Atmospheric Modeling IV, Chemistry and Aerosols

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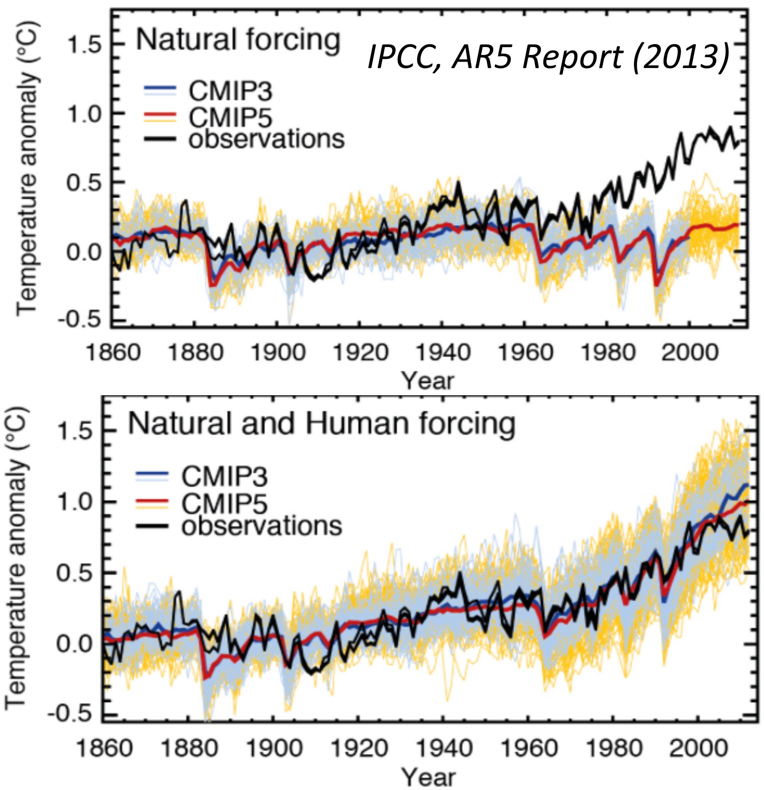
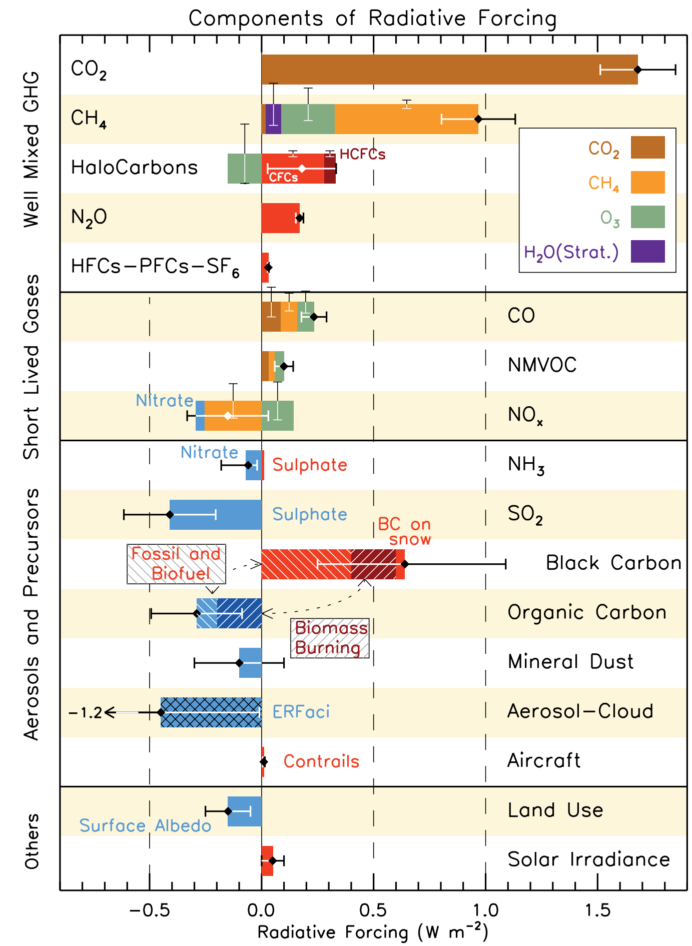
Importance of Chemistry and Aerosols

