Documentation for CESM CAM4 and 5 with Chemistry (and Prescribed Dynamics); Running an existing component set (on yellowstone)

More information on how to run CESM:
http://www.cesm.ucar.edu/models/cesm1.1/cesm/doc/userguide/book1.html
To start, check out the latest version of the model: http://www.cesm.ucar.edu/models/cesm1.1/

Skip this step if you are working on yellowstone.

This documentation is for the release Version cesm1_1! CESM1.1 contains NO scientifically validated component sets and as such is not to be used for scientific simulations.

Creating, building and running

Pick One Component Set (see table), or find a list of all supported compsets:
http://www.cesm.ucar.edu/models/cesm1.1/cesm/doc/modelnl/compsets.html

Compsets	Model (phys)/ radiation	Chemistry	Components / Meteorology
B_2000_TROP_MOZART (BMOZ) B_2000_MOZSOA_CN	CAM4, active	trop_mozart +soa chemistry	All active + CLM/CN
F_2000_TROP_MOZART (FMOZ) F_2000_MOZSOA_CN (FMOZSOA)	CAM4, passive	trop_mozart +soa chemistry	Prescr. ocn/ice, CLM/CN
F_SD_CAMCHEM_CN F_SD_BAM_CN F_TROP_STRAT_CHEM_CN (FTSC)	CAM4, passive	trop_mozart trop_bam trop/ strat_mozart	Prescr. ocn/ice, CLM/ CN, offline: GEOS5 Prescr. ocn/ice, CLM/CN
B_2000_CN_CHEM (B2000CNCHM) B_1850_CN_CHEM (B1850CNCHM) B_1850-2000_CN_CHEM (B20TRCNCHM) F_1850_CN_CHEM (F1850CNCHM)	CAM4, active CAM4, passive	super_fast_llnl	MEGAN VOC emis CLM/CN
B_2000_MOZMAM_CN (BMOZMAM) F_2000_MOZMAM_CN (FMOZMAM) F_2000_STRATMAM3_CN F_2000_STRATMAM7_CN	CAM5, active CAM5 passive	trop_mozart mam trop/ strat_mozart mam	All active, CLM/CN Prescr. ocn/ice, CLM/CN

Roadmap for a CAM-Chem model run (Quickstart):

1. Create a new case called <case_name>:

CESM_ROOT = <release tag> (intern)

On yellowstone: /glade/p/cesm/cseg/collections/cesm1_1

Go to your model directory **CESM_ROOT**, then **cd scripts** and invoke:

create_newcase -case $HOME/<case_name> -res f19_f19 -compset <COMPSET> -mach yellowstone (change **'yellowstone'** to your computer name)

f19_f19: data ocean (finite volume of the atmosphere)

f19_g16: active ocean

A new directory **<case_name>** is created in your **<home_dir>** (below, **<case_dir>** is **<home_dir>/<case_name>**)

2. Setup your run: invoke ./cesm_setup
3. Make changes to defaults if desired (see description below)
   - edit **env_build.xml** to change calendar type (NO_LEAP, GREGORIAN), CAM_CONFIG_OPTS (e.g., to point to new mechanism file), different vertical levels. If you have to rebuild the model, make sure to invoke *.clean_build first
4. Configure and build the model in **<case_dir>**: **./*.build** file
5. Make changes to your namelist variable (if desired): edit file **user_nl_cam**, **user_nl_clm** ect. in **<case_dir>** to modify paths to emissions, output variables. **NOTE: changes in user_nl* files do not require new configuration or build.**
6. Invoke **./preview_namelists**
7. Check your model setup in CaseDocs: e.g., atm_in (namelist), chem_mech.in (chemistry mechanism)

- Check run setup: **env_run.xml.** The default is a test run -- 5 days.. **NOTE: changes can be performed any time during the run**

8. **./*.submit** (or bsub < ./*.run on yellowstone)
   - default for model output is in **<run_dir>: /glade/scratch/<username>/<case_name>/run**
   - namelist that was used for run in **<run_dir>/atm_in**

Modification of the run (no changes to the model configur1ation):

