

# Chemistry-Climate Modeling

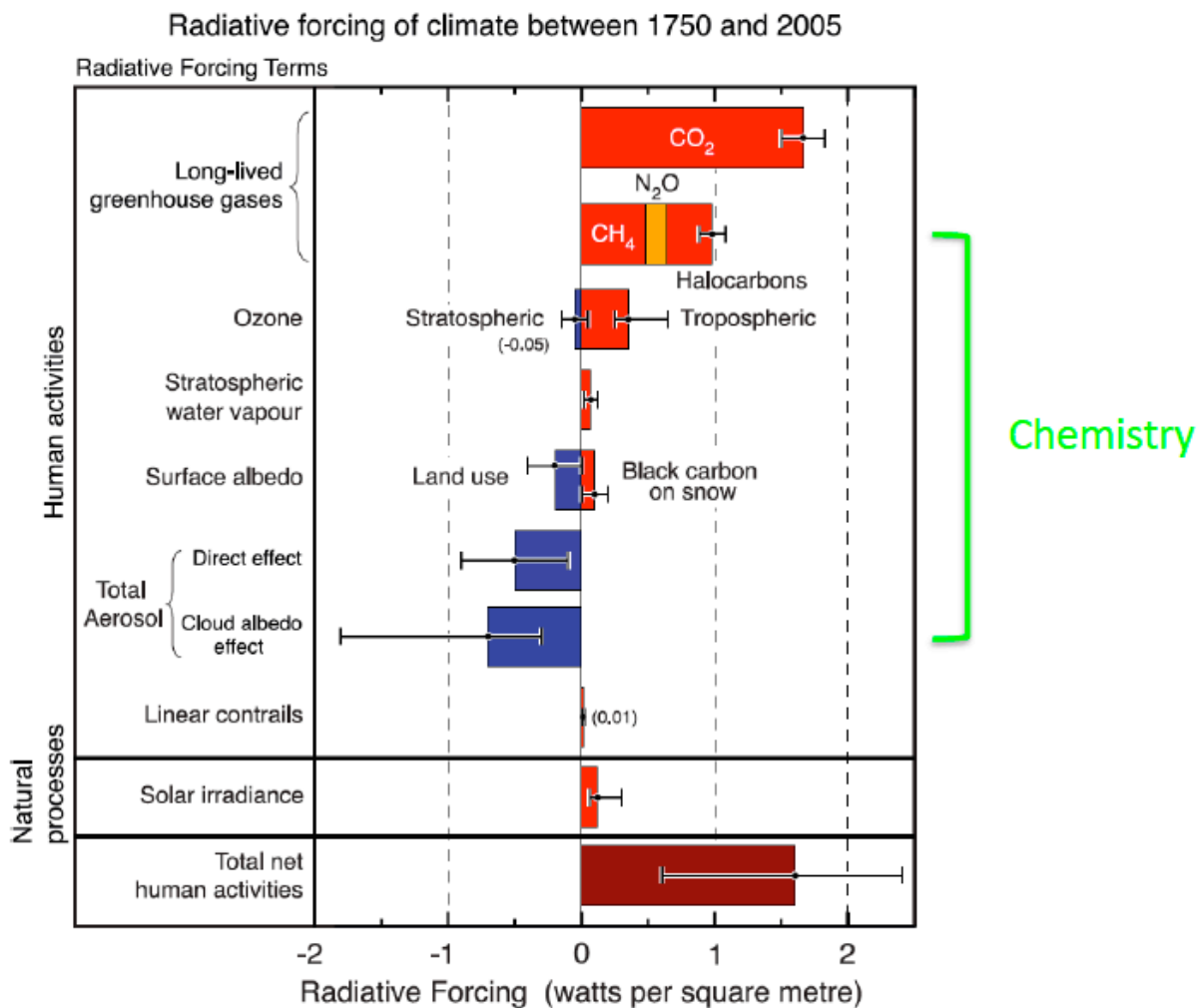
Simone Tilmes  
NESL: ACD/CGD



CESM Tutorial 2012, Chemistry / Aerosols

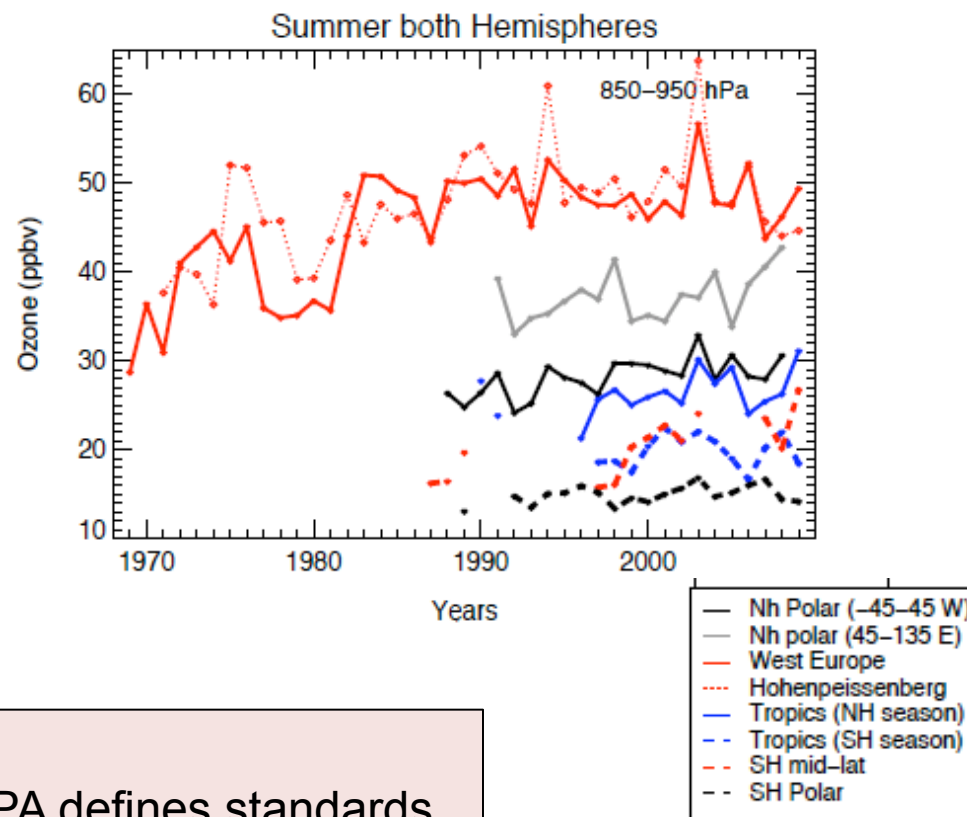
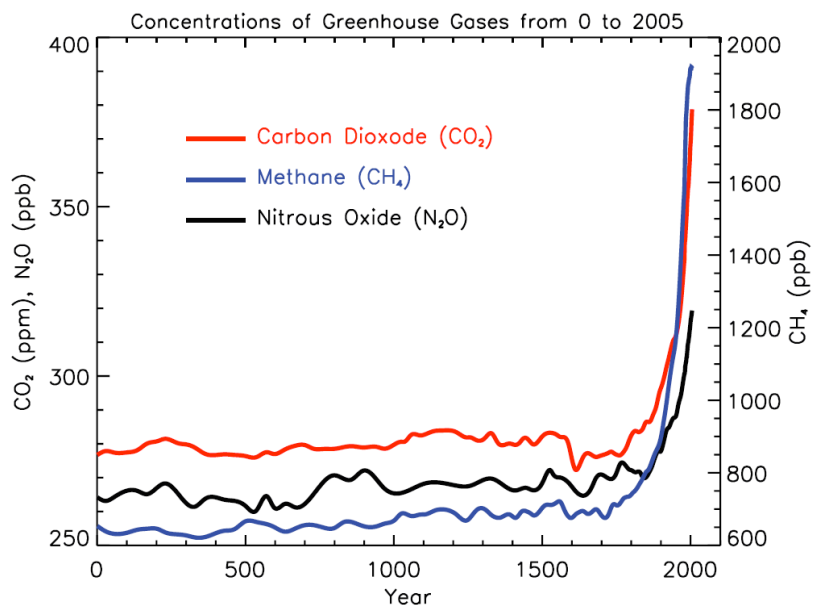


