

NorESM and chemistry

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- Introduction
- Chemical schemes
- Chemical preprocessor
- Coupling
- Emissions
- Task

- CAM

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- CAM-Oslo

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- CAM \otimes Chemistry

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- CAM-Oslo \otimes Chemistry ?

Overview

- Tracers

DMS	SO ₂	SO ₄	BC	OC	SS	DUST	(H ₂ O ₂)	Total
1	1	6	6	3	3	2	(1)	23

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Some extra information

- MSA is formed, and added to OC aerosol
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What is lacking?

- Evolution of oxidants since industrial period
- Short time scales - possible non-linearities are missed
- Consistency for impact of SLCF: e.g., emissions affecting O₃ versus emissions affecting BC

Where

- `noresm/models/atm/cam/src/chemistry`

Where

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Three types of subdirectories

- Common: `mozart`
- Specific for aerosols: `bulk_aero`, `modal_aero`
- The actual schemes:

<code>pp_none</code>	<code>pp_super_fast_llnl</code>
<code>pp_super_fast_llnl_mam3</code>	<code>pp_trop_bam</code>
<code>pp_trop_ghg</code>	<code>pp_trop_mam3</code>
<code>pp_trop_mam7</code>	<code>pp_trop_mozart</code>
<code>pp_trop_strat_bam_v1</code>	<code>pp_waccm_ghg</code>
<code>pp_waccm_mozart</code>	<code>pp_waccm_mozart_v1</code>

Example:

- `pp_trop_mozart`

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Content of directory

```
chem_mech.doc      chem_mech.in
chem_mods.F90     m_het_id.F90
mo_adjrxn.F90     mo_imp_sol.F90
mo_indprd.F90     mo_lin_matrix.F90
mo_lu_factor.F90  mo_lu_solve.F90
mo_nln_matrix.F90 mo_phtadj.F90
mo_prod_loss.F90 mo_setrxn.F90
mo_sim_dat.F90    m_rxn_id.F90
mo_spc_id.F90
```

Chemistry: Mozart - tropospheric chemistry

Number of species

- 103 species (including Pb and Rn²²²)

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1	2	2/1	4	4	1	1

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Some specification

- Conversion of hydrophobic to hydrophilic OC and BC ($\tau = 1$ to 2 days)
 - OC1 \rightarrow OC2
 - BC1 \rightarrow BC2
- Nitrate equilibrium (Metzger et al., 2002)
- Oxidants calculated on-line
- SOA production calculate on-line
- Heterogeneous chemistry: influenced by aerosols surface area
- No MSA taken into account

SOA-production in Mozart

Emissions of SOA precursors [Tg/yr]

		Anthrop.	BB	Biogenic
C10H16	Lumped monoterpenes (α -pinine)			90.7
TOLUENE	Lumped aromatics	31.5	2.8	
BIGALK	Lumped alkenes C>3	77.6	1.4	

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C10H16 + NO₃
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TOLUENE + OH
BIGALK + OH

Current SOA production in Mozart

- 10 Tg/yr
- No SOA production from isoprene

CAM combined with Mozart

- Standard

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CAM-Oslo combined with Mozart

Be carefull about

- Naming: SO_2 , DMS, SO_4 both in CAM-Oslo as in Mozart
- OFF-LINE CAM-Oslo influenced by radiative active chemical species: O_3 , CH_4
- Deposition of radiative active species: BC, DUST

Emitted species in CAM-Oslo

- BC/OC/SO₂

Type	Volcanic	Biomass burning	Anthropogenic
# layers	9	8	2

- DMS (only at surface)
- OC from the ocean
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Some specifications

- Emissions files explicitly named in `emissions.F90`
- Works mainly with decadal data for fossil fuel and bb emissions
- For monthly varying emissions: applied constant between begin/end of month
- Units of off-line emissions: kg/m²/s

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Stratosphere

- Stratospheric sulphate aerosol is prescribed.

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Described in the (atmospheric) namelist

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- 2D (molecules/cm²/s): `srf_emis_specifier`
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`CYCLICAL` (needs `srf_emis_cycle_yr`)

`SERIAL`

`INTERP_MISSING MONTHS` (easy for transient decadal emissions)

`FIXED` (needs `srf_emis_fixed_ymd`)

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Application of monthly varying emissions

- Interpolated between middle of months
- Disadvantage: simulations starting 1 January, ending 31 December

Preprocessing: modify/generate a chemistry scheme (1)

In the compset (where you define the case)

```
CAM_CONFIG_OPTS="  -phys cam4  
                  -cam_oslo aeronline  
                  ...  
                  -chem trop_mozart  
                  -usr_mech_infile <description file>"
```

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Examples of <description file>

- noresm/models/atm/cam/chem_proc/inputs/ **trop_mozart_mech.in**
- noresm/models/atm/cam/chem_proc/inputs/
super_fast_LLNL.lut.fixed_ch4.isoprene+O3.in

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Results of pre-processing

cases/<expname>/Buildconf/camconf/chem_proc/source

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SPECIES

Solution S04, DMS -> CH3SCH3, CB1 -> C, MSA -> CH3SO3H, MPSOA ->
C12, MPMSA -> CH3SO3H, MPSO4GA -> S04, ...

Fixed ...

Col-int ...

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Implicit (all others)

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CHEMISTRY

Photolysis ...

Reactions ...

Heterogeneous (wet deposition)

Ext Forcing (3D sources from file, or from lightning parametrization)

Coupling of CAM-Oslo and Mozart (1)

Rationale

- Everything is introduced by CPP-keys

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The same code can give

- CAM-Oslo (original) parallel with Mozart (original)
- CAM-Oslo combined with Mozart-chemistry

Coupling of CAM-Oslo and Mozart (2)

Sulphur cycle

- Units of DMS, SO_2 , SO_4 in CAM-Oslo: converted from [S] to real molecular mass
- Introduce MSA tracer, and formation reaction in Mozart
- Aqueous SO_4 and gas-phase H_2SO_4 formation: use H_2SO_4 , SO_4 , and MSA production rates from Mozart
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- Use CAM-Oslo aerosols (externally and internally mixed)
- Hygroscopic growth: take into account internal mixture

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CAM-Oslo SO₄ used in nitrate equilibrium calculation

Further points of interest

Emissions/speciation

- ACCMIP, RCP45, RCP85: readily available for Mozart
- RCP26, RCP60: possible

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Development

- Coupling with the land model (NO, CO, VOC) and ocean model (DMS)
- There exists more elaborate descriptions of SOA formation

Task 1

- Create/test a case: CAM-Oslo parallel with super_fast_chemistry

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Task 2

- Create/test a case: CAM-Oslo parallel with super_fast_chemistry with modified reaction constant

Task 1

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- (Hint: look at B_1850_CN_CHEM case, and N_1850_AEROSLO case)
- (Hint: think about double-used names as SO₄ - modify aerosoldef.F90, calccol.F90, cam_diagnostics.F90 in SourceMods/src.cam)

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- (Hint: think about double-used names as `SO4` - modify `aerosoldef.F90`, `calccol.F90`, `cam_diagnostics.F90` in `SourceMods/src.cam`)

Task 2

- Create/test a case: CAM-Oslo parallel with `super_fast_chemistry` with modified reaction constant
- (Hint : look at `noresm/models/atm/cam/chem_proc/inputs` at `super_fast_LLNL.lut.fixed_ch4.isoprene+03.in`)