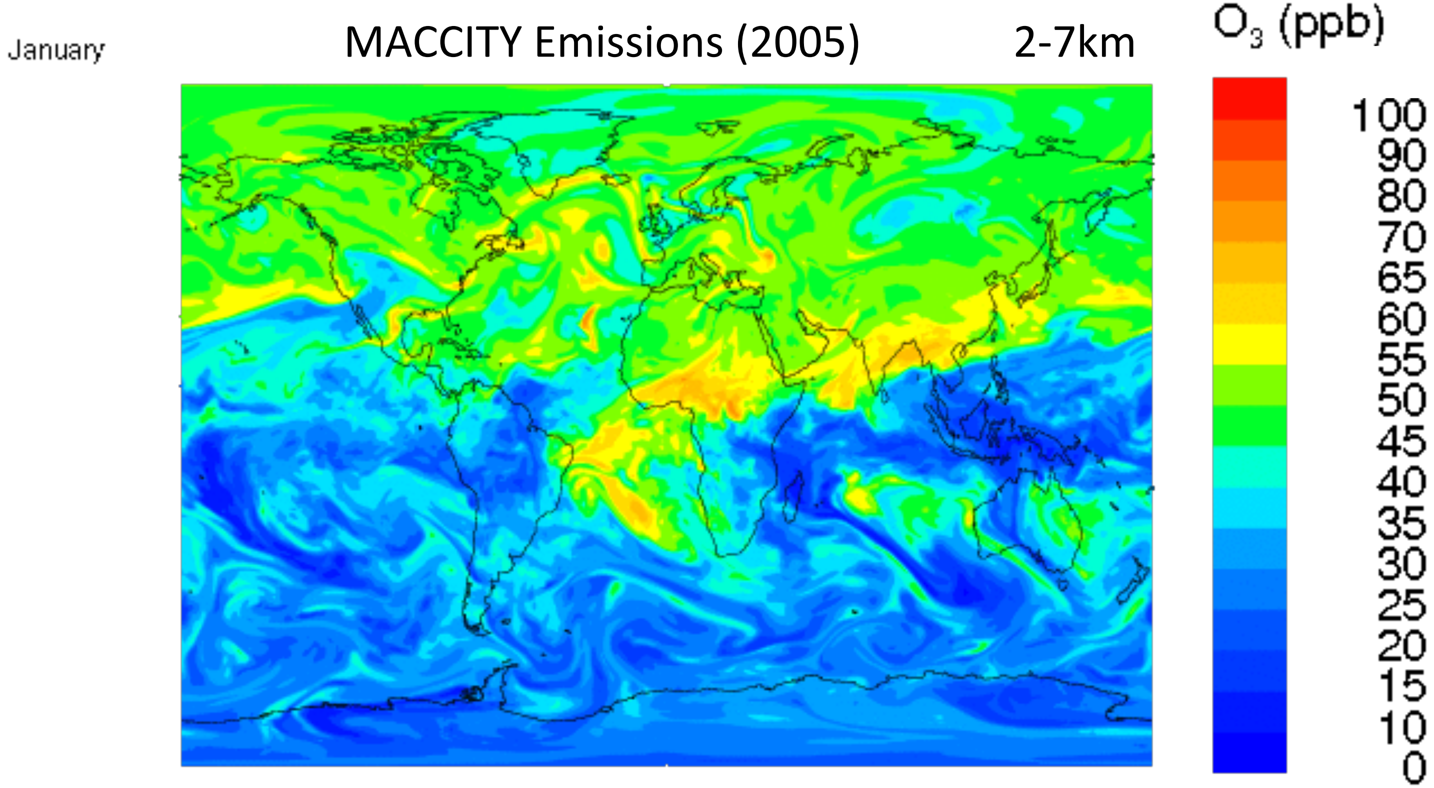




Importance to represent climate gases for radiative forcing: (CO_2), CH_4, O_3, H_2O

Chemistry and aerosols interact with the climate system,
-> need to be well describe in climate models

Interactive Modeling with Chemistry

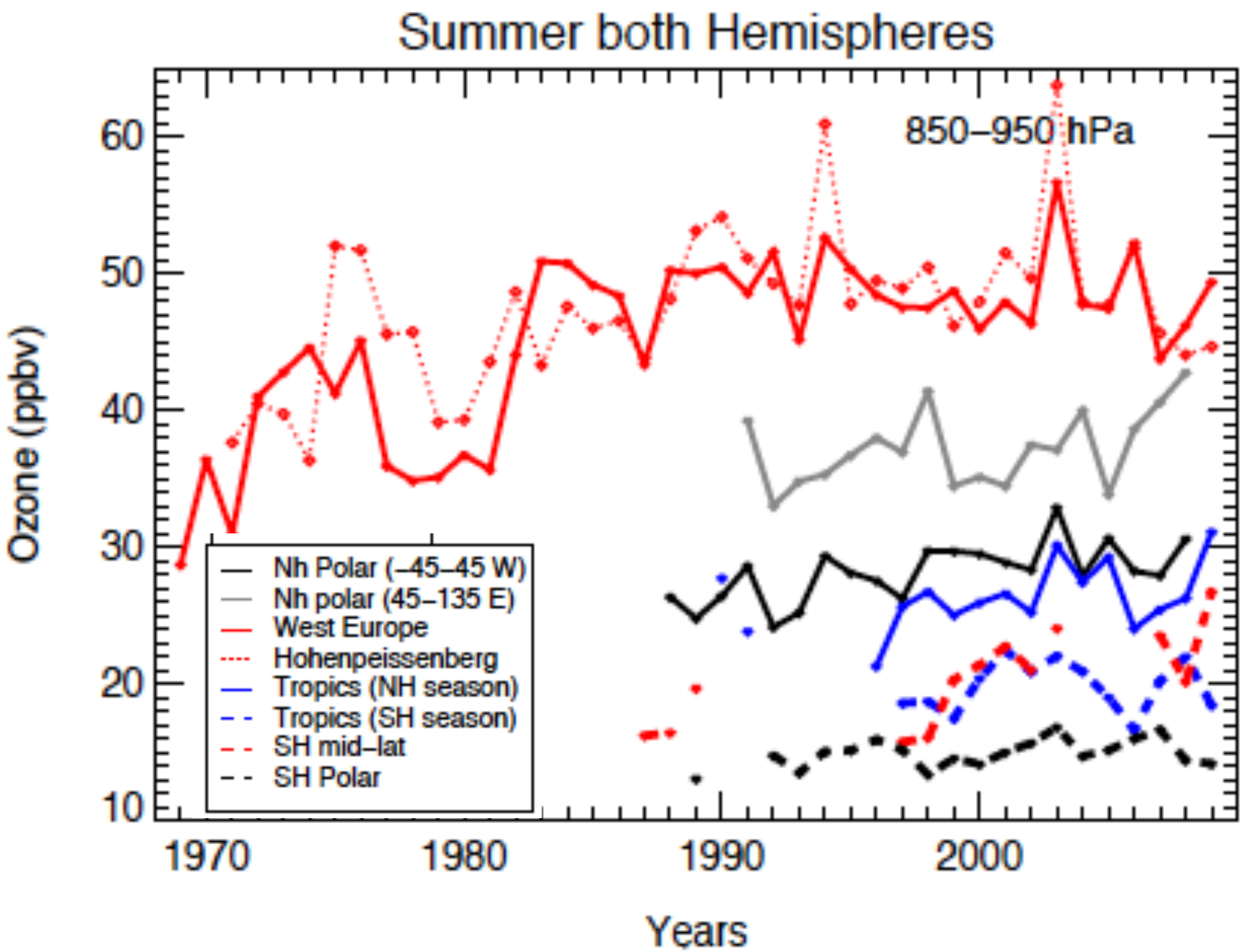


Tropospheric ozone is an important pollutant. It's distribution is dependent on:

- Changes in precursors: NO_x ($NO + NO_2$), CO, volatile organic compounds (VOCs) and other emissions
- Implications for air quality and ecosystem: EPA defines standards for air quality (75 ppb)
- Meteorology and Removal

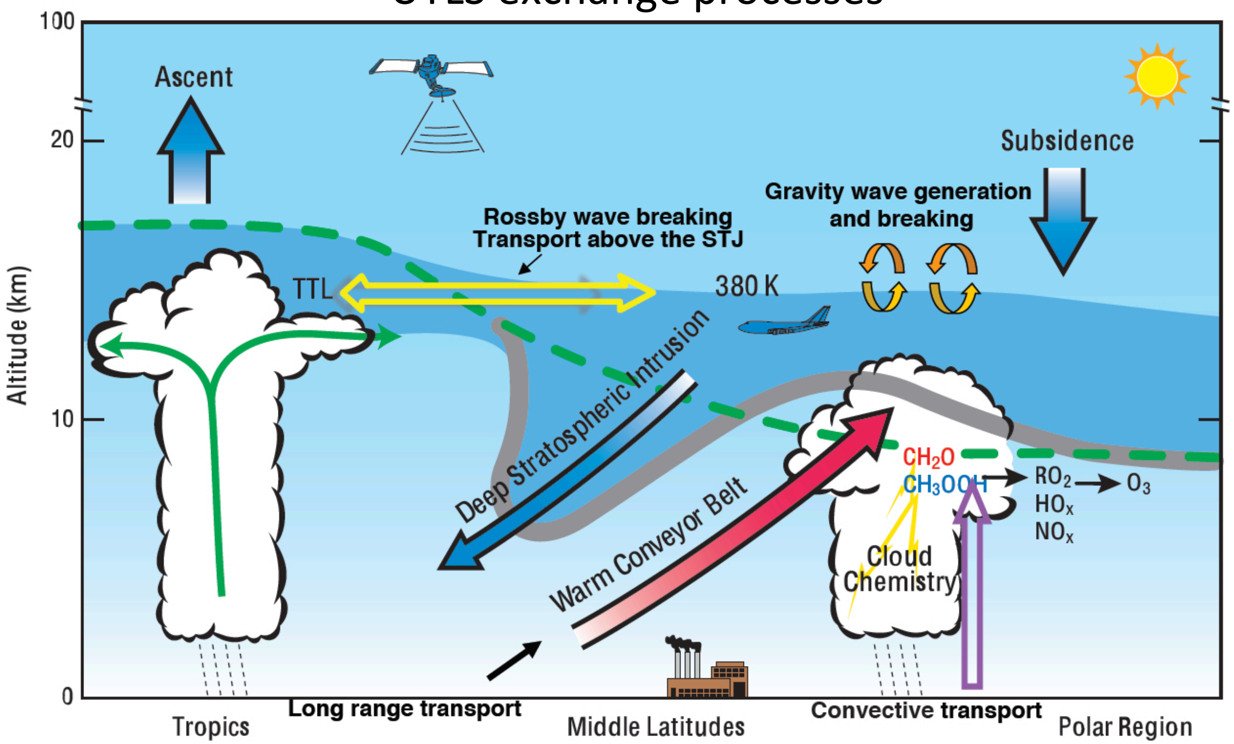
-> Interaction with Radiation (climate gas)

Interactive Modeling with Chemistry



Importance of the Stratosphere, and Exchange Processes

UTLS exchange processes



Stratosphere-Troposphere Analyses of Regional Transport (2008)

- Exchange of chemistry and aerosol due to stratospheric/troposperic transport
- Impact of halogen loading on stratospheric ozone (ozone hole) and impact on climate (importance of very short-lived species)