# Atmospheric Chemistry and Climate



Forster and Ramaswamy. AR4 Chapter 2

# Changing Atmospheric Composition



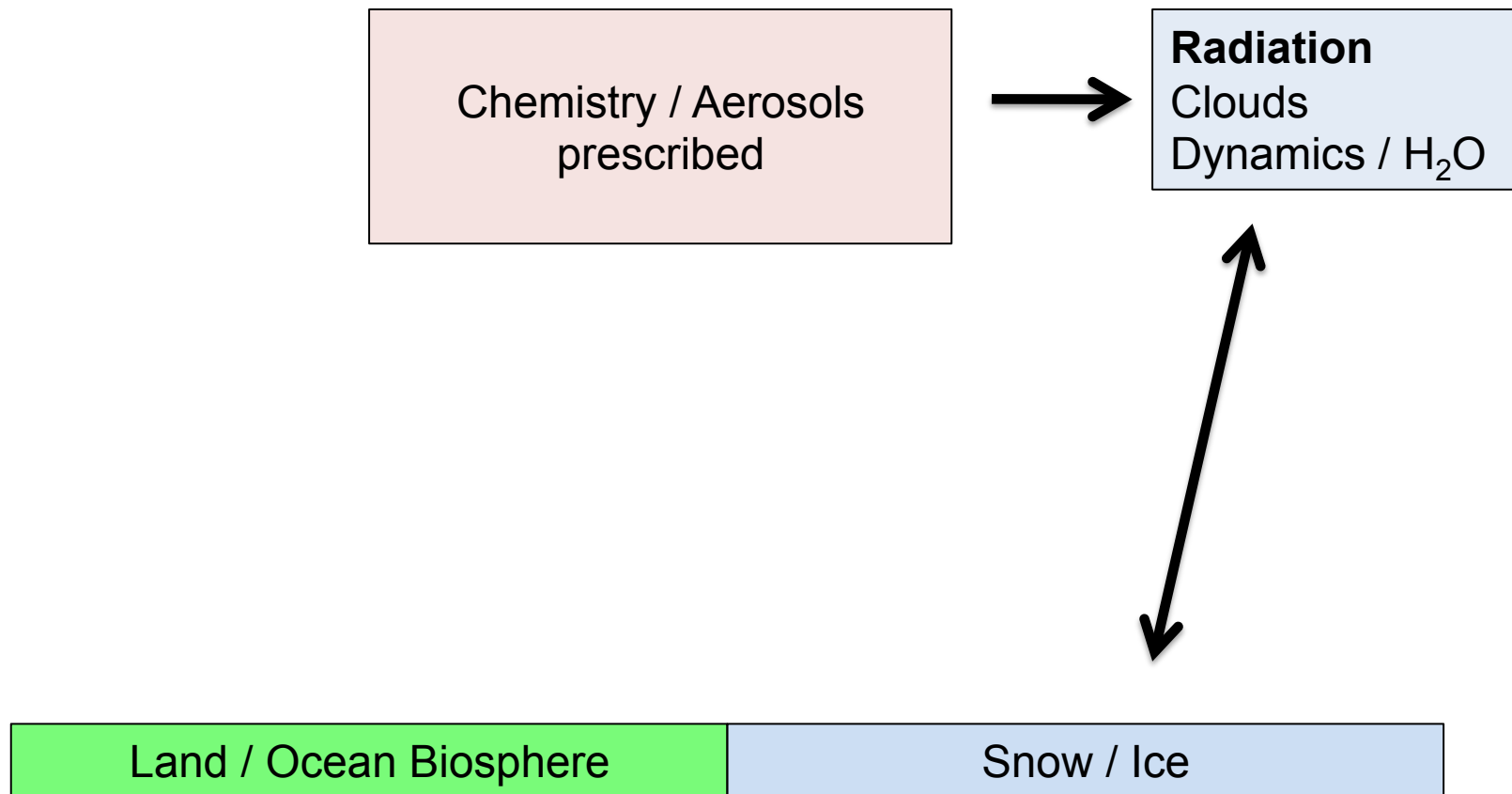
Implications for Climate  
Implications for Air Quality: EPA defines standards  
for air quality (currently 75 ppb)

