Intent of Chemistry Infrastructure

- User-friendly
 - Less code editing for each experiment
 - Fewer hidden side effects (WSM6 doesn't work with Aerosol Indirect?)
 - User can add reaction without having to install some unix tool (yacc)
- Explicit
 - Data describes what chemicals are present and their properties
 - Data describes chemical interactions
 - No code choices about configuration ("if MAM") or code choices based on name ("if hno3")
- Flexible
 - User can add a species to aerosol without rewriting aerosol scheme code
 - User can add a reaction without a complicated user process
- Separated concerns
 - Radiation code is ignorant of which aerosol is being implemented
- Traceable
 - What was the chemistry specified in that experiment?
 - Which emissions did we use?

Generalize interaction of model with external data





Atmosphere Host Models (CCPP)

- CAM (part of CESM, using coupler to surface models) [FV, MPAS, FV3, SE, SE-RR]
- MPAS-A (Includes MPAS, and surface models)
- WRF
- NOAA models



Standard Arrhenius, including (1 + E*P) factor from some pollution modeling

Parameter	Value	Default	Units	Comment
А	Number	1e-8	1/sec*(1/ndens)^(n_react-1)	Always positive number
с	Number	0	к	typical ranges: -1500:1500
D	Number	300	к	typically 300
В	Number	0	none	Sometimes called -n
E	Number	0	1/Pa	Almost always 0

hemical Potential Heating	cph	
Rate:		
Reactants:	CLm + H	
Products:	HCL + e	
ajc : 2019-12-13 :	Add A Comment. Your initials and date will be prepended automatically.	

Musica Development Pathways

MICM (box model) with CCPP

- Photodecomp (j-rates)
- Actinic flux
- Reaction kinetics
- no emissions
- gas phase only
- Database-driven
- -> aerosols

MICM in CAM/CESM without CCPP

CCPP into CAM (or rebuild CAM around CCPP and new versions of physics packages)

CAMP: Combined Aerosol/gas phase solver

Others: Emissions, Evaluation, Assimilation



MICM O atom [mole/mole] at 52 hPa

00 UTC 20 January 1979



WACCM O atom [mole/mole] at 52 hPa

00 UTC 20 January 1979



MICM/Chapman in CAM

Full WACCM



analy 10.16 (214 (16.4))

4.75e-12 4.50e-12 4.25e-12 4.00e-12 3.75e-12 3.50e-12

3.25e-12 3.00e-12 2.75e-12 2.50e-12 2.55e-12 2.55e-12 1.55e-12 1.55e-12 1.55e-12 1.00e-12 5.50e-13 5.50e-13 0.00

MUSICA Status

Musica v0 is cam-chem running with a spectral element dynamical core including regional refinement.

- Improved ozone over (CONUS) regionally-refined region (Forrest)

Box chemistry solver with CCPP: "MICM" <u>https://github.com/NCAR/MusicBox</u>

- MICM scheme: https://github.com/NCAR/MICM_chemistry/blob/master/src/chemistry_driver.meta https://github.com/NCAR/MICM_chemistry/blob/master/src/chemistry_driver.F90
- Incorporated (MICM-chapman) in atmosphere model
- Works with a web-service preprocessor
- Will replace this with a combined gas/aerosol multiphase solver (CAMP) without a preprocessor. Allows runtime specification of chemistry.

Both MICM and CAMP use (very similar) specification of molecular properties and chemical reactions CCPP in CAM has some ways to go.