-> local changes of short time scales are important

Modeling without Chemistry-Climate Interactions in CESM

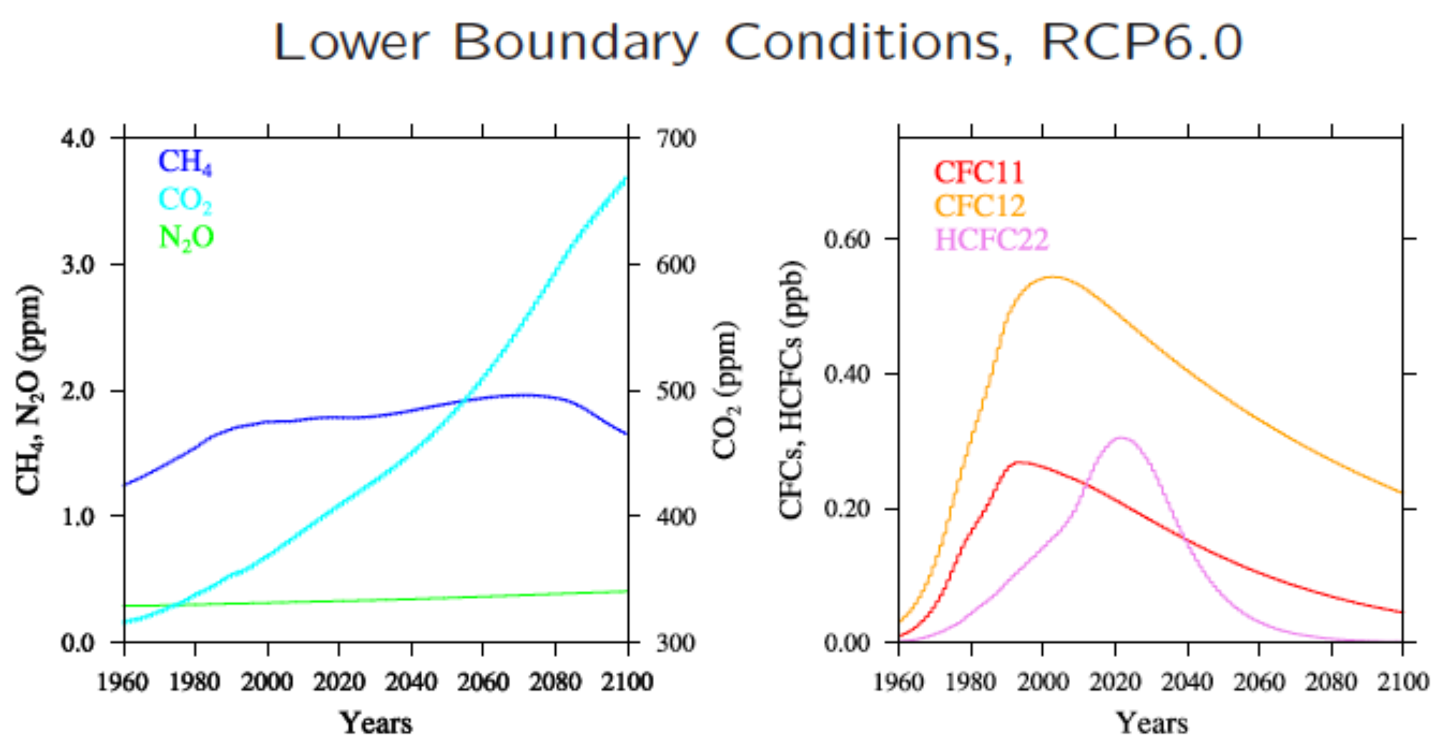
- **CAM4:** Chemistry (including ozone) and aerosols are prescribed for the entire atmosphere (usually monthly fields), also run with the Bulk Aerosol Model (BAM)
- **CAM5:** Aerosols are calculated (Modal Aerosols Model MAM), coupled with simple chemistry ("fixed" oxidants) (prescribe: N_2, O_2, H_2O, O_3, OH, NO_3, HO_2; chemically active: H_2O_2, H_2SO_4, SO_2, DMS, SOAG)

  Limited interaction between Chemistry and Climate

  -> prescribed fields have to be derived using chemistry-climate simulations
- Prescribed ozone is used for radiative calculated

Modeling without Chemistry-Climate Interactions in CESM

- Greenhouse gases are prescribed in monthly fields of CO_2, CH_4, O_3, N_2O, CFCs) through lower boundary conditions. All CFCs can be combined to effective CFC emissions.



Aerosols

Direct Effects:

- Radiation (scattering/absorbing)

Indirect Effects (in CAM5):

- Changes in cloud properties (consistency, reflectivity), precipitation

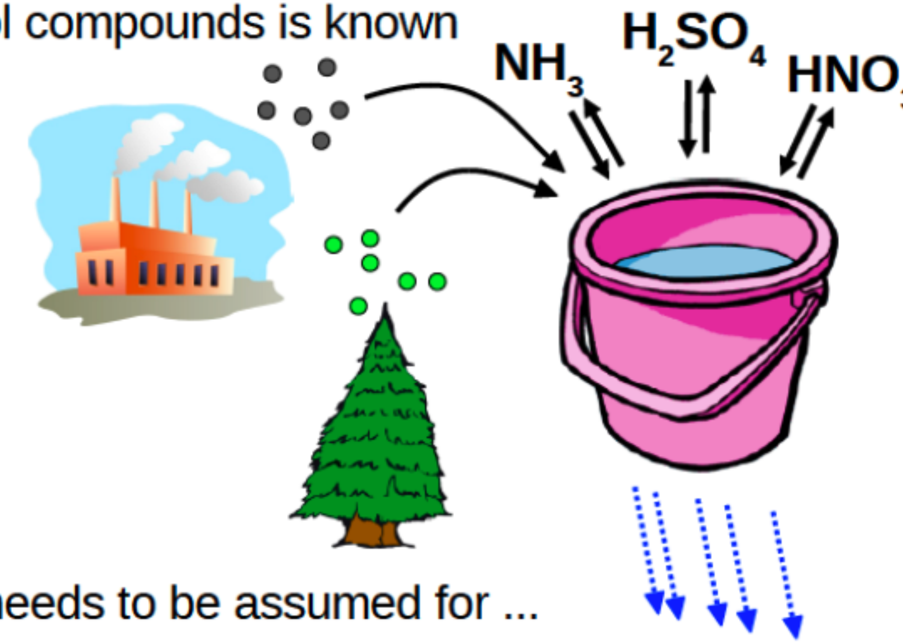
Controlled by: Emissions, nucleation processes, deposition, chemistry

Aerosols in CESM:

- Bulk Aerosols Model (BAM)
- Modal aerosol Model (MAM)

Bulk aerosol scheme

- Only total mass of aerosol compounds is known
- No information on
  - Particle number
  - Aerosol size distribution



- Aerosol size distribution needs to be assumed for ...
  - radiative transfer
  - response of cloud properties to aerosol number
- Can't do aerosol nucleation
- **Numerically efficient**
- **Useful when focus is on complex gas phase / aerosol chemistry**