# Modeling without Chemistry-Climate interactions CCSM CAM4

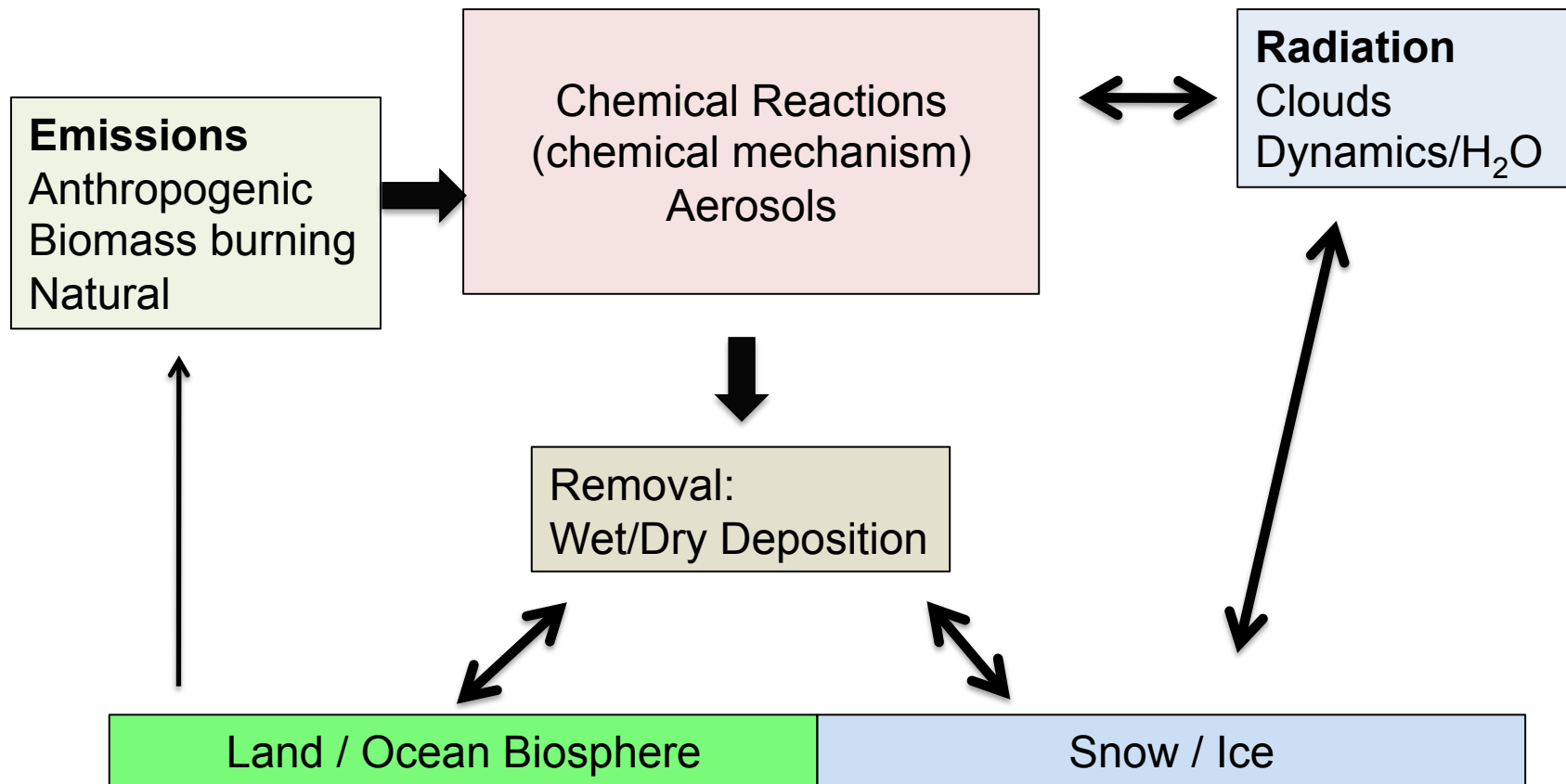
- Chemistry and aerosols are prescribed in CAM4:  
(prescribed monthly fields of CO<sub>2</sub>, CH<sub>4</sub>, O<sub>3</sub>, N<sub>2</sub>O, CFCs)
- Aerosols are calculated in CAM5 (Modal Aerosols Model MAM), but not coupled with chemistry

**No interaction between Chemistry and Climate**

# Chemistry in CESM CAM4

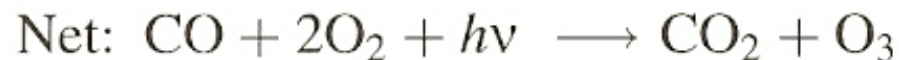
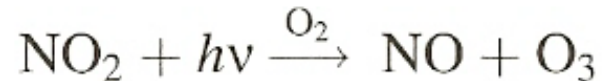
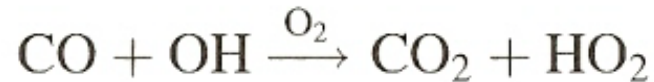


# Chemistry in CESM CAM4 Chem



# Modeling with Chemistry

- Represent Climate gases: (CO<sub>2</sub>), CH<sub>4</sub>, O<sub>3</sub>, H<sub>2</sub>O
- Tropospheric/Stratospheric Chemistry: 122 species to cover around 300 main reaction. NO<sub>x</sub> (NO + NO<sub>2</sub>), CO, volatile organic compounds (VOCs), are key species controlling Ozone, OH determines oxidation capacity, CH<sub>4</sub> lifetimes



# Modeling with Chemistry

## Define Chemical Mechanism: Options in CAM4-Chem

### Superfast Chemistry:

12 species, simple chemistry mechanism, CH<sub>4</sub> prescribed  
LINOZ + Cariolle in stratosphere, fully coupled

### Bulk Aerosol Model (BAM):

Includes Black Carbon, Organic Carbon, Sea Salt, Dust  
(prescribed monthly fields of CO<sub>2</sub>, CH<sub>4</sub>, O<sub>3</sub>, OH, HO<sub>2</sub>, NO<sub>2</sub>, N<sub>2</sub>O, SO<sub>2</sub>/SO<sub>4</sub>)

### BAM and tropospheric chemistry (trop\_mozart):

Tropospheric mechanism, 103 species (MOZART: *Emmons et al.*, 2010)  
Stratospheric chemistry is prescribed: (O<sub>3</sub>, HNO<sub>3</sub>, CH<sub>4</sub>, CO)  
Emissions, Dry/Wet Deposition

### Plus stratospheric chemistry (trop-strat mozart):

Tropospheric and Stratospheric mechanism (122 species) including  
stratospheric heterogeneous reactions, about 300 reactions

