



CAM-Chem and WACCM

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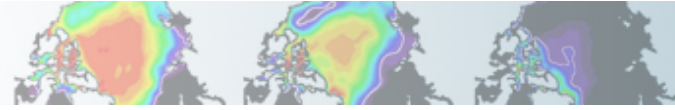
U.S. DEPARTMENT OF
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WACCM Compsets & Scientifically Validated Resolutions

- **B Compsets:** Fully active atmosphere (CAM), land (CLM), ocean (POP), sea ice (CICE); stub land ice (SGLC)
 - **B_1850_WACCM** (short name **B1850W**): Pre-industrial (perpetual year 1850AD)
 - **B_1850_WACCM_CN** (**B1850WCN**): Pre-industrial with carbon-nitrogen cycle in CLM. **Scientifically validated at 1.9x2.5_gx1v6.**
 - **B_1850-2000_WACCM_CN** (**B20TRWCN**): 20th Century (1850-2000 transient) with carbon-nitrogen cycle in CLM. **Scientifically validated at 1.9x2.5_gx1v6.**
- **F Compsets:** Fully active atmosphere (CAM), land (CLM); prescribed sea ice (CICE); data ocean (SST data mode); stub land ice (sglc)
 - **F_1850_WACCM** (**F1850W**): Pre-industrial (perpetual year 1850AD)
 - **F_2000_WACCM** (**FW**): Present-day (perpetual year 2000AD)



Building WACCM

- Create a new case with the perpetual year 2000 at 4x5 degrees:

```
> cd $CCSMROOT/scripts
```

```
> create_newcase
```

```
-case ~/case/f2000.track1.4deg.001
```

```
-compset FW
```

```
-mach bluefire
```

```
-res f45_f45
```

```
-skip_rundb
```



Changing a reaction rate

- The **chemistry preprocessor**: generates CAM Fortran source code to solve chemistry.
- Input: a simple ASCII file listing chemical reactions and rates.
- Sample input files are in `$CCSMROOT/models/atm/cam/chem_proc/inputs`

```

SPECIES
  Solution
  O3, O, O1D -> O, O2, O2_1S -> O2, O2_1D -> O2
  End Solution

  Fixed
M, N2
  End Fixed
End SPECIES

Solution Classes
  Explicit
  CH4, N2O, CO, H2, CH3CL, CH3BR, CFC11, CFC12
  End explicit
  Implicit
  O3, O, O1D, O2, O2_1S, O2_1D
  End implicit
End Solution Classes

CHEMISTRY
  Photolysis
[jo2_a] O2 + hv -> O + O1D
  End Photolysis

  Reactions
[cph1,cph] O + O3 -> 2*O2      ; 8e-12, -2060
  End Reactions
END CHEMISTRY

```

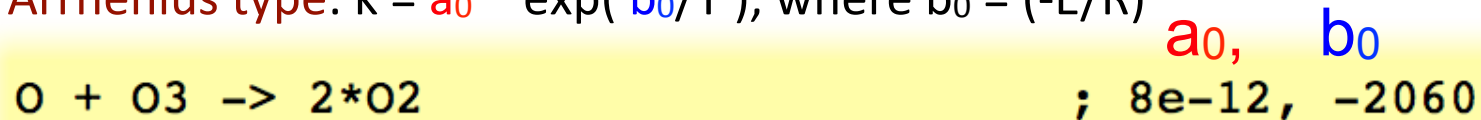


Modifying the chemical preprocessor input file

- **Temperature-independent rates:** k [$\text{cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$] = a_0



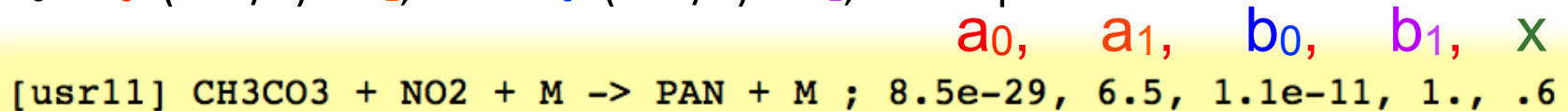
- **Arrhenius type:** $k = a_0 * \exp(b_0/T)$, where $b_0 = (-E/R)$



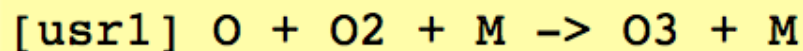
- **Troe rate constant:** $k = \alpha^x / (1 - \beta^2)$, where:

$$\alpha = k_0 * M / k_\infty, \quad \beta = \log_{10}(\alpha), \quad M = \text{air density (molec cm}^{-3}\text{)}, \quad T = \text{temperature (K)}$$

$$k_0 = a_0 * (300/T)^{a_1}, \quad k_\infty = b_0 * (300/T)^{b_1}, \quad x = \text{“exponential factor”}$$



- **User-specified reaction rate:**



rate defined in routine mo_usrrxt.F90



Building the model with new chemistry

- Copy a sample preprocessor input file to the case directory and edit it:

```
> cd $CASEROOT
> source Tools/ccsm_getenv
> cp $CCSMROOT/models/atm/cam/chem_proc/inputs/
  waccm3_57spc_JPL06_ccmval_clbrfam.in my_waccm_mech.in"
> nedit my_waccm_mech.in &
```

- Modify the temperature-dependence of the reaction $O + O_3 \rightarrow 2*O_2$, changing the exponent term from -2060 to -2050:

```
[cph1,cph] O + O3 -> 2*O2 ; 8e-12, -2050
```



Building the model with new chemistry

- Edit the file `env_conf.xml` in the case directory to add the CAM configure option `-usr_mech_infile` pointing to the new preprocessor input file:

```
> xmlchange -file env_conf.xml -id CAM_CONFIG_OPTS -val "-  
phys cam4 -chem waccm_mozart -usr_mech_infile $CASEROOT/  
my_waccm_mech.in"
```

- IF you had previously configured this case, you would need to clean up via:

```
> configure -cleanall
```

- Now configure the case:

```
> configure -case
```

These same steps may be used to change chemistry in CAM-Chem compsets as well.



Accessing 'use_cases'

- We have set up further specific atmosphere runs. List is in:
`$CCSMROOT/models/atm/cam/bld/namelist_files/use_cases`
 - An example: WACCM REFB1 used for WMO ozone assessment runs:
`waccm_refb1`. Others include chemistry and future emissions.
 - To use this, just need an `xmlchange` command to modify `CAM_NML_USE_CASE` in `env_conf.xml`: before `configure`
- ```
> xmlchange -file env_conf.xml -id CAM_NML_USE_CASE -val
"waccm_refb1"
```
- Now: `reconfigure` (`configure --cleanall` then `configure --case`)
  - If you look in `$CASEROOT/Buildconf/cam.buildnml.csh` you will see changes
  - Exercise: Set up a new FW case (`create_newcase`), then issue the above `xmlchange` command, `configure` and compare the `cam.buildnml.csh` file
  - Note: you can make your OWN `use_cases` too.