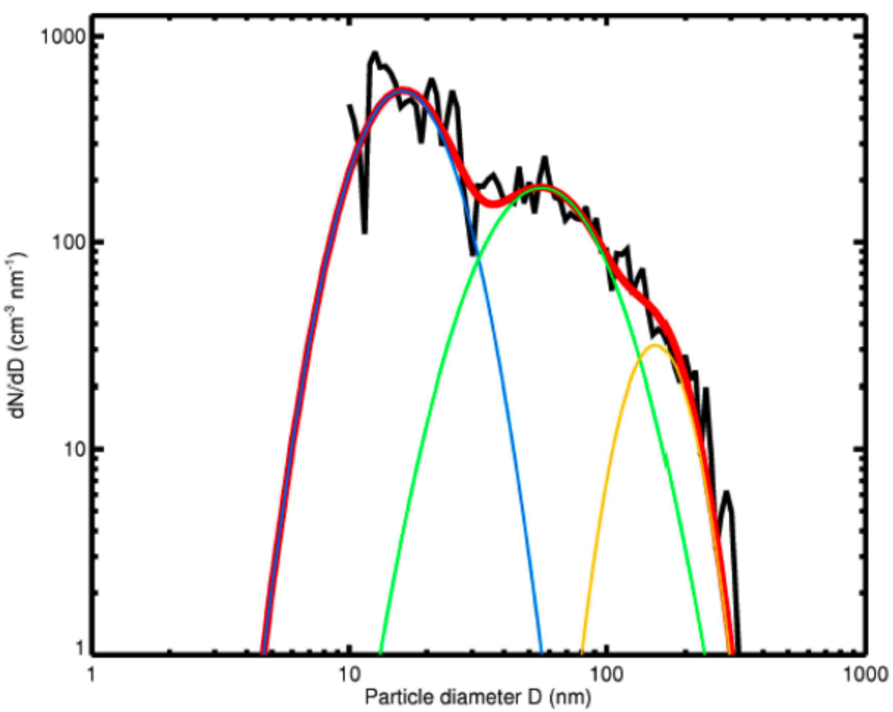
From J. Kazil, CIRES

Modal Aerosol Model (MAM)

Representation of Sulfates, Black Carbon Organic Carbon, Organic Matter (OC, SOA), Mineral Dust and Sea-Salt

CESM CAM5
Aerosol size distribution using 3 modes
Other versions exist with 4 and 7 modes.

Twin Otter data (black)



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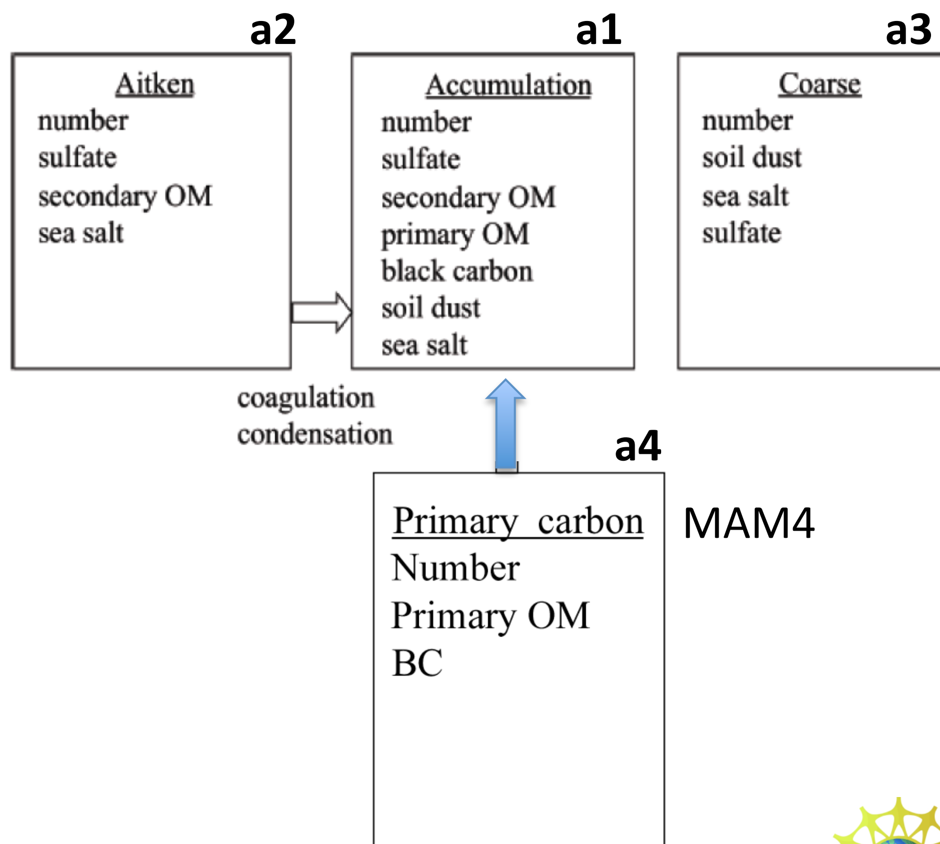
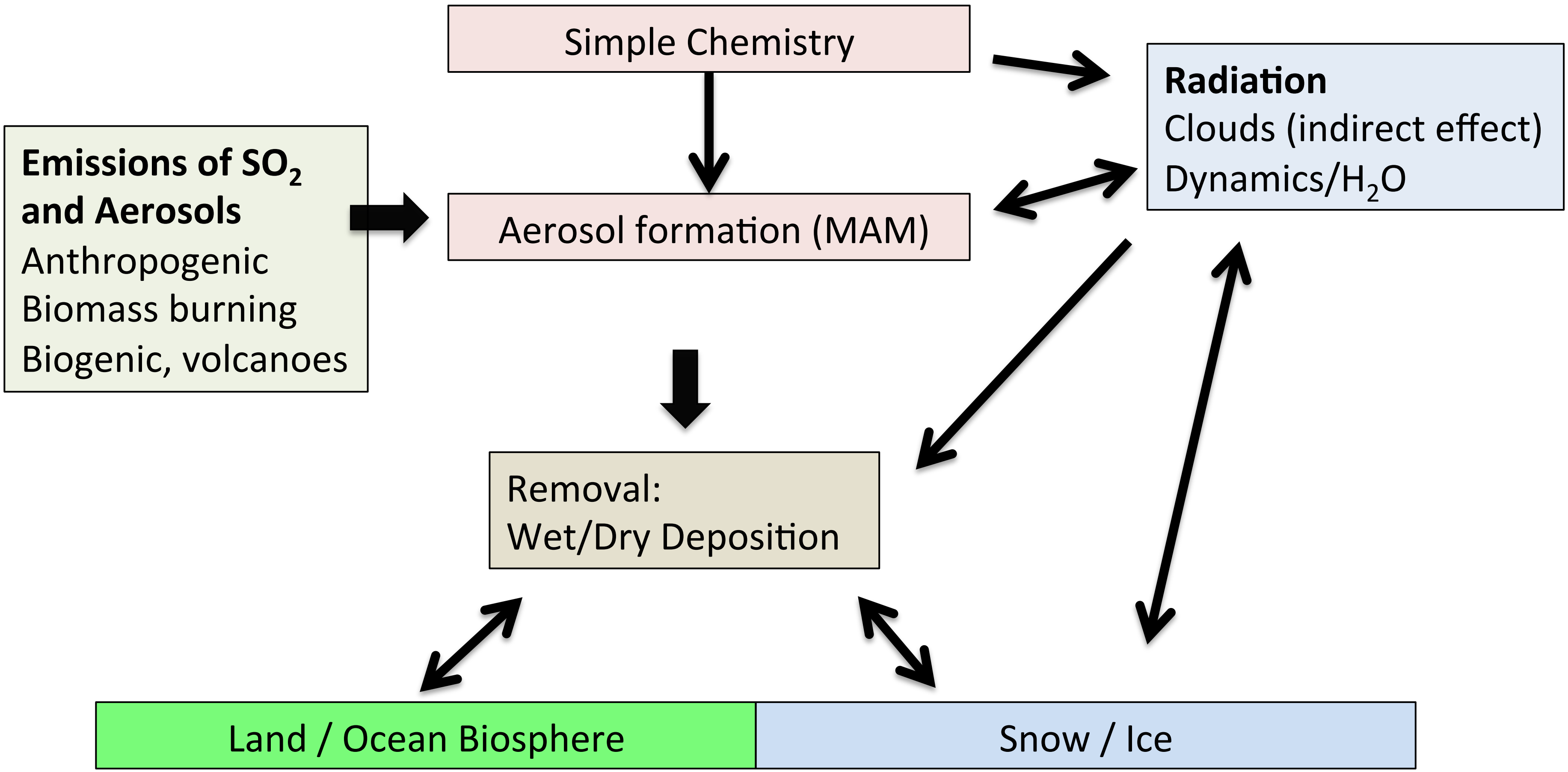