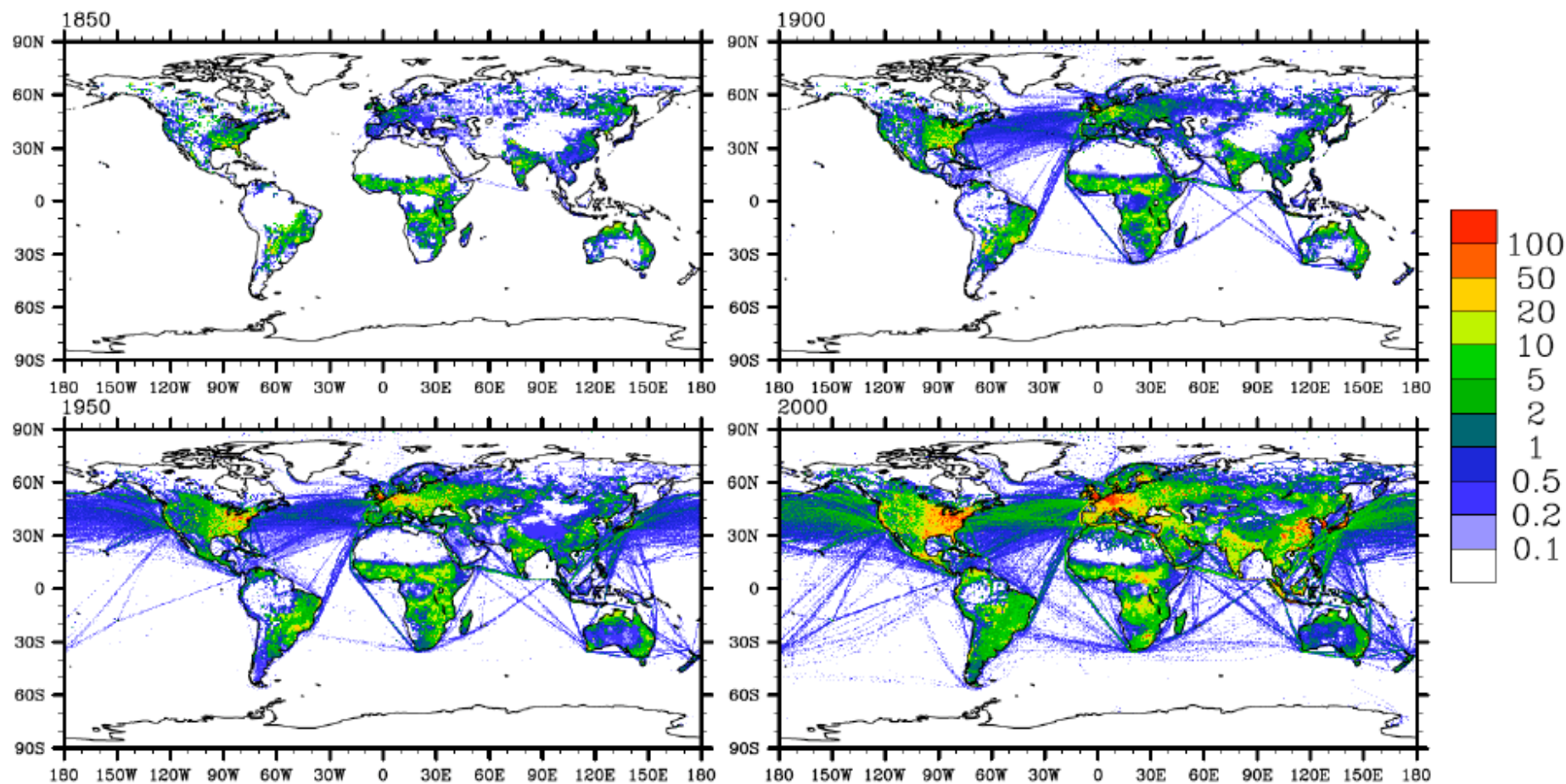


# CAM-Chem with Tropospheric Chemistry

*Lamarque et al., 2012, GMD*

**Emissions:** surface emissions fields, fixed boundary conditions, calculated using vegetation type (biogenic, VOC) , external forcings (aircraft emissions)

# Example: NO<sub>x</sub> emissions



*Lamarque et al., 2010*

Anthropogenic + biomass burning + ships: kg(N)/year

# CAM-Chem with Tropospheric Chemistry

*Lamarque et al., 2012, GMD*

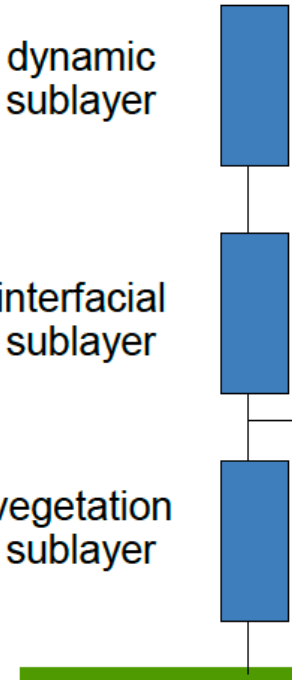
**Emissions:** surface emissions fields, fixed boundary conditions, calculated using vegetation type (biogenic, VOC), external forcings (aircraft emissions)

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

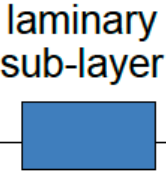
# Dry Deposition Velocity

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

$R_a$   
Resistance of:



$R_b$   
Resistance of:

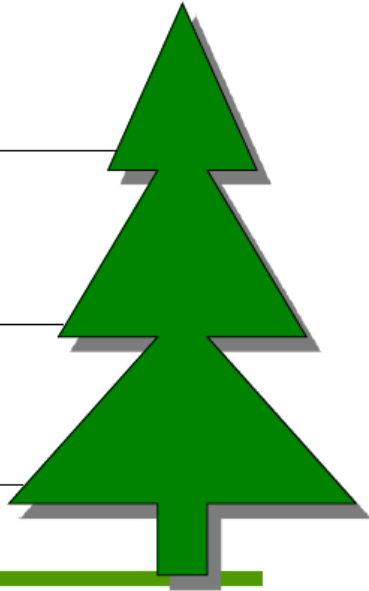


$R_c$   
Resistance of:

wet surface

stomata

dry surface



Deposition flux:

$$F = -v_d C$$

C: concentration of species am 10m



# CAM-Chem with Tropospheric Chemistry

*Lamarque et al., 2012, GMD*

**Emissions:** surface emissions fields, fixed boundary conditions, calculated using vegetation type (biogenic, VOC) , external forcings (aircraft emissions)

**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).

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

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

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

# CAM-Chem with Online/Offline Meteorology

## Fully coupled model:

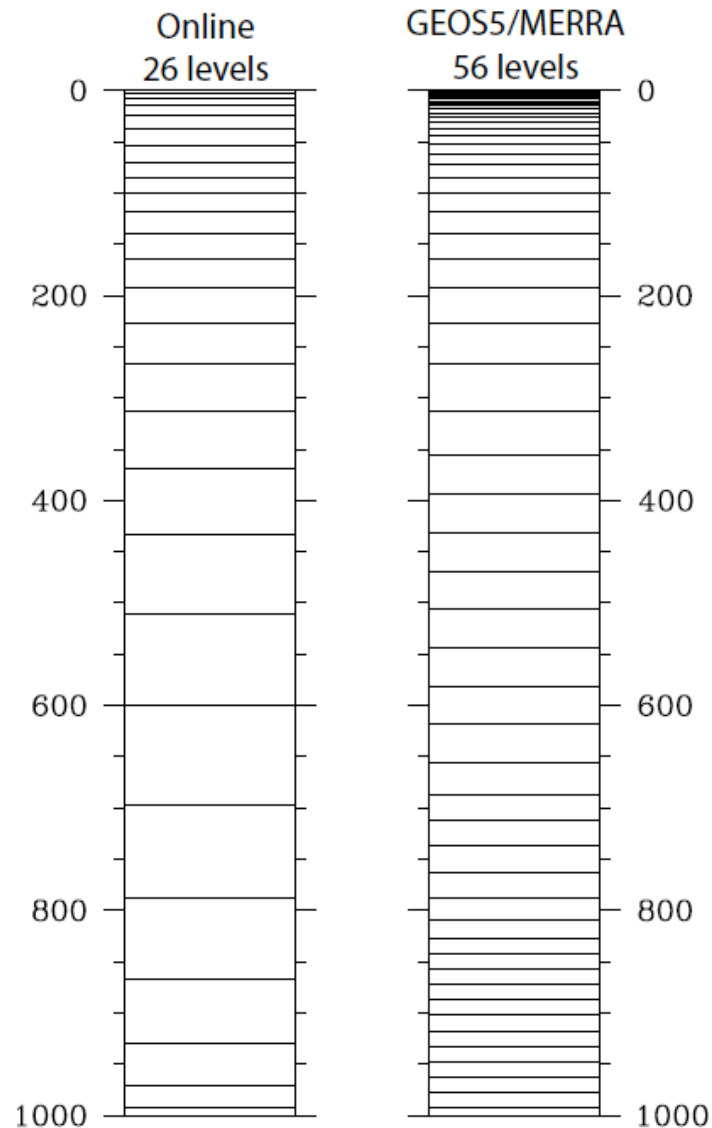
Chemistry interacts with radiation, atmosphere, land, ocean

