Atmosphere Modeling IV, Chemistry and Aerosols

Presented by Louisa Emmons, ACOM

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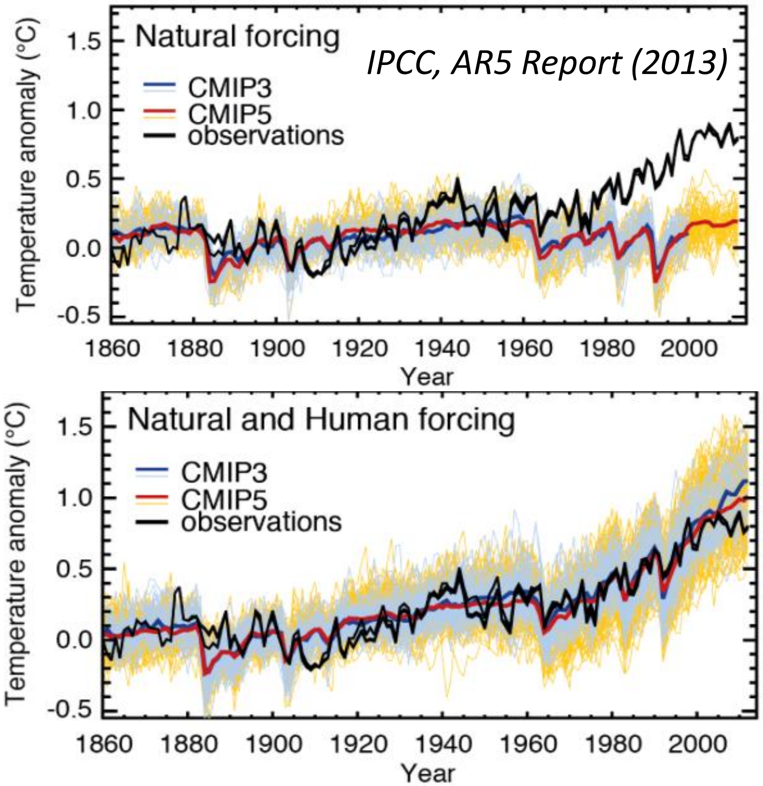
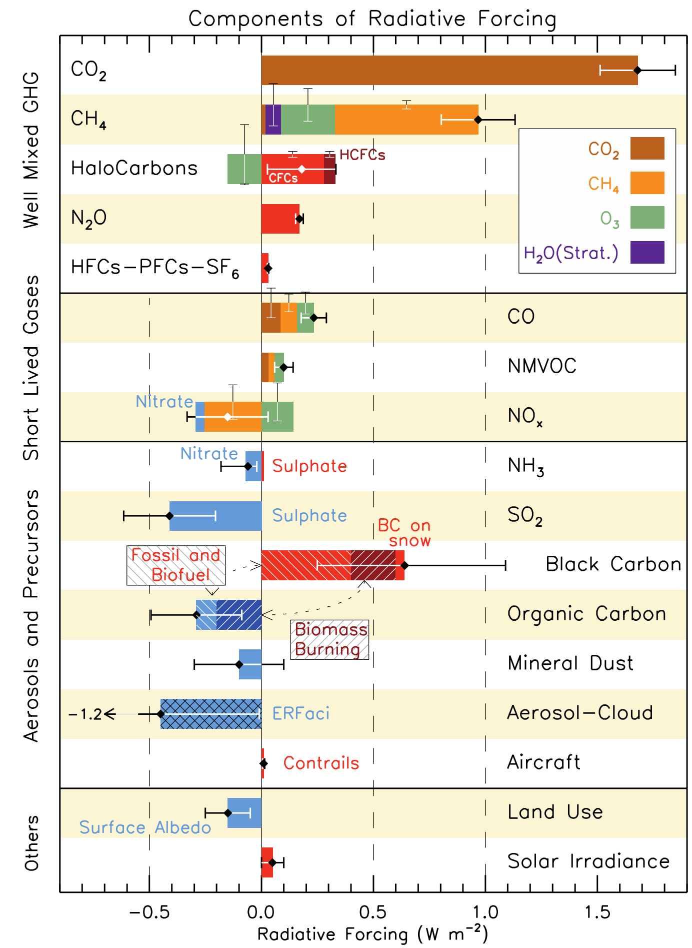
WACCM Liaison: Mike Mills

Importance of Chemistry and Aerosols for Climate



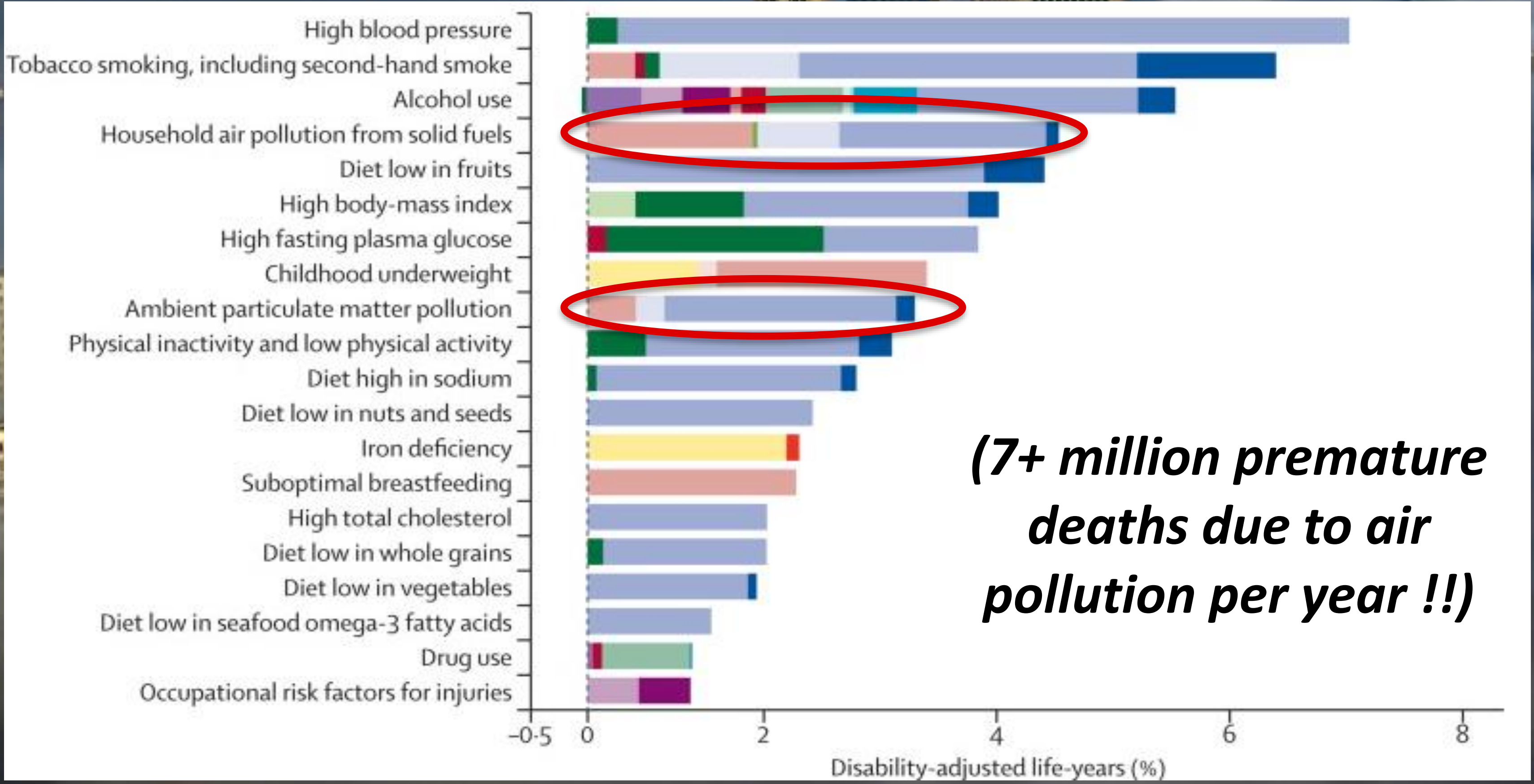


Chemistry is needed to represent atmospheric composition for radiative forcing:
(CO_2), CH_4, O_3, H_2O and secondary aerosols