Liu et al., 2016

Chemistry and Aerosols in CESM CAM5



Important processes for simulating Aerosols (and Chemistry)

Emissions and external forcings: surface emission: anthropogenic aerosols; altitude dependent emissions: biomass burning, aircraft.

Chemical mechanism: simple chemistry for aerosol production

Dry Deposition: uptake of chemical constituents by plants and soil (CLM), depending on land type, roughness of surface, based on resistance approach

Wet Deposition: uptake of chemical constituents in rain or ice (linked to precipitation, both large-scale and convective).

Important processes for simulating Aerosols

Emissions and external forcings: surface emission: anthropogenic aerosols; altitude dependent emissions: biomass burning, aircraft.

```
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        'bc_a4        -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/trop_mozart_aero/emis/ar5_mam3_bc_e
        'num_a1       -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/trop_mozart_aero/emis/ar5_mam4_num_
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```

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Bulk Aerosol Model (BAM)

Representation of Sulfates, Black Carbon, Organic Carbon, Organic Matter (OC, SOA), DMS, Mineral Dust and Sea-Salt

```
    SPECIES

      Solution
  H2O2, SO2, SO4, DMS -> CH3SCH3
  OC1 -> C, OC2 -> C
  CB1 -> C, CB2 -> C
  SSLT01 -> NaCl, SSLT02 -> NaCl, SSLT03 -> NaCl, SSLT04 -> NaCl
  DST01 -> AlSiO5, DST02 -> AlSiO5, DST03 -> AlSiO5, DST04 -> AlSiO5
      End Solution

      Fixed
  M, N2, O2
  O3, OH, NO3, HO2
      End Fixed
```

```
CHEMISTRY
     Photolysis
     End Photolysis

     Reactions
   CB1 -> CB2     ; 1.006e-05
   OC1 -> OC2     ; 1.006e-05
     End Reactions