## Specified Sea/Ice distribution

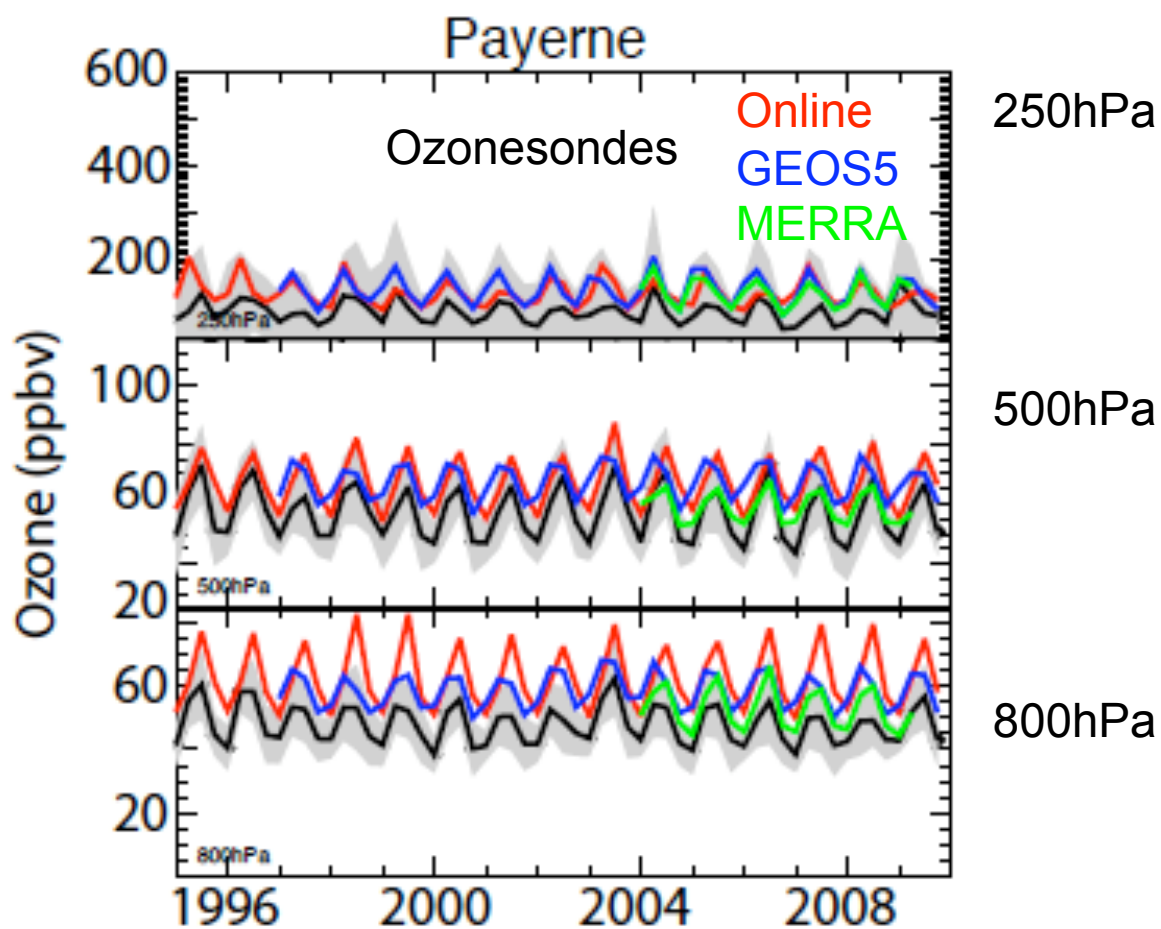
## Specified Dynamics (offline) model:

