Discussion of chemistry in CESM2

- Chemistry mechanisms available in CESM
- Plans for Chemistry Module

CAM5/CAM6-MAM4

with MAM-SOA scheme, MAM4 modified for volcanic aerosols

Prescribed oxidants (read from file): O3, OH, NO3, HO2

Solved species: H2O2, H2SO4, SO2, DMS, SOAG , H2O,
bc_a1, bc_a4, pom_a1, pom_a4,
so4_a1, so4_a2, so4_a3, soa_a1, soa_a2,
dst_a1, dst_a2, dst_a3, ncl_a1, ncl_a2, ncl_a3,
num_a1, num_a2, num_a3, num_a4

MAM7 works in CAM6

Reactions (aerosol formation and transformations in code):

H2O2 + hv ->

HO2 + HO2 -> H2O2

H2O2 + OH -> H2O + HO2

DMS + OH -> SO2

DMS + OH -> .5 * SO2 + .5 * HO2

DMS + NO3 -> SO2 + HNO3

SO2 + OH -> H2SO4

MOZART-4 to MOZART-T1

Improved treatment of SOA precursors:

- Replace lumped aromatic “TOLUENE” with specific BENZENE, TOLUENE, XYLENES
- Updates to isoprene oxidation scheme
- Updated oxidation of terpenes: replaced “C10H16” with MTERP ($C_{10}H_{16}$), BCARY ($C_{15}H_{24}$)
  or
  speciated monoterpenes (APIN, BPIN, MYRC, LIMON) and MBO
- Improved treatment of organic nitrates (replace ONIT with more specific nitrates from alkanes, isoprene, etc.)

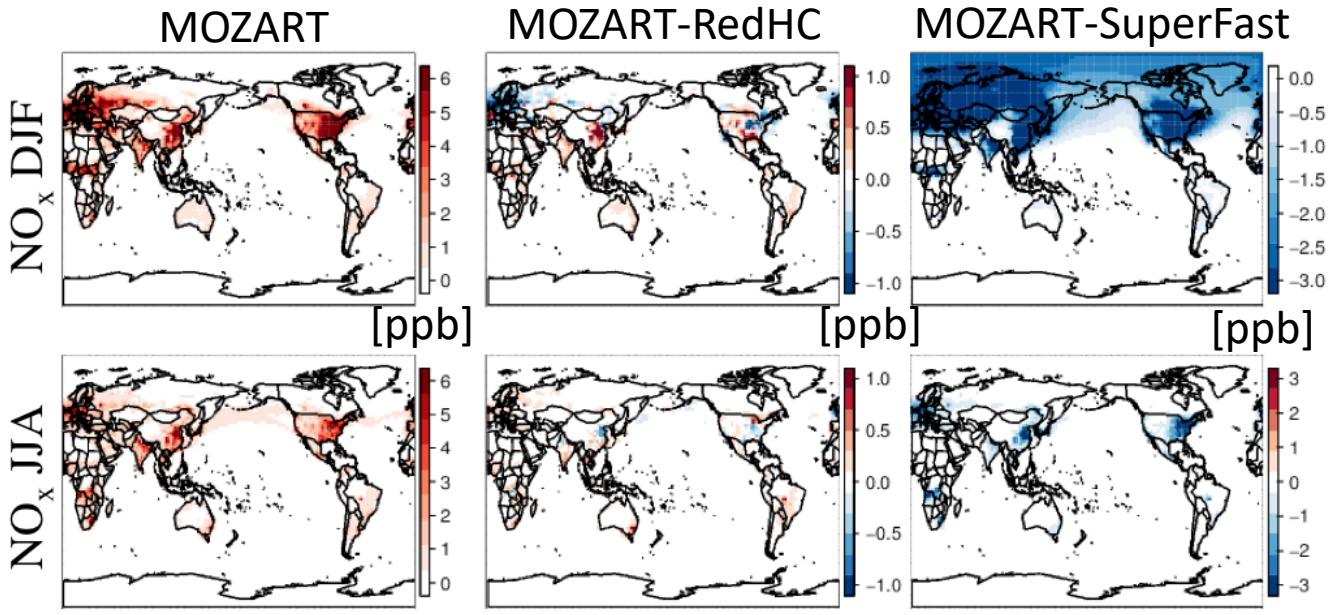
Paper in preparation describing CESM2 chemistry
(Emmons et al., for JAMES)