     Ext Forcing
   SO2 <- dataset
   SO4 <- dataset
     End Ext Forcing
```

The chemistry preprocessor: tool that generates CAM Fortran source code; numerically solve a set of differential equations which
represent the chemical reactions -> temporal evolution of the chemical tracers

Modal Aerosol Model: CAM5 and CAM5-chem

CAM5:	**CAM5-Chem**:
Fixed: (N_2, O_2 H_2O,) O_3, OH, NO_3, HO_2 (prescribed with monthly mean values) **Chemically active**: H_2O_2, H_2SO_4, SO_2, DMS, SOAG Chemistry: photolysis of H_2O_2, includes DMS, [usr_HO2_HO2] HO2 + HO2 -> H2O2 H2O2 + OH -> H2O + HO2 [usr_SO2_OH] SO2 + OH -> H2SO4 DMS + OH -> SO2 **Aerosol formation of SO_4:** Chemically: from SO_2 -> H_2SO4 aq-phase (H_2O_2, O_3), nucleation, H_2SO_4 deposition	Comprehensive tropospheric and stratospheric chemistry Photolysis, DMS, [OH_OH_M] OH + OH + M -> H2O2 + M [OH_H2O2] H2O2 + OH -> H2O + HO2 [usr_HO2_HO2] HO2 + HO2 -> H2O2 + O2 [H2O2_O] H2O2 + O -> OH + HO2 [CL_H2O2] CL + H2O2 -> HCL + HO2 [usr_HO2_aer] HO2 -> 0.5*H2O2 (not in CAM5) [usr_SO2_OH] SO2 + OH -> H2SO4 DMS + OH -> SO2 **-> much more comprehensive description of chemistry (including H_2O_2 and Ozone)** **-> impact on SO_4 formation**

Important processes for simulating Aerosols

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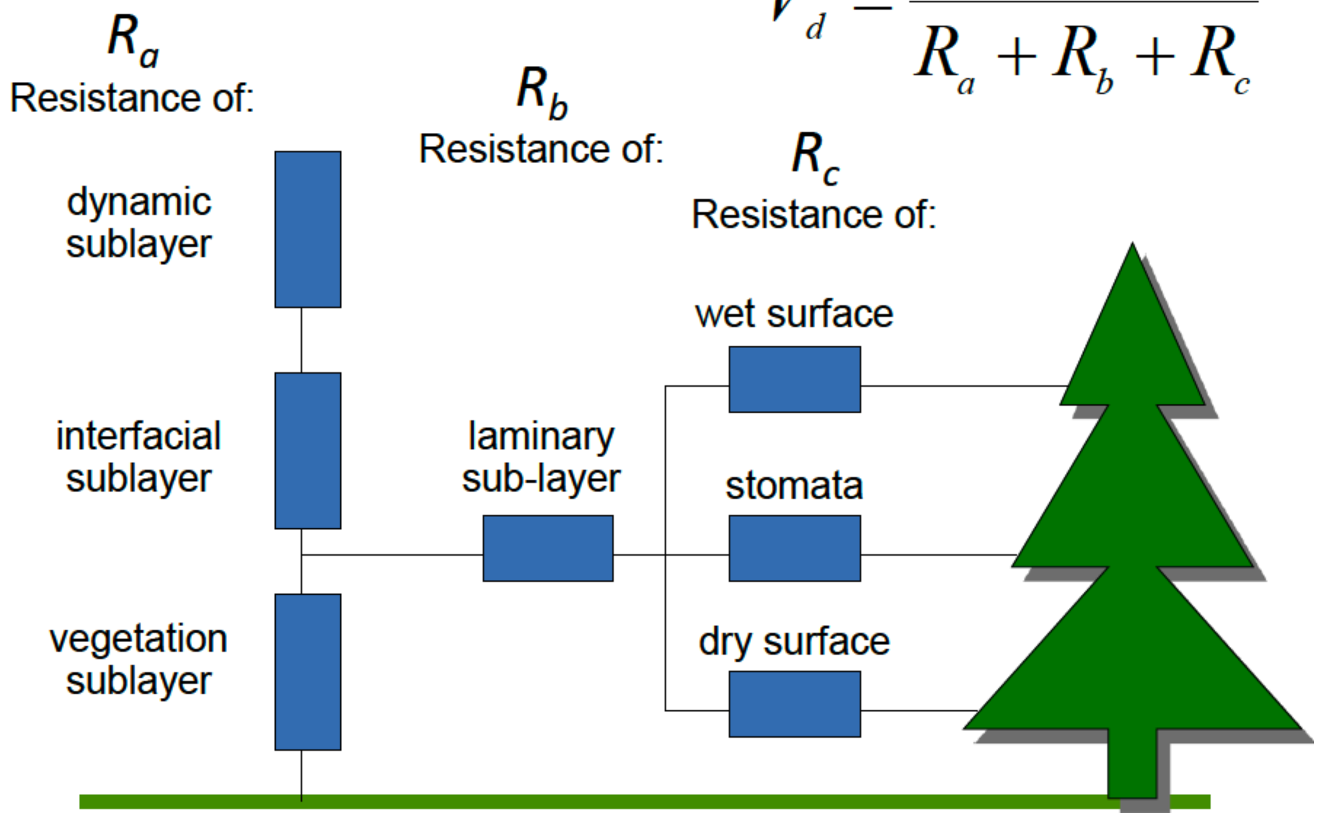
Dry Deposition Velocity

$$V_d = \frac{1}{R_a + R_b + R_c}$$



Deposition flux: $$F = -v_d C$$

C: concentration of species am 10m

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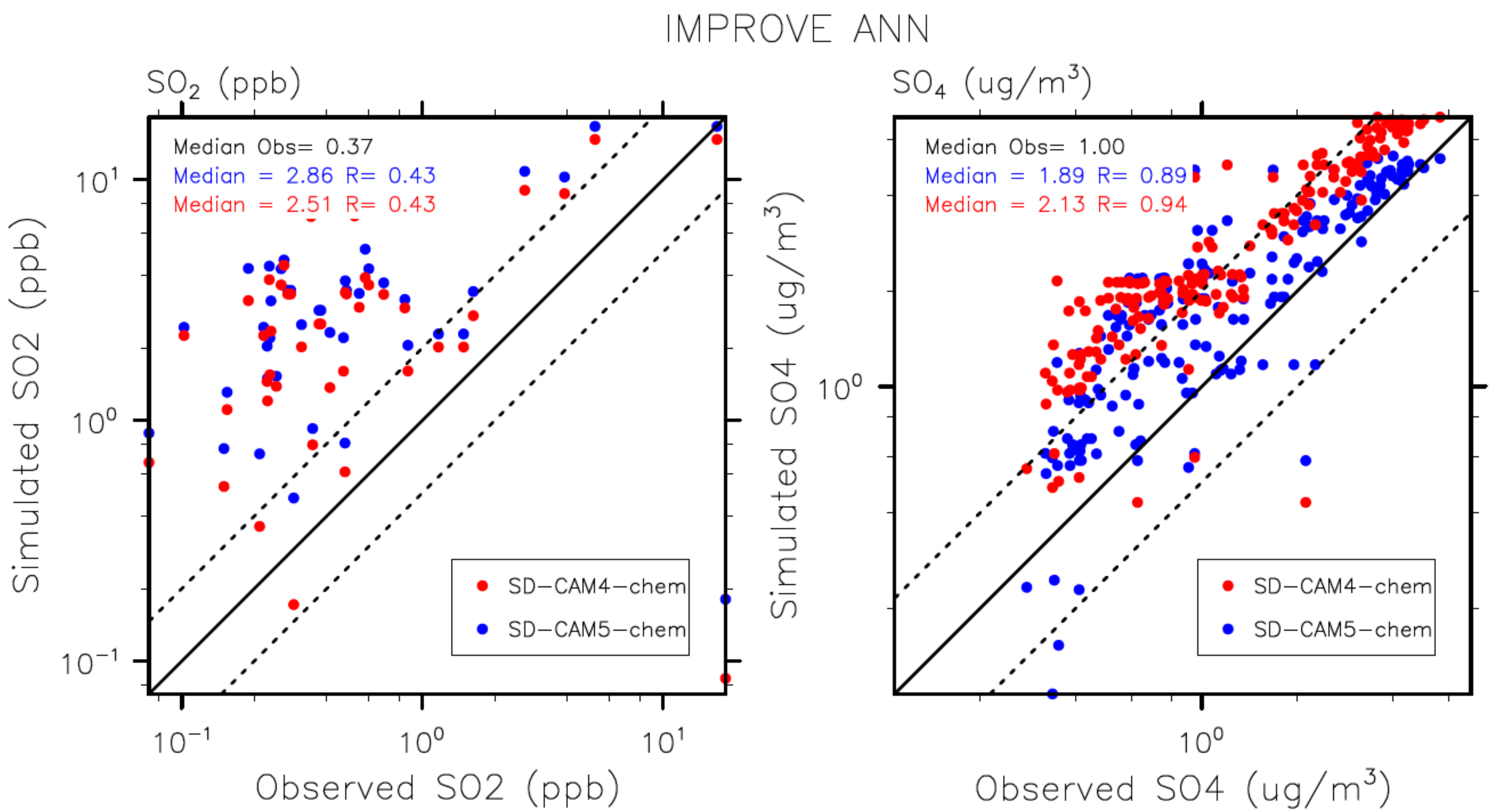
- Removal is modeled as a simple first-order loss process