Meteorological Data are prescribed or nudge (%) for defined altitudes

Nudging: the amount and altitudes of nudging can be defined



# CAM-Chem with Online/Offline Meteorology

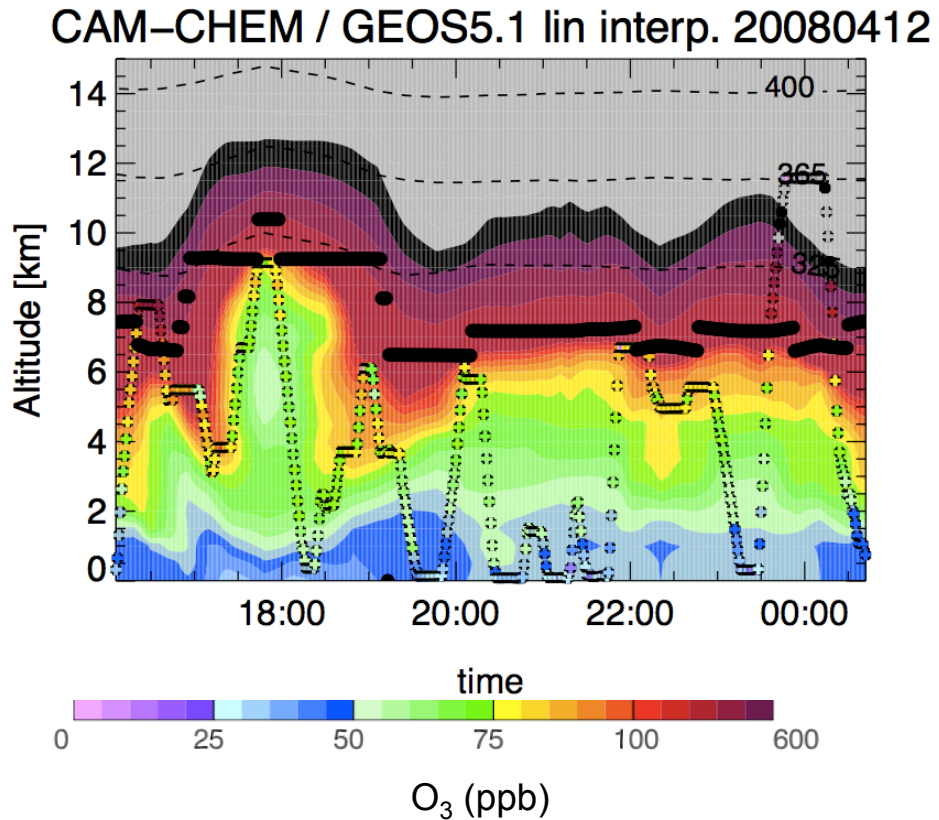


*Lamarque et al., 2012*





# CAM-Chem with Offline Meteorology

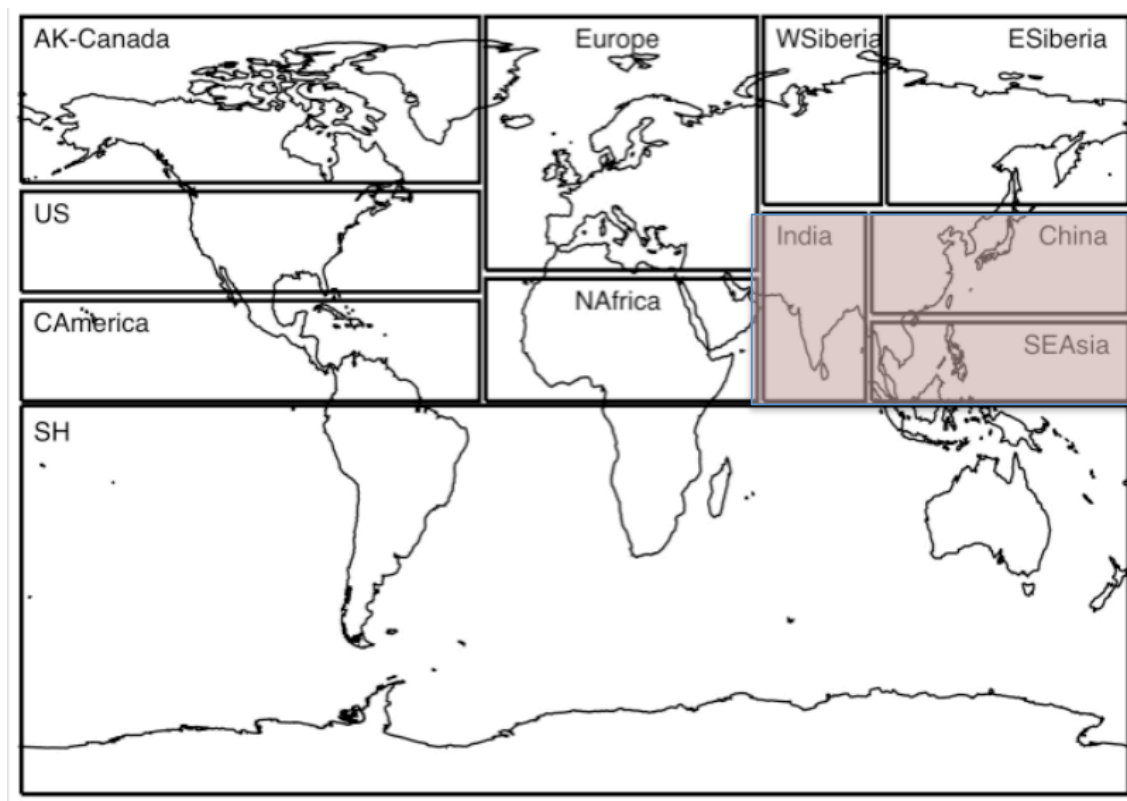


**Comparisons to Aircraft  
campaigns:**  
Model output on the  
flight path for direct comparison



# O<sub>3</sub>, CO, BC tags with Offline Meteorology

*Emmons et al., 2012, GMDD*



## The Model for Ozone and Related chemical Tracers (MOZART4)

Resolution: T85 (1.4°x1.4°)

Meteorology: NCEP/GFS

Emissions: Streets ARCTAS emissions + daily fires (C.Wiedinmyer)

Vertical Injection of Fire Emission between 0-6 km

CESM Tutorial 2012, Chemistry / Aerosols

# Importance of Fire Emissions

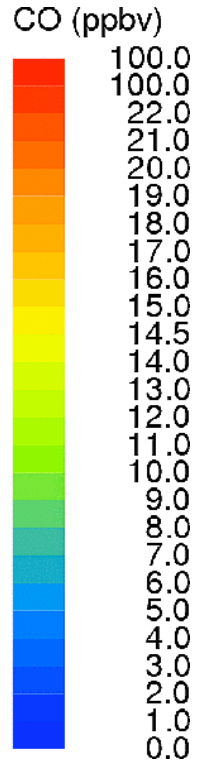
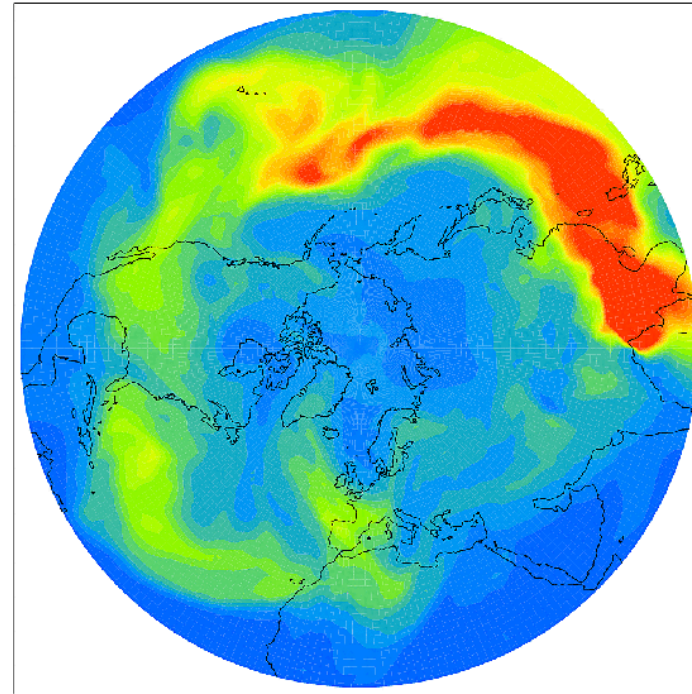
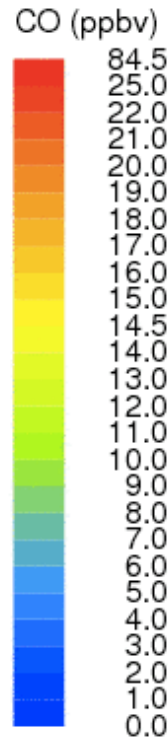
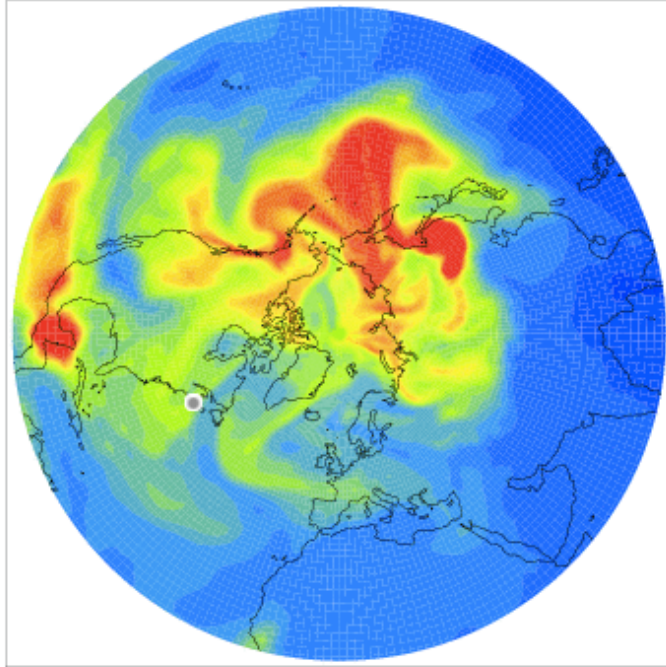
April

without South Asia and SH

South Asia and SH only

Fire Emissions (no SAsia/SH) 080431

Fire Emissions SAsia/SH 080405



CO averaged column between surf. and 200 hPa

# Aerosols

## Direct Effects:

- Radiation (scattering/absorbing)