CAM-chem chemistry choices (CAM6/MAM4)

- MOZART-TS1 – comprehensive Troposphere and Stratospheric chemistry w/VBS-SOA (222 species)
- MOZART-T1 – Troposphere only, stratospheric compounds specified from climatology w/VBS-SOA (187 species)
- VSL halogens (still needs porting to CESM2)

Not supported, but presented in Brown-Steiner et al. (GMD, 2018): https://doi.org/10.5194/gmd-2018-16)

- Super Fast (P. Cameron-Smith, LLNL)
- Reduced Hydrocarbon (ACCMIP)



WACCM

TSMLT: Troposphere-Stratosphere-Mesosphere-Lower Thermosphere

- Includes MOZART-TS1 and mesospheric and ion chemistry, MAM4
- 232 species
- 150 photolysis and 447 kinetic reactions
- *Mechanism to be used for CMIP6*

SC: Specified Chemistry

MA: Middle Atmosphere

- Only Stratosphere-Mesosphere-Lower Thermosphere chemistry (only CH4 chemistry in the troposphere; no NMHCs)

MA-D-region:

Differences between mechanisms

CAM-chem does not include excited state O2, so 2 reactions must be combined:

Reactants		Products	Rate Constant	T	TS	W
O1D + O2	->	O + O2	3.30e-11 exp(55/T)	x	x	
O1D + O2	->	O + O2	6.60e-12 exp(55/T)			x
O1D + O2	->	O + O2_1S	2.64e-11 exp(55/T)			x

CAM-chem does not include NO produced in ionosphere and from solar proton events

To reduce species in Troposphere-only, H is not included:

e.g., H2 + O -> OH + H becomes H2 + O -> OH + HO2

Next Steps and Questions

- Online TUV for radiative transfer (to account for impact of aerosols) being implemented; LUT for cross-sections and quantum yields remains
- Nitrate aerosol scheme using MOSAIC with MAM4 being finalized; requires full chemistry
- Are additional chemistry mechanisms needed?
  - e.g., updated reduced HCs for climate runs with nitrate aerosols
  - Expanded terpene chemistry in progress
- Are any chemistry-related processes needed?
  - Heterogeneous reactions on specific aerosols (e.g., sulfate vs dust, not total SAD)
- Other topics?

Workshop: FUNDAMENTALS OF ATMOSPHERIC CHEMISTRY AND AEROSOL MODELING

NCAR AUG 13-15, 2018

To be announced soon

- Will introduce the fundamentals of atmospheric chemistry and aerosol modeling across different scales (box models, regional, and global models)
- Will teach the science behind atmospheric modeling, covering three main themes; transport, chemistry and aerosols
- Up to 40 students, postdocs, early career professors and researchers with a general background in atmospheric chemistry, but not necessarily in modeling
- https://www2.acom.ucar.edu/workshop/fundamentals-atmospheric-chemistry-and-aerosol-modeling-2018

MICM: Model Independent Chemistry Module

Goal: to create a unique chemistry module that can be implemented in any atmosphere model used at NCAR (and possibly others)

Approach:

1. MICM will create an interface flexible enough to be incorporated in any atmosphere model
2. MICM will provide a framework for developers (inside and outside NCAR) to test and incorporate updated/new approaches or methods
3. Physical parameterizations in atmosphere model will take care of physical processes (rainout, diffusion, deposition)

Chemistry Café

The Chemistry Café is a database of all chemical reactions used in CAM-chem, WACCM and WRF-Chem, allowing for identical mechanisms to be produced in formats for the CESM (MOZART) preprocessor or KPP (for WRF-Chem or BOXMOX).

Will be the framework for storing associated data (Henry's Law constants, photolysis data) in addition to kinetic reaction rate constants

Plan for the next year