We here distribute the emissions input that is not size resolved into the different modes by applying a mass fraction of 0.1 for the Aitken mode and 0.9 for the accumulation mode*

(based on the work of Elleman and Covert, 2010). Emissions into these two modes are then distributed within WRF-Chem into the size bins of the MOSAIC aerosol module.

WRF-Chem species	Emissions input species
E_PM25	PAL + PCA + PFE + PK + PMFINE + PMG + PMN + PMOTHR + PSI + PTI
E_NA	PNA
E_CL	PCL
E_EC	PEC
E_ORG	POC
E_SO4	PSO4
E_NO3	PNO3
E_NH4	PNH4
E_PM_10	PMC

References

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