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

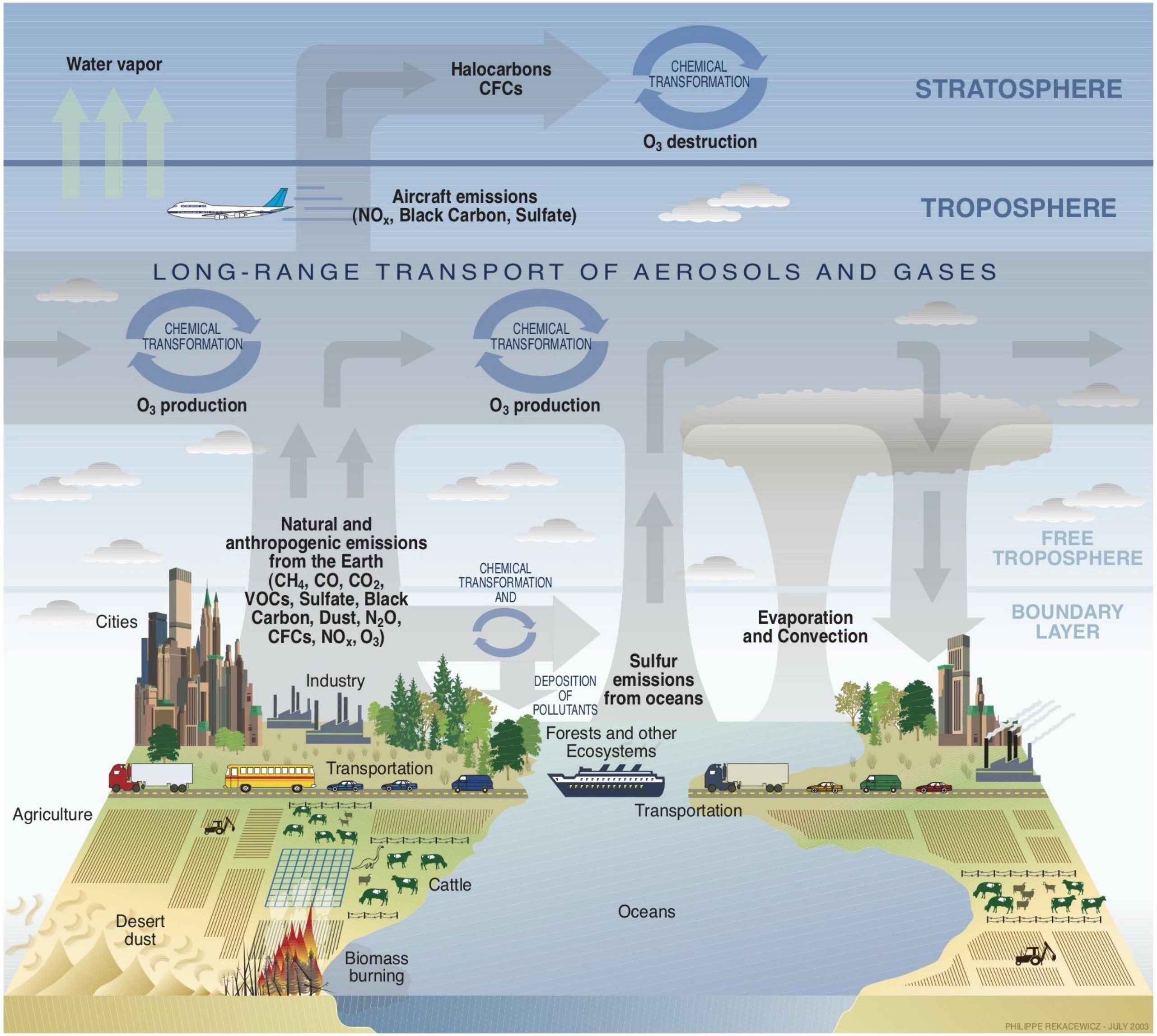
Poor air quality is a major health issue

Health Burden of Global Air Pollution is Enormous

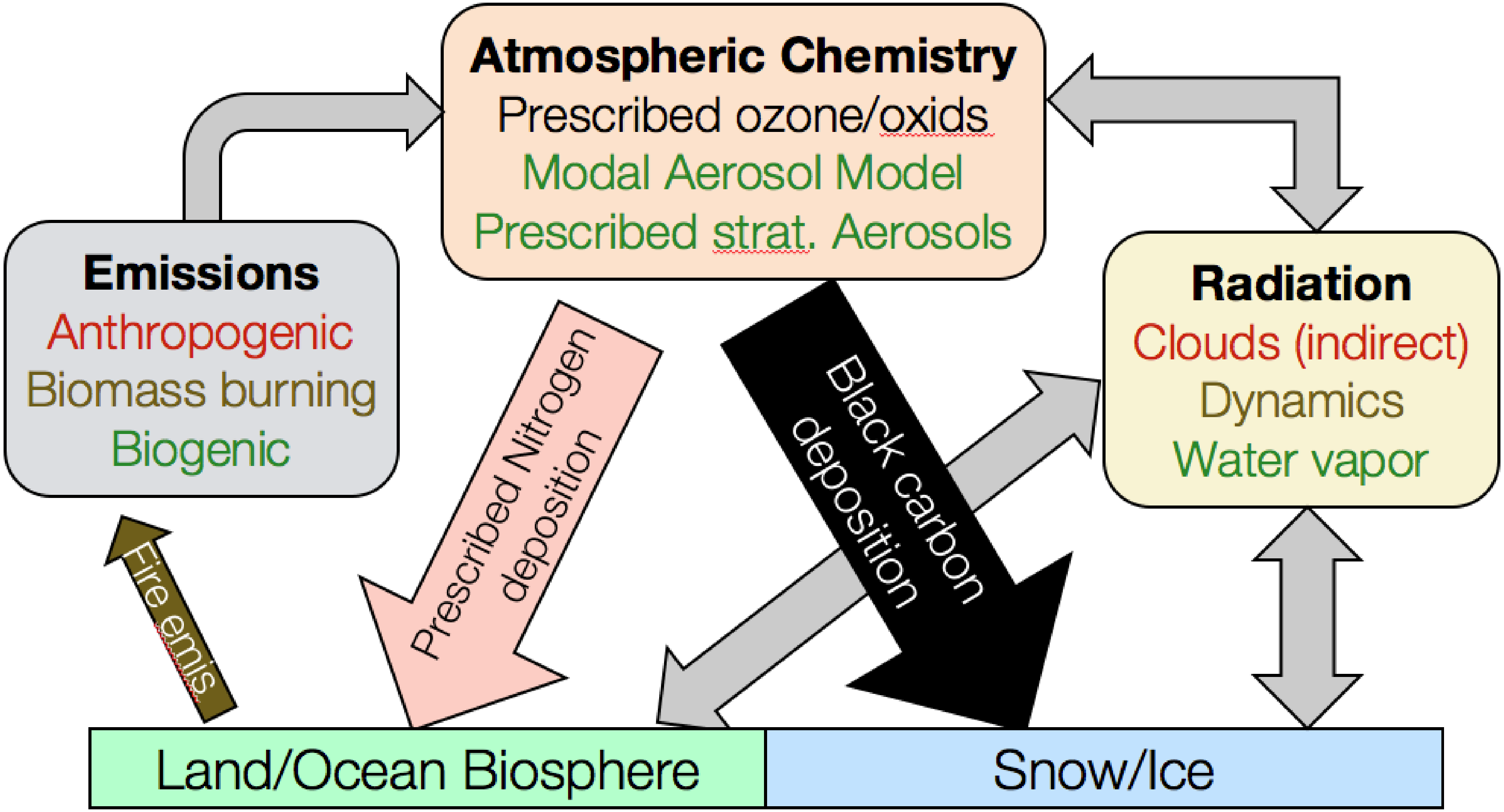


(7+ million premature deaths due to air pollution per year !!)