## Indirect Effects:

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

**Controlled by:** Emissions, Nucleation processes, Deposition

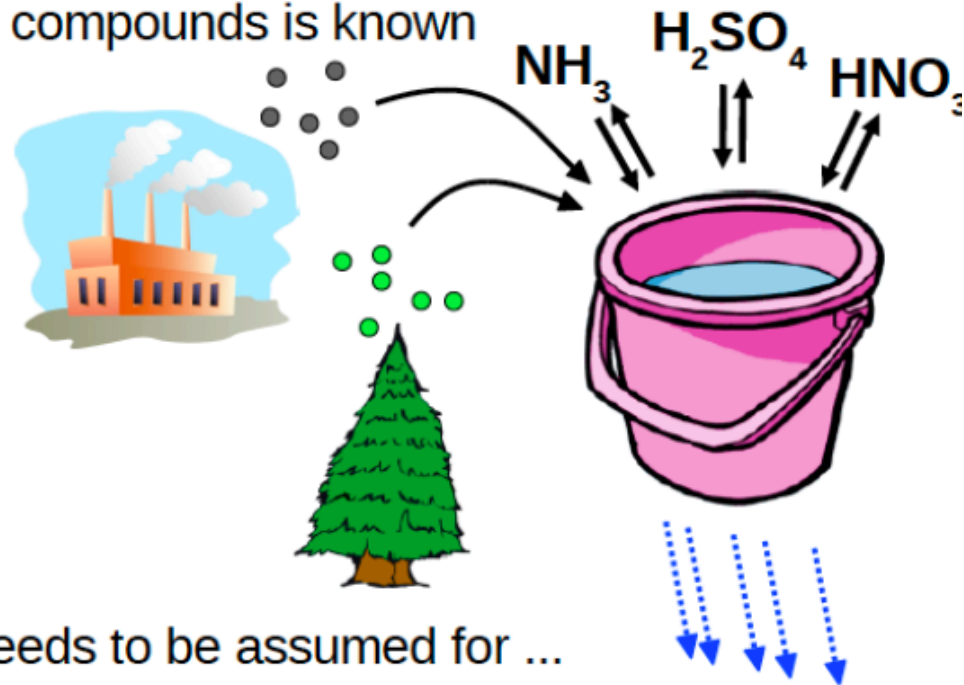
## Aerosols in CESM:

- 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

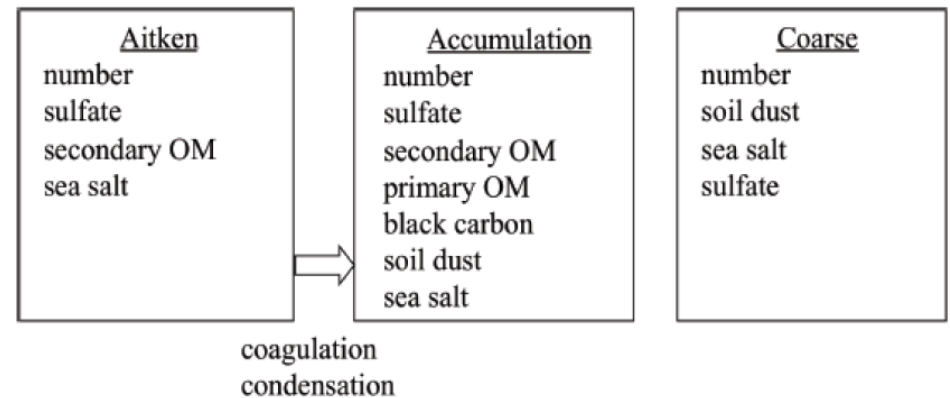
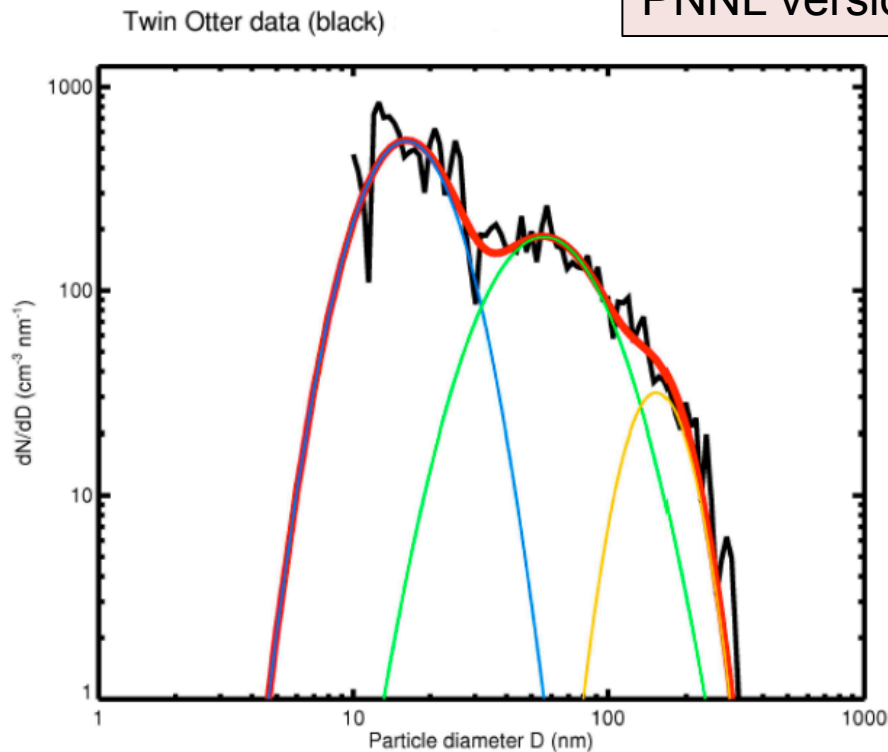


- Aerosol size distribution needs to be assumed for ...
  - radiative transfer
  - response of cloud properties to aerosol number
- Can't do aerosol nucleation
- **Numerically efficient**
- **Useful when focus is on complex gas phase / aerosol chemistry**

# Modal Aerosol Model (MAM3)

## CESM CAM5

Aerosol size distribution using 3 modes  
 PNNL version exists with 7 Modes.