1. edit **env_run.xml** to change run specifications, run type (startup, branch), start date (RUN_STARTDATE), run time, output, restart, type of archiving
2. open ***.run** to change run specific parameters, NOTE: there is a new 'small' queue for <2hour runs available that will be treated like premium but is cheaper.
3. after these changes you can just resubmit the run

Some additional useful information:

CONTINUE_RUN: needs to be set to TRUE to continue a run for several time segments

RESUBMIT: set value to the number of segments you want to run (value counts down during the simulation)

REST_OPTION: will write out restart files in the frequency chosen (e.g., nmonths every months)

REST_N: frequency of restart file output, 0: no restart file

DOUT_L_MS: archiving to mss is not a default and needs to be set

Archiving:

–short-term archiving in /glade/scratch/<username>/archive

–long-term archiving on the mass store

Modification of the namelist (can be done during the run, no compilation required):
(nl definitions**:** http://www.cesm.ucar.edu/cgi-bin/eaton/namelist/nldef2html-pub)

edit **user_nl_cam** in your <case_dir> to change your namelist, for example, emissions, met fields, model output etc. Examples:

add aircraft of satellite obs. track option:

```
&satellite_options_nl
  sathist_fincl   =  species
  sathist_hfilename_spec   = '%c.cam2.aircraft.%y-%m-%d-%s.nc'
  sathist_track_infile          = '<aircraft track file location>'
```

running with MEGAN emissions:

```
&megan_emis_nl
 megan_factors_file            = '/glade/user/emmons/megan/megan21_emis_factors_c20120313.nc'
 megan_specifier               = 'ISOP = isoprene',
'C10H16=myrcene+sabinene+limonene+carene_3+ocimene_t_b+pinene_b+pinene_a+phellandrene_a+thuje
ne_a+terpinene_a+terpinene_g+terpinolene+phellandrene_b+camphene+bornene+fenchene_a+ocimene_al+
ocimene_c_b+camphor+linalool+terpineol_4+terpineol_a+cineole_1_8+linalool_OXD_c',
  'CH3OH = methanol',
  'C2H5OH = ethanol',
 'CH2O = formaldehyde',
 'CH3CHO = acetaldehyde',
  'CH3COOH = acetic_acid',
 'CH3COCH3 = acetone',
 'HCOOH = formic_acid',
 'HCN = hydrogen_cyanide',
  'NH3 = ammonia',
 'C2H6 = ethane',
 'C2H4 = ethene',
 'C3H8 = propane',
 'C3H6 = propene',
  'BIGALK = pentane + hexane + heptane + tricyclene',
 'BIGENE = butene',
 'TOLUENE = toluene'
```

Modification of the chemistry mechanism, example:

1. copy an input file in $CCSMROOT/models/atm/cam/chem_proc/input to your directory and name it: **my_mech.in**
2. edit **my_mech.in**
3. edit **env_build.xml** and add to :
   <entry id="CAM_CONFIG_OPTS" ... usr_mech_infile my_mech.in" />
4. if needed, modify source code (for example for wet-dep or dry-dep) and place in appropriate subdirectory of **<case_dir>/SourceMods/**:

- files originally in /models/atm/cam/src/chemistry/mozart/ go in **<case_dir>/SourceMods/src.cam/**
- files originally in models/drv/shr/ (e.g., seq_drydep_mod.F90) go in

<case_dir>/SourceMods/src.share/

5. invoke ***.clean_build** and ***.build** to rebuild your model
6. if you have trouble configuring (e.g., errors in your mechanism file), edit the **configure** script: **env_case.xml** commenting out the line: rm -rf $CASEBUILD. This allows you to track down how far the pre-processor got, etc. However, you have to invoke **cesm_setup** –clean and **cesm_setup** again

Add new species:

If you add a species that is not listed in the species_name_table list, you can map it to one of the species in the list, as done in the subroutine seq_drydep_init.F90
Add your new species in the masterlist: models/atm/cam/bld/namelist_files/master_drydep_list.xml

if you want to add a species that will be dry deposited, you might have to adjust the following routines:
– models/drv/shr/seq_drydep_mod.F90 -> test_name
– models/atm/cam/src/chemistry/mozart/mo_drydep.F90 (subroutine drydep_xactive)
– models/lnd/clm/src/biogeochem/DryDepVelocity.F90
You have to modify the setup of the mechanism if you add more species: models/atm/cam/src/chemistry/…

Available Deposition Schemes:

Dry Deposition:
namelist options in drv_flds_in (drydep_inparm):
drydep_list = list of species (controlled through the masterlist now)
drydep_method =
'table' (prescribed method in CAM)
'xactive_atm' (interactive method in CAM)
'xactive_lnd' (interactive method in CLM)

Wet Depostion (wash out):
namelist options in atm_in (wetdep_inparm)
gas_wetdep_list = list of species
gas_wetdep_method =
'NEU' (J Neu's scheme)
'MOZ' (MOZART scheme)

Available Chemistry Mechanisms:

MOZART4 Chemistry: trop_mozart (103 species) including HCN,CH_3CH + C_2H_2, HCOOH
MOZART4 trop-start mozart (122 species) including stratospheric heterogeneous reactions
MOZART4 +mam 4 additional reactions on aerosols
MAM get information from the Chemistry (SO2, DMS, H2SO4) to calculate the aerosol modes. If chemistry is not included, these values are prescribed using a climatology.
Superfast Chemistry (15 species)

Emissions: Default path on Yellowstone: /glade/p/cesm/cseg/inputdata/atm/cam/chem/emis
For trop_mozart (MOZART-4):
MOZART-4 standard emissions (Emmons et al., GMD, 2010)
/glade/p/cseg/cesm/inputdata/atm/cam/chem/emis/1992-2010/

Default for offline model runs:
–Anthropogenic: POET, with REAS over Asia (time-varying for 1997-2010; 1997 used for 1992-1996).
–Biomass burning: GFED-v2 - 1992-1996: avg of 1999-2007; 1997-2008: for each year/month; 2009-2010: FINN.
–Biogenic, soil, ocean, volcano: POET, GEIA,

Species emitted for standard mozart-4 chemistry:
NO, CO, C2H6, C2H4, C3H8, C3H6, BIGALK, BIGENE, TOLUENE
ISOP, C10H16, CH2O, CH3CHO, CH3OH, C2H5OH, CH3COCH3, MEK
CB1, CB2, OC1, OC2, SO2, DMS, NH3, HCN, CH3CN, C2H2, HCOOH

If running with FINN fire emissions, also have:
NO2, BIGALD, CH3COCHO, CH3COOH, CRESOL, GLYALD, HYAC, MACR, MVK

Improved Climatology for the Stratosphere based on IPCC model runs based on WACCM
(O_3, NOy, CH_4, CO)

ACCMIP and RCPs, speciated for trop_mozart:
/glade/p/cesm/cseg/inputdata/atm/cam/chem
1850-2000_emis
2000-2100_RCP45
2000-2100_RCP85

If running with MEGAN, must create emissions files for all MEGAN species, with the biogenic emissions removed (if have other types, such as bb).

Aircraft emissions (time-dependent, 3D, for NO, CO, SO2, BC, etc.):
/glade/p/cesm/cseg/inputdata/atm/cam/chem/emis/

For MAM surface and external forcings:
/glade/p/cesm/cseg/inputdata/atm/cam/chem/trop_mozart_aero/emis/

Available Meteorological Datasets: (ESG)
the location is:
http://www.earthsystemgrid.org/browse/viewDataset.htm?datasetId=f9a382be-53c5-11e0-80e4-00c0f03d5b7c

for MERRA, and

http://www.earthsystemgrid.org/browse/viewDataset.htm?datasetId=9d662678-4e5c-11e0-80e4-00c0f03d5b7c

GEOS5: 1.9x2.5, 0.5x0.6 2004-present
MERRA: 1.9x2.5 0.5x06, 1979-present

On Yellowstone:
/glade/p/cesm/cseg/data_tmp/