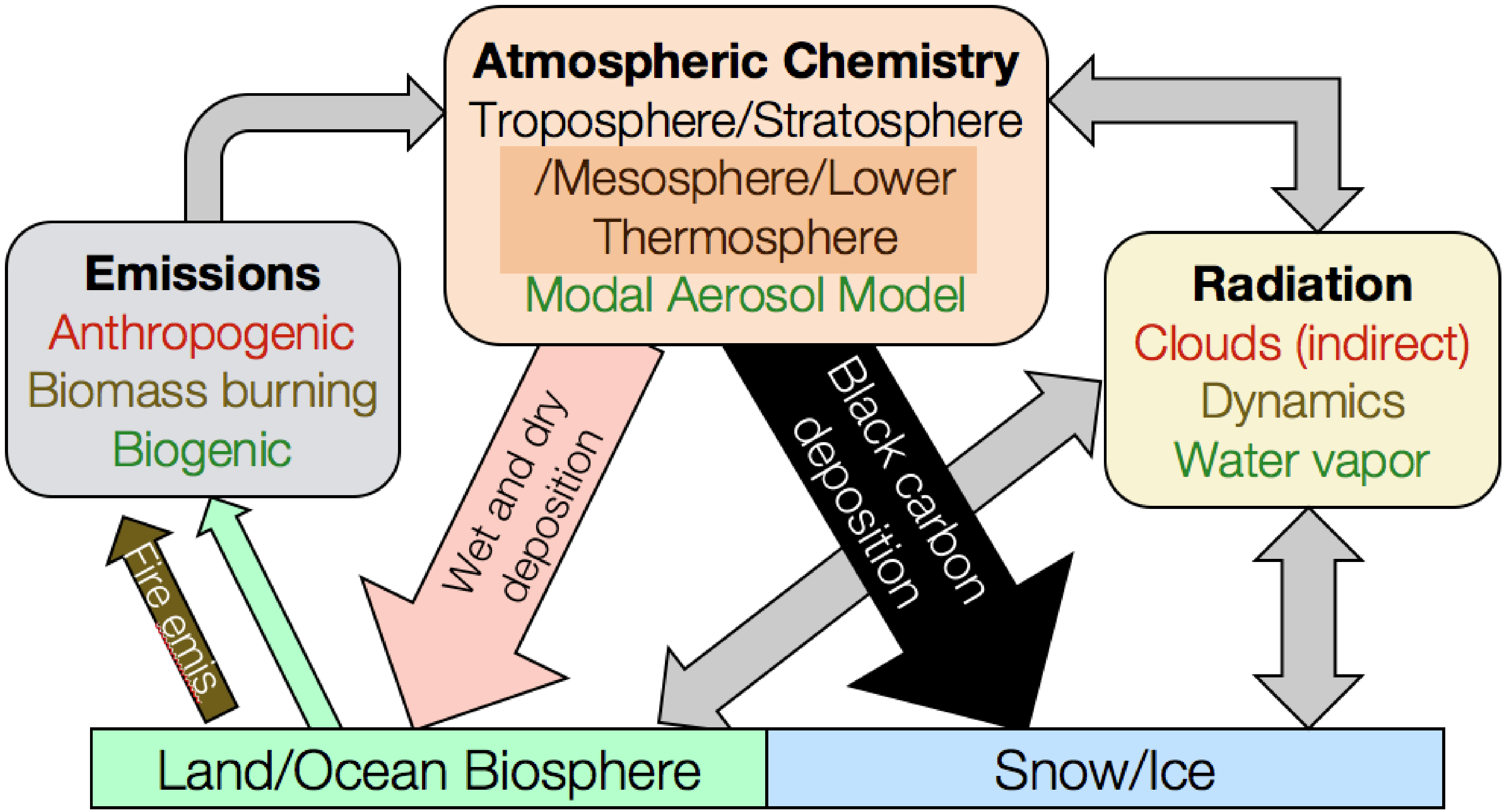
Simulation of atmospheric composition requires many components



Chemistry-Climate Interactions in CESM2: CAM6



Chemistry-Climate Interactions in CESM2: CAM-chem or WACCM



CAM6 vs CAM-chem

Same atmosphere, physics, resolution

Different chemistry and aerosols -> emissions and coupling

- **CAM6:** Aerosols are calculated, using simple chemistry ("fixed" oxidants) (prescribed: 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 interactions between Chemistry and Climate

  -> prescribed fields have to be derived using chemistry-climate simulations

  - Prescribed ozone is used for radiative calculations
  - Prescribed oxidants is used for aerosol formation
  - Prescribed methane oxidation rates
  - Prescribed stratospheric aerosols
  - Prescribed nitrogen deposition
  - Simplified secondary organic aerosol description

Modeling Chemistry-Climate Interactions in CESM2

Surface emissions and concentrations

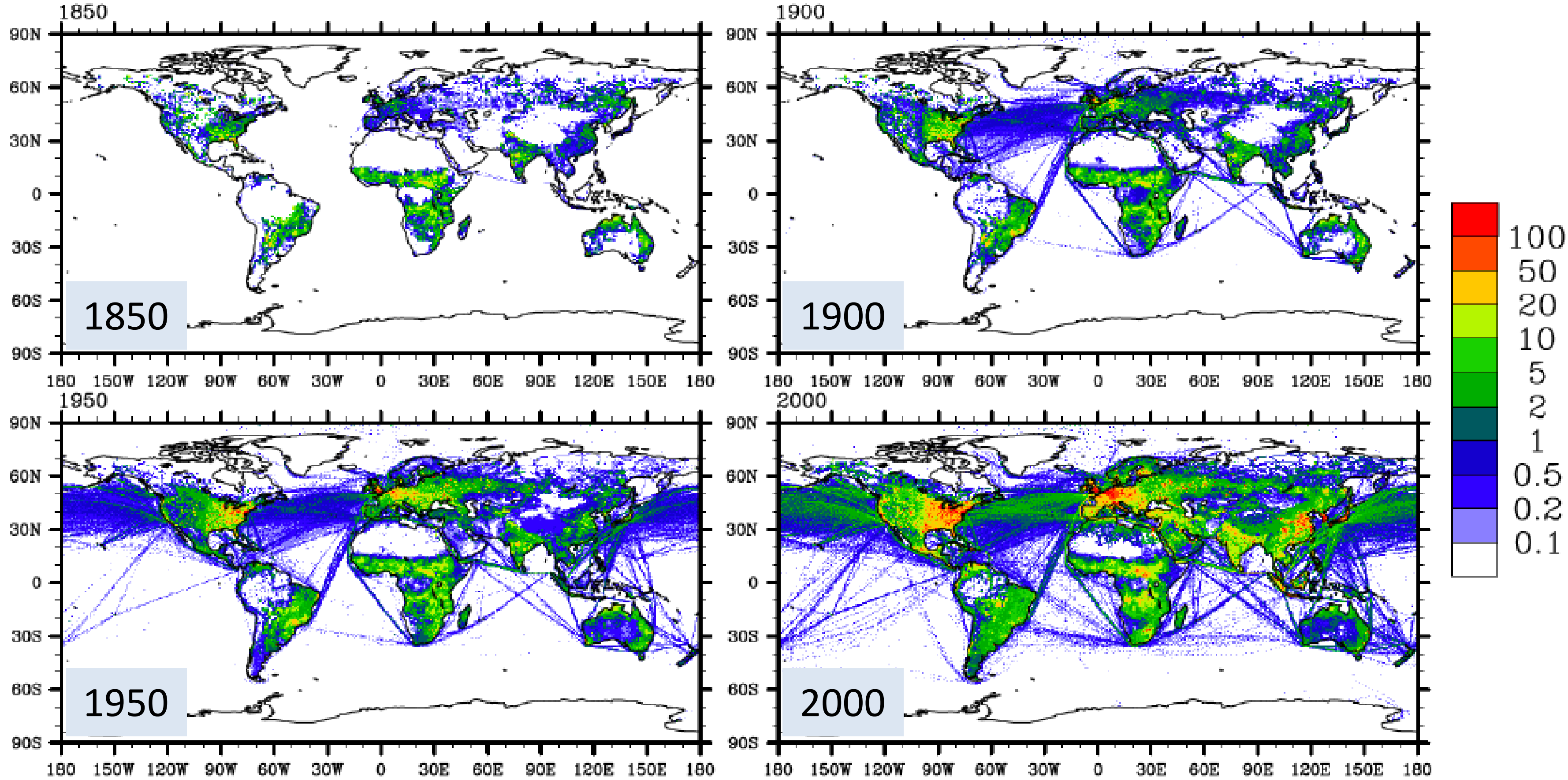
- emissions: anthropogenic, biogenic, biomass burning, ocean, soil, volcanoes
- surface concentrations (greenhouse gases)