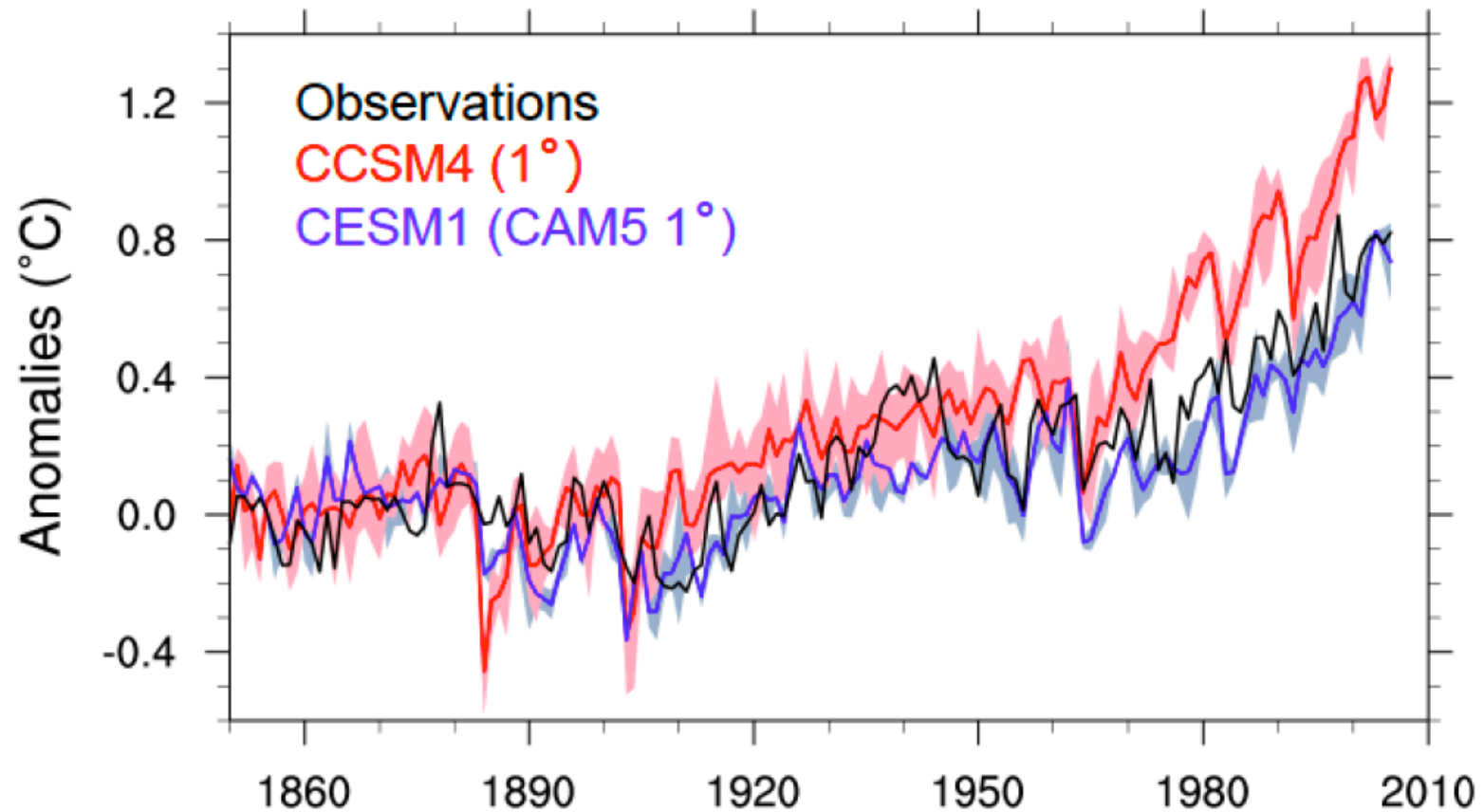


*Liu et al., 2011*

*From J. Kazil, CIRES*



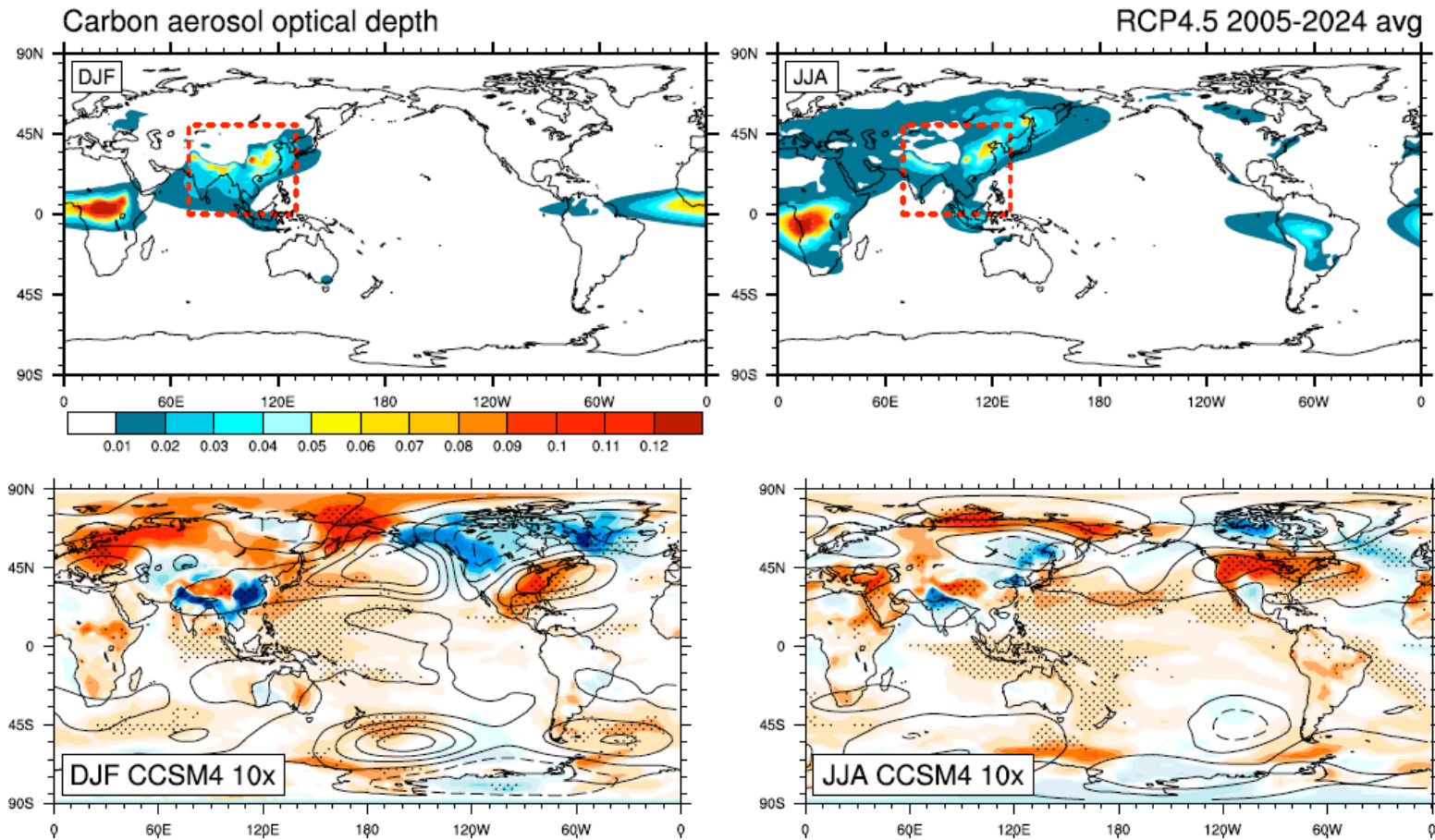
# Modal Aerosol Model (in CESM)





# Single forcing Experiment

*Teng et al., 2012*



**10x increase of organic and black carbon over South-East Asia  
-> temperature response in the US**

# Modal Aerosol Model (in CESM)

MAM available with CAM5 physics

Adds ~ 25 species and simple chemistry (“fixed” oxidants)

Work in progress:

CAM5Chem: Chemistry is couple to MAM3

Better description of SOA