$$X_{iscav} = X_i \times F \times (1 - \exp(-\lambda \ \Delta t))$$

- X_{iscav} is the species mass (in kg) of Xi scavenged in time
- F is the fraction of the grid box from which tracer is being removed, and λ is the loss rate.

Performance of the Models: SO_2 and SO_4 in Comparison to IMPROVE



Use the AMWG Diagnostics tool to evaluate your Model!

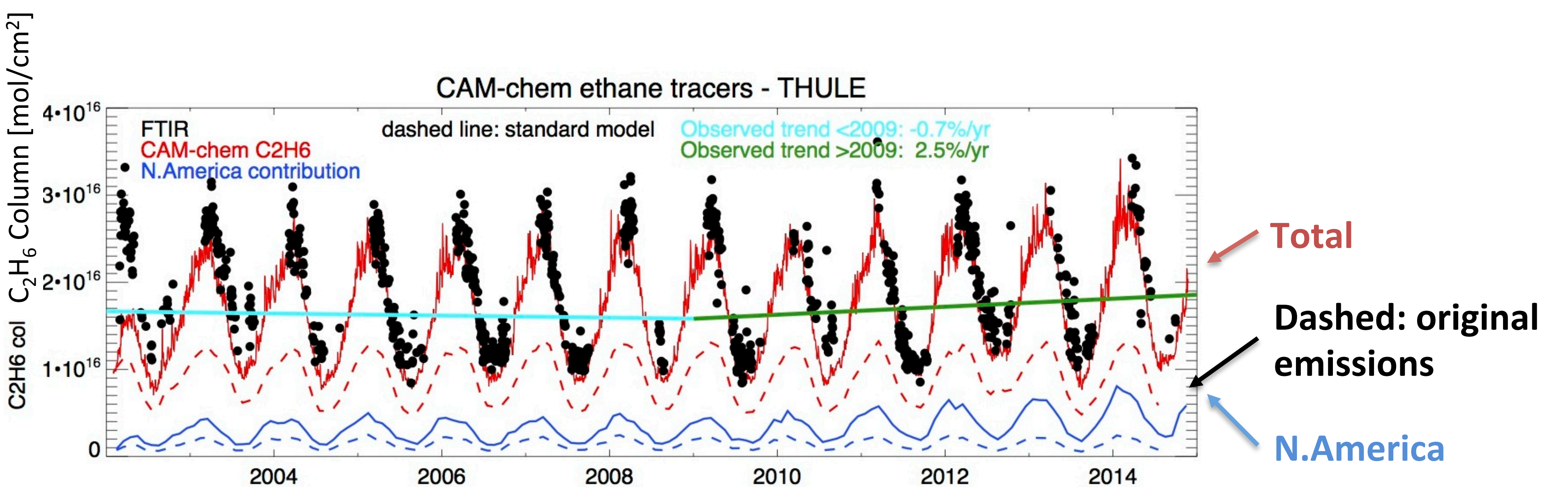
Synthetic tracers to study source contributions in CAM

Example Ethane: C2H6

Standard emissions inventories used in global models do not reproduce observations.

Long-term ground-based FTIR observations document changes in trends due to oil and gas extraction in the US

FTIR C_2H_6 and CAM-chem tracers – Thule, Greenland



In order to match observations, the HTAP2 anthropogenic inventory has been doubled globally for all years, and additionally the N. America emissions are increased 0.2 Tg/yr after 2009.

Synthetic tracers to study source contributions

For compounds with simple chemistry (e.g., only react with OH), tracers can be added to a CAM (with prognostic aerosols) simulation

Add to usr_mech_infile (copy chem_mech.in) new species and reactions

For example, ethane (C2H6) has emissions and is only chemically lost with OH, so can be simulated with specified OH fields:

C2H6 + OH -> {ignored product}

And additional tracers representing different source types or regions can be added:

C2H6_BB + OH -> prod [*for biomass burning*]
C2H6_NAM + OH -> prod [*for N.America only*]

WACCM and CAM-Chem Customer Support

CGD Forum: http://bb.cgd.ucar.edu/

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