Chemical mechanism: important for chemistry and 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).

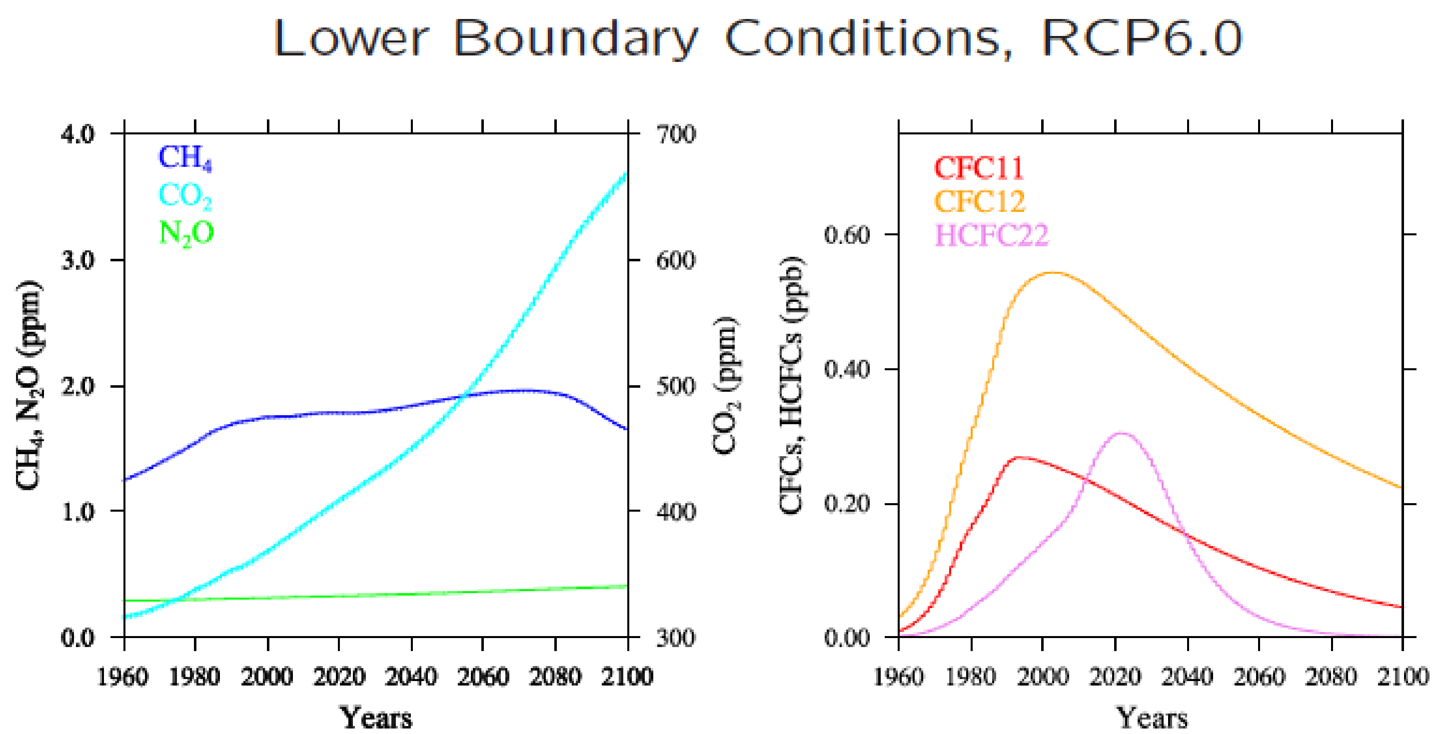
Example: NOx Emissions



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

Modeling Chemistry-Climate Interactions in CESM2

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



Modeling Chemistry-Climate Interactions in CESM2

Surface emissions and concentrations

- emission: anthropogenic, biogenic, biomass burning, ocean, soil, volcanoes
- surface concentrations (greenhouse gases)

Chemical mechanism: important for chemistry and aerosol production

- WACCM and CAMchem: 483 reactions and 231 solution species
- CAM6: 6 chemical reactions and 25 solution species (much simpler)

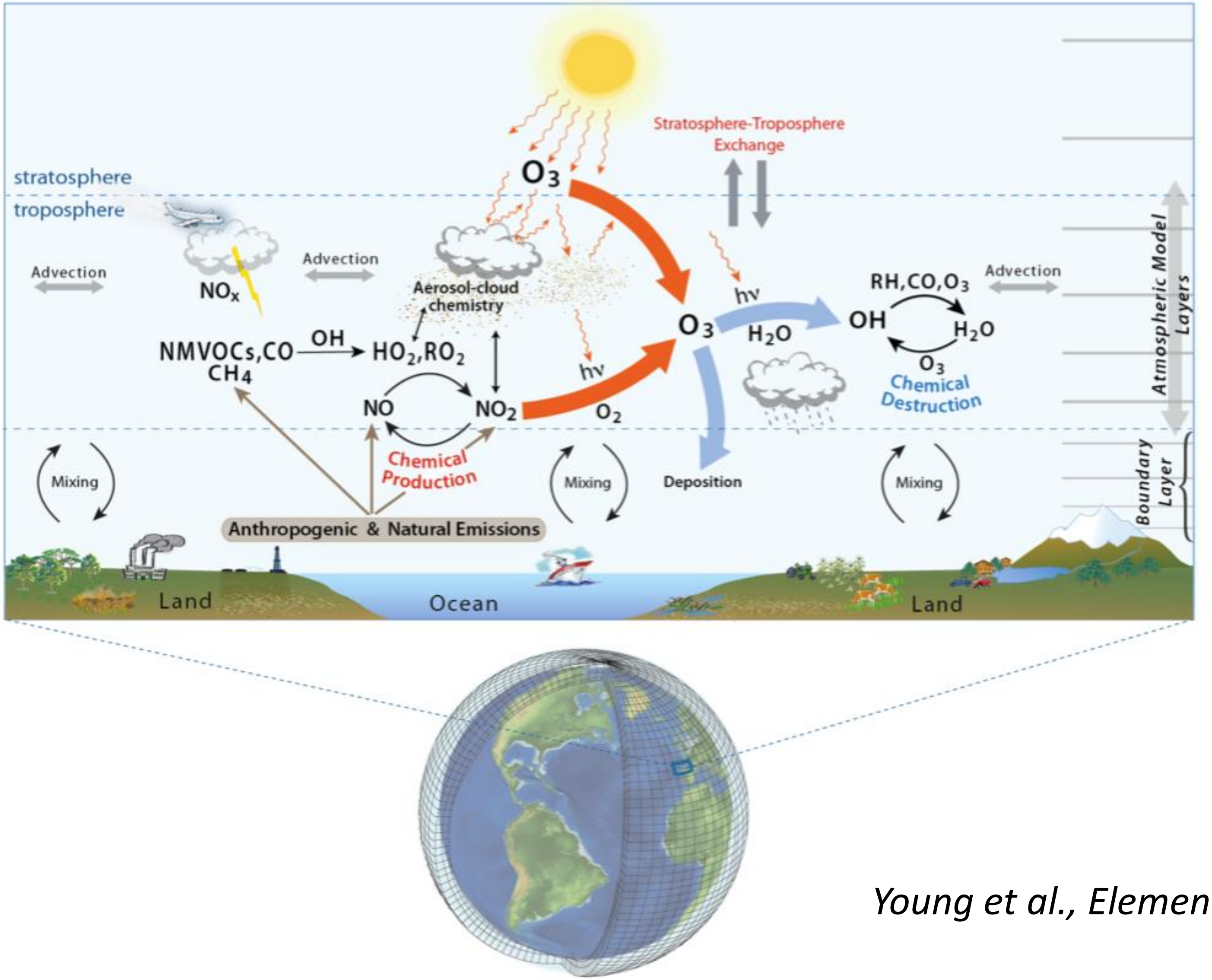
Dry Deposition: uptake of chemical constituents by plants and soil (CLM), depending on land type, roughness of surface, based on resistance approach

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

Modeling Chemistry-Climate Interactions in CESM2

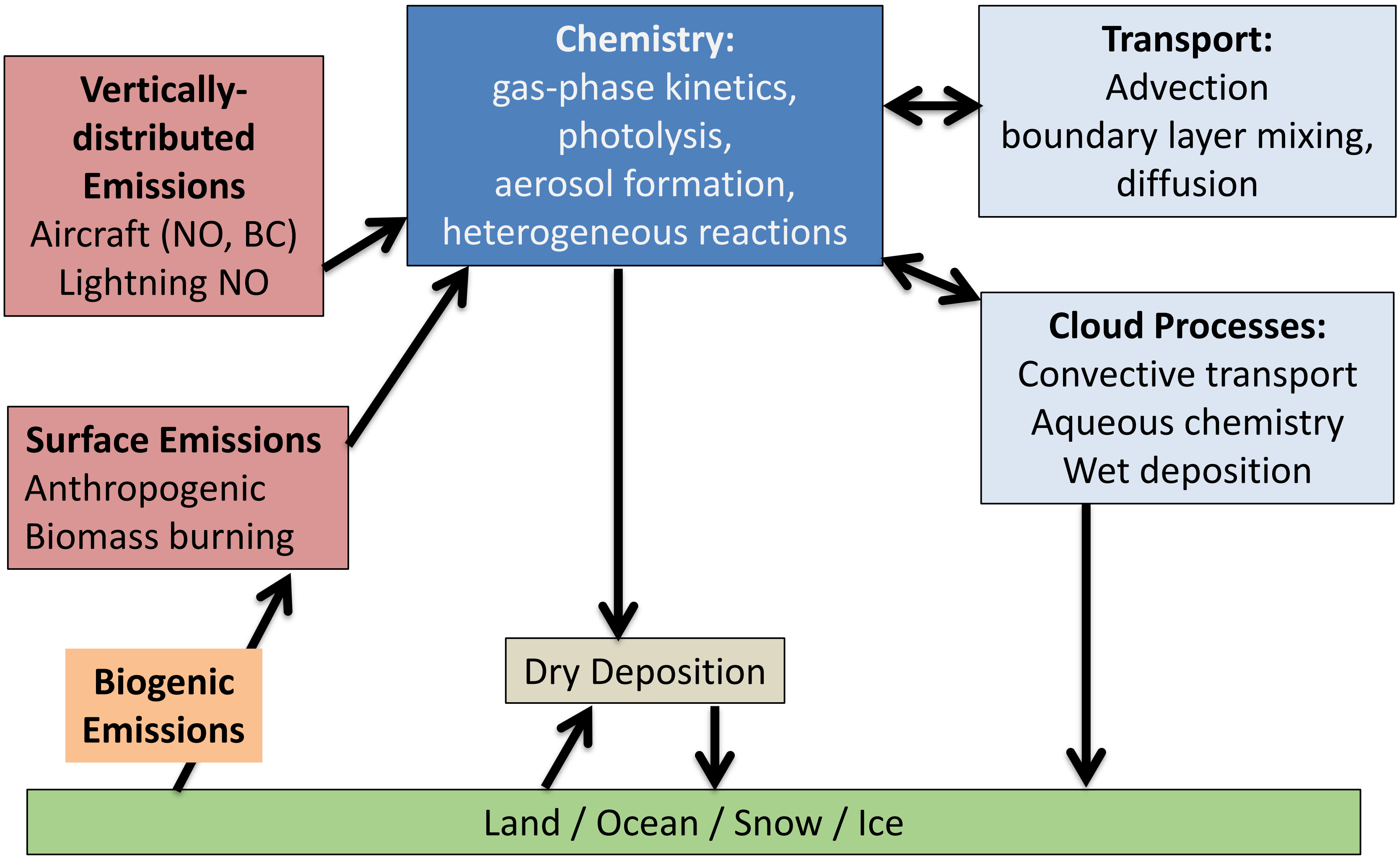
Mechanism (pre-processor code)	Model: Chemistry Description	#Species	#Reactions
TSMLT1 (pp_waccm_tsmlt_mam4)	WACCM: Troposphere, stratosphere, mesosphere, and lower thermosphere	231 solution, 2 invariant	583 (433 kinetic, 150 photolysis)
TS1 (pp_trop_strat_mam4_vbs)	CAM-chem: Troposphere and stratosphere	221 solution, 3 invariant	528 (405 kinetic, 123 photolysis)
MA (pp_waccm_ma_mam4)	WACCM: Middle atmosphere (stratosphere, mesosphere, and lower thermosphere)	98 solution, 2 invariant	298 (207 kinetic, 91 photolysis)
MAD (pp_waccm_mad_mam4)	WACCM: Middle atmosphere plus D-region ion chemistry	135 solution, 2 invariant	593 (489 kinetic, 104 photolysis)
SC (pp_waccm_sc_mam4)	WACCM: Specified chemistry	29 solution, 8 invariant	12 (11 kinetic, 1 photolysis)
CAM	CAM: Aerosol chemistry	25 solution, 7 invariant	7 (6 kinetic, 1 photolysis)

Tropospheric Ozone Chemistry



Young et al., Elementa, 2017

Models treat each process as a separate module



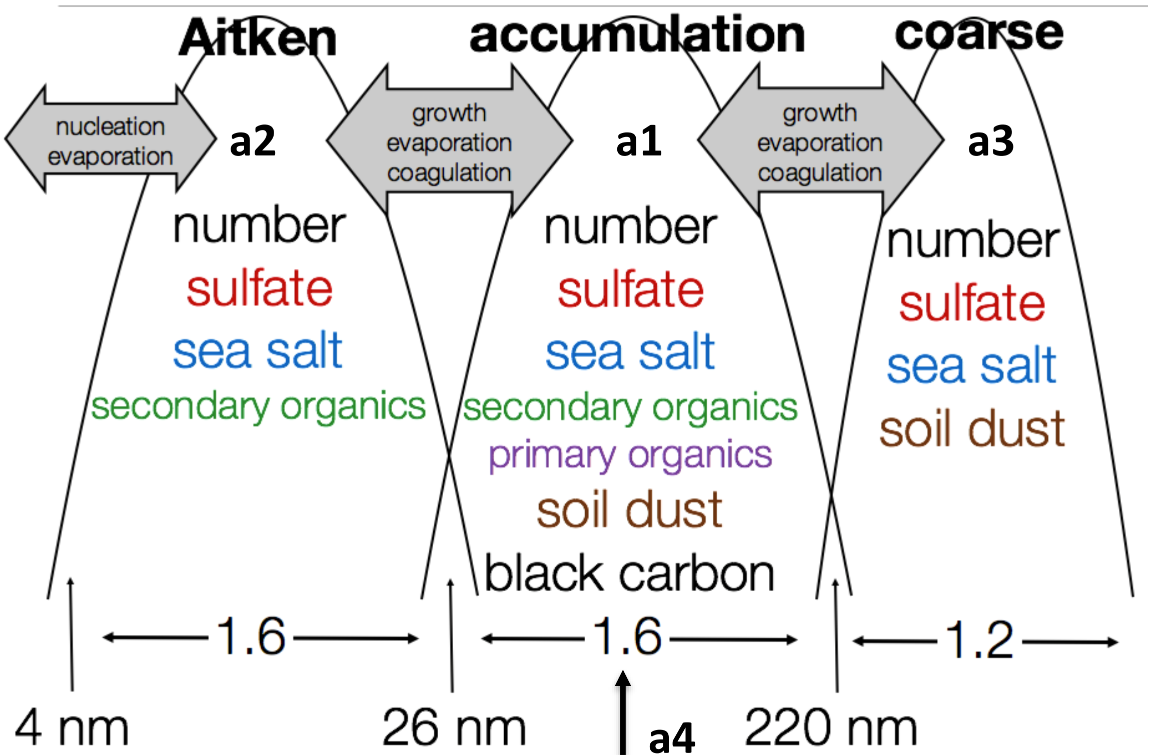
Solution for each chemical species *i*

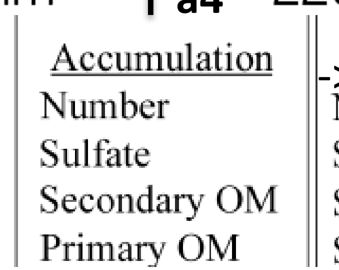
$$\frac{\partial c(i)}{\partial t} = Production(i) - Loss(i) = E_i + C_i + A_i + T_i + W_i + D_i$$

- For each compound, at each timestep, the change in concentration is the sum of the change in concentration for each process:
  - E_i: Emissions
  - C_i: Gas-phase-Chemistry
  - A_i: Aerosol-processes
  - T_i: Advection + Diffusion
  - W_i: Cloud-processes (wet deposition)
  - D_i: Dry deposition

- For compounds with short lifetimes the order of operators can affect results

Modal Aerosol Model (MAM4)



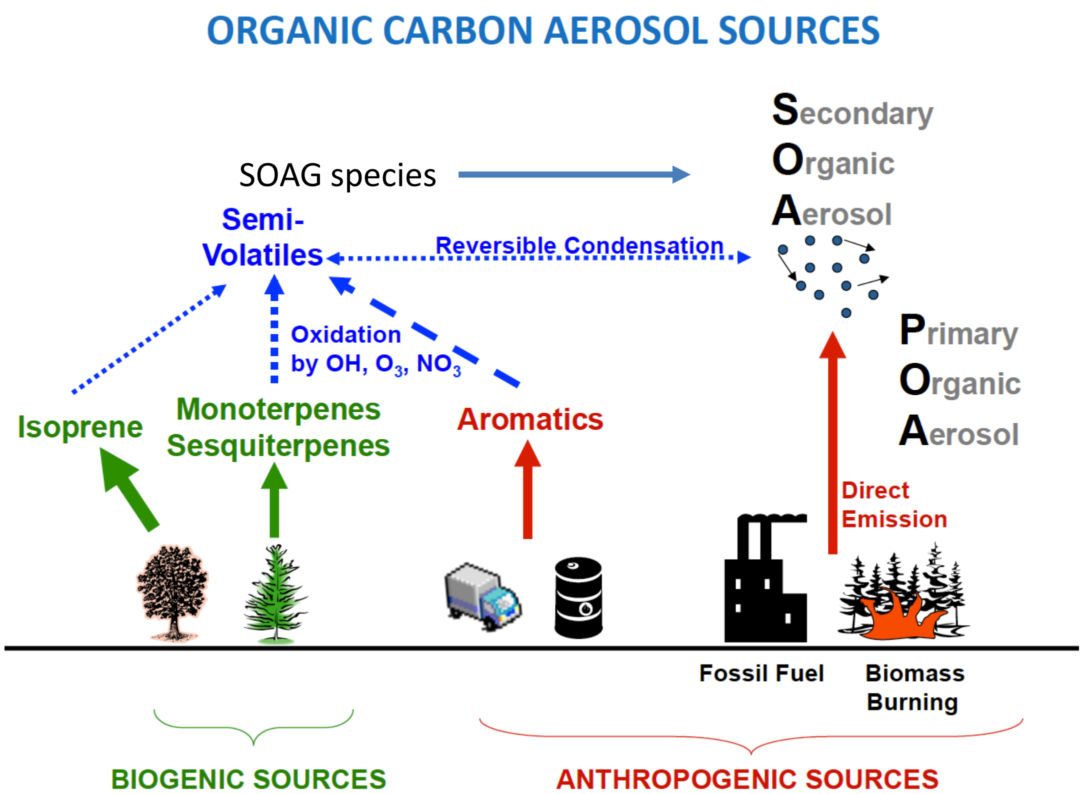


-> changes the lifetime of BC

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

Liu et al., 2016

Secondary Organic Aerosol Description in WACCM and CAM-chem



Modified after C. Heald, MIT Cambridge

Simplified Chemistry (CAM6):

- SOAG (oxygenated VOCs) derived from fixed mass yields
- no interactions with land

Comprehensive Chemistry:

- SOAG formation derived from VOCs using Volatility Basis Set (VBS) description
- 5 volatility bins
- Interactive with land emissions

-> more physical approach

Modeling Chemistry-Climate Interactions in CESM2

Surface concentrations and emissions

- surface concentrations (greenhouse gases)
- emission: anthropogenic, biogenic, biomass burning, ocean, soil, volcanoes

Chemical mechanism: important for chemistry and aerosol production

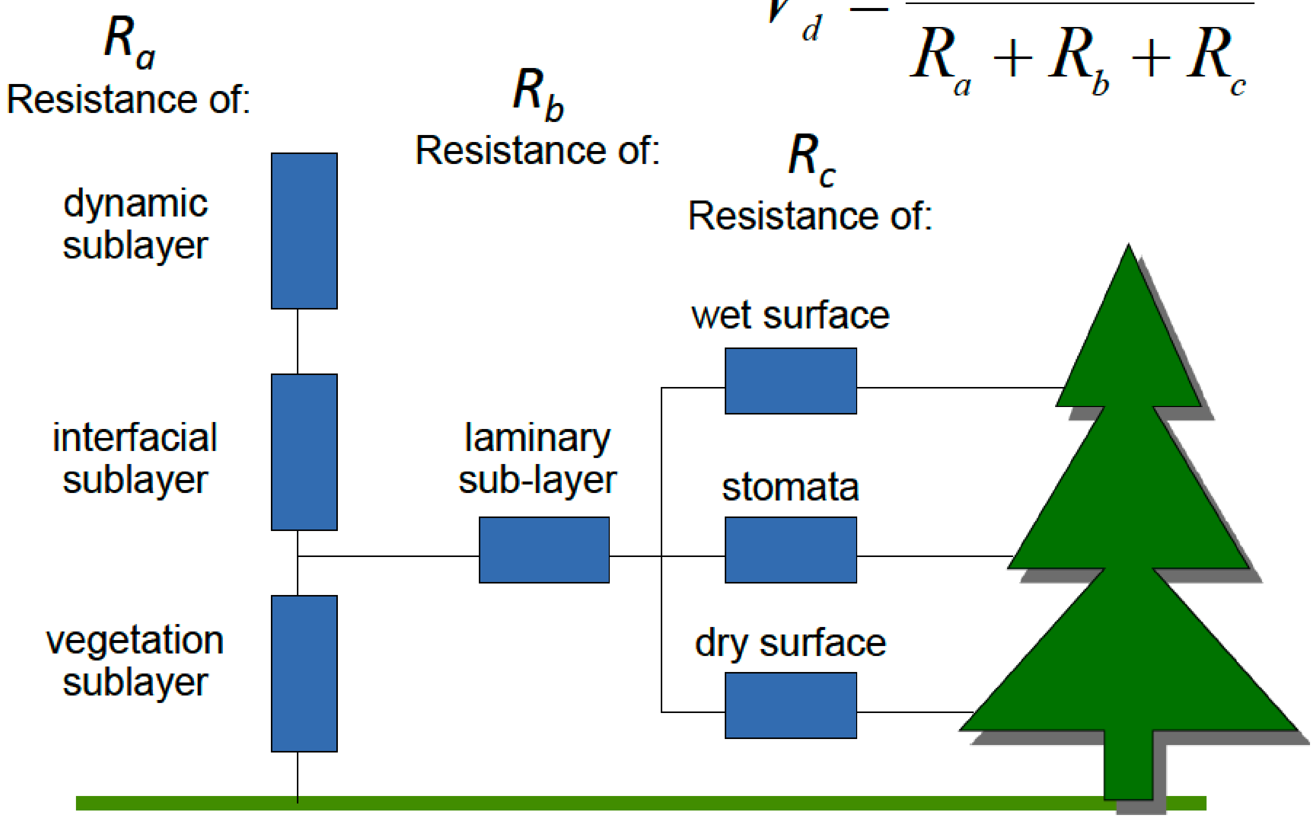
- WACCM and CAMchem: 417 reactions and 220 solution species
- CAM6: 6 chemical reactions and 26 solution species (much simpler)

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).

Dry Deposition

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



Varies with surface type (vegetation, ocean, etc.)
Key component of ozone budget
Important for sticky and soluble gases: HNO_3, CO, OVOCs, etc.

Important processes for simulating Aerosols

Surface concentrations and emissions

Chemical mechanism: important for chemistry and 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).

- 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.

Compsets define the specifics of emissions, chemistry, and deposition!

CAM-chem – Spectral Element

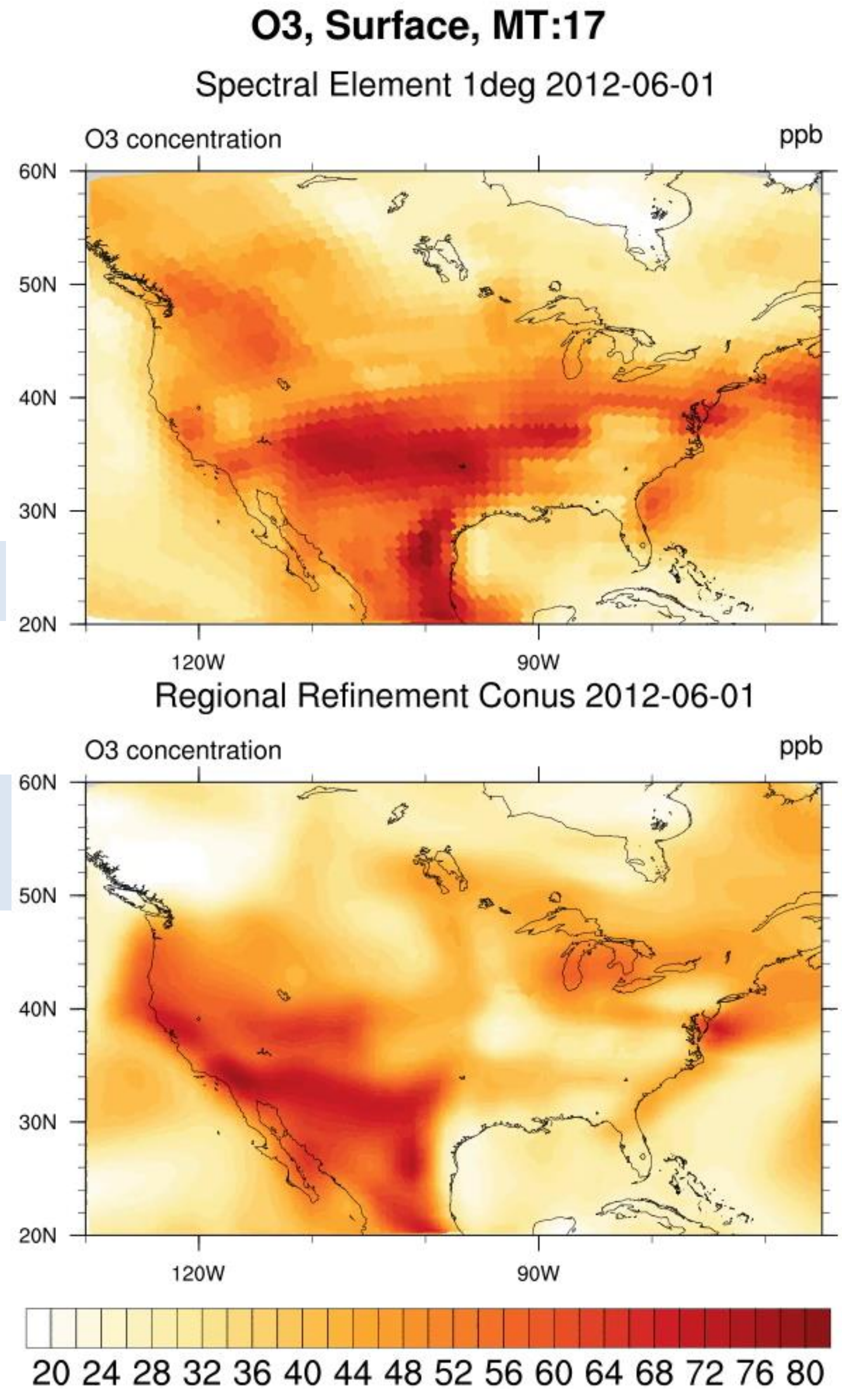
CAM6-chem with Spectral Element and Regional Refinement is running with ~14 km over U.S. (~1° elsewhere)

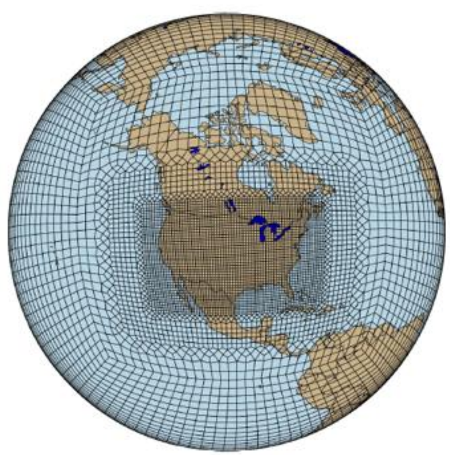
Current science goals:

- Studying air quality and health impacts in U.S.
- Evaluating importance of greater chemical complexity vs. higher horizontal resolution

ne30

CONUS
ne30x8





NSF NCAR

AMWG Diagnostic Package includes WACCM and Chemistry diagnostics

Chemistry Set Description

1 Tables / Chemistry of ANN global budgets
2 Vertical Contour Plots contour plots of DJF, MAM, JJA, SON and ANN zonal means
3 Ozone Climatology Comparisons Profiles, Seasonal Cycle and Taylor Diagram
4 Column O3 and CO lon/lat Comparisons to satellite data
5 Vertical Profile Profiles Comparisons to NOAA Aircraft observations
6 Vertical Profile Profiles Comparisons to Emmons Aircraft climatology
7 Surface observation Scatter Plot Comparisons to IMROVE

WACCM Set Description

1 Tables of regional min, max, means
2 Seasonal cycle line plots of SP, SM, EQ, NM, NP zonal means (vertical log scale)
3 Vertical seasonal cycle plots of SP, SM, EQ, NM, NP zonal means (vertical log scale)
4 Vertical contour plots of JUN, DEC, DJF, MAM, JJA, SON and ANN zonal means (vertical log scale)
5 Horizontal contour plots of JUL, AUG, JJA, DJF and ANN zonal means

User Support: CAM-Chem Wiki page

https://wiki.ucar.edu/display/camchem/Home

Advanced Changes	• Data Assimilation • Online Air-Sea Interface for Soluble Species • Updating Gas-phase Chemistry • Tagging CO and simple tracers • Clone a Case • Create a Branch • Biogenic Emission Options (MEGAN)
Model Component Descriptions	• Wet Deposition • Dry Deposition • Gas-phase Chemistry • Emission Inventories • Aerosols
Processing	• Pre-processing • Using CAM-chem output • Automated CESM diagnostic package • GitHub Tutorial
User Community	• Current Users/Projects • Chemistry-Climate Working Group Publications • UCAR Publications

WACCM and CAM-Chem Customer Support

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

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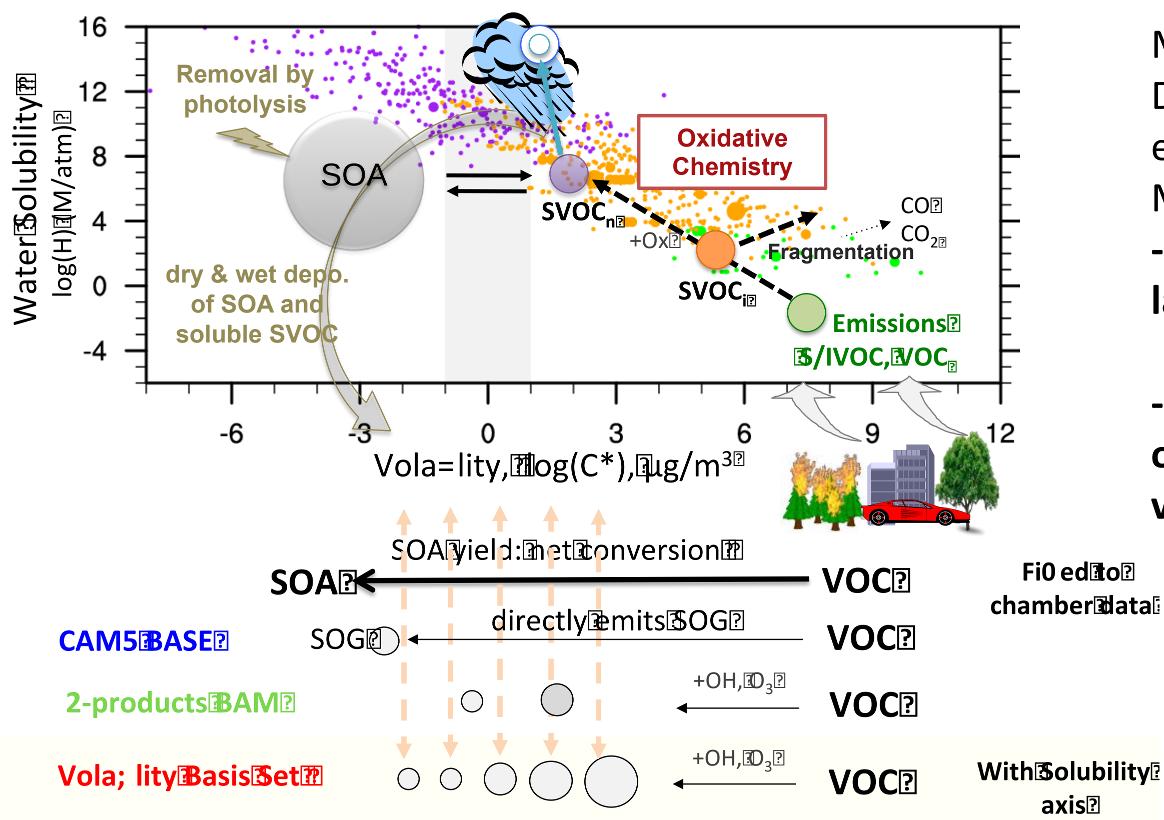
NCAR | UCAR | COMMUNITY EARTH SYSTEM MODEL CESM ™

Extras

New Secondary Organic Aerosol approach in CESM2 CAM-chem and WACCM

Simplis=c ways of trea=ng the complex SOA lifecycle



More physical approach

Direct coupling to biogenic emissions changes from MEGAN

-> couples SOA formation to land use and climate change

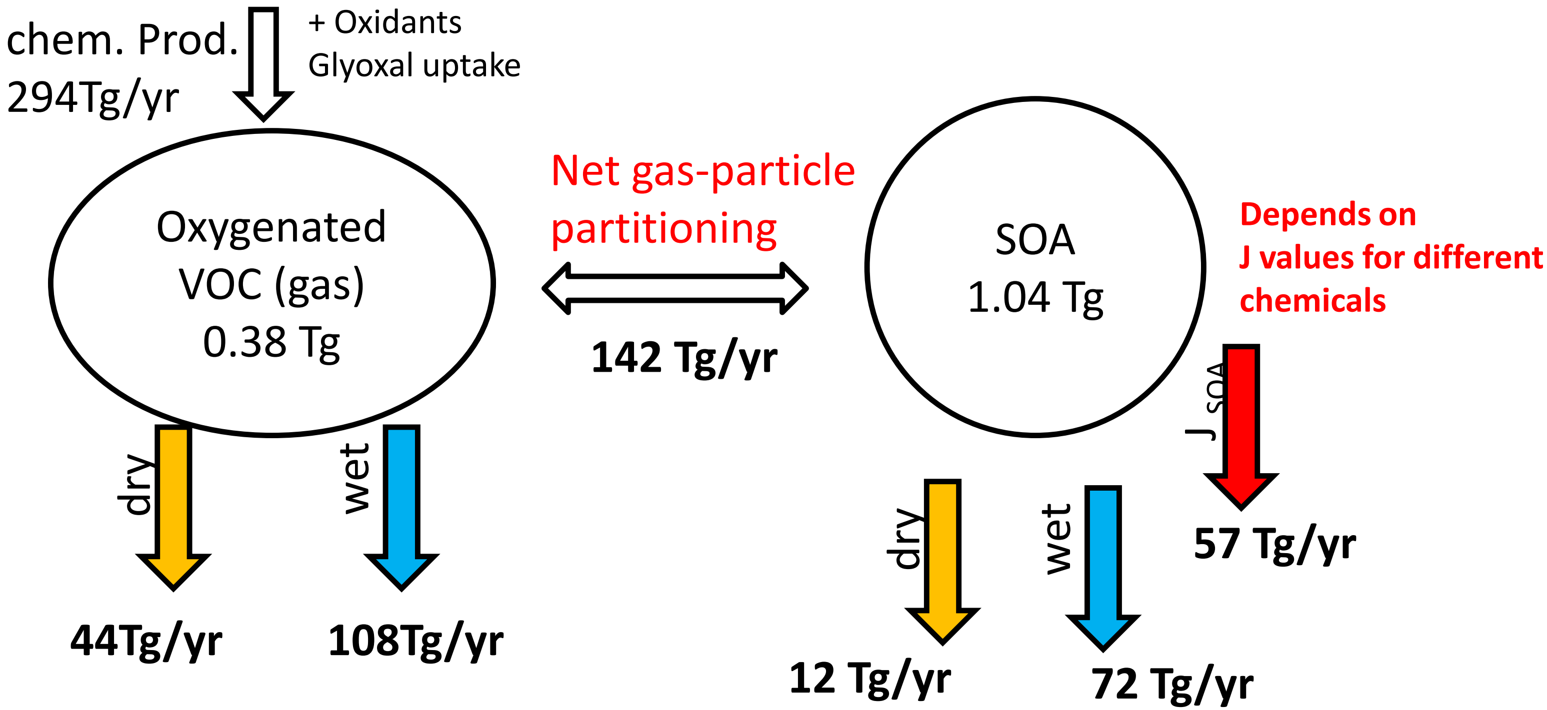
-> VBS (volatility bin scheme) only works in full chemistry version at this point

Most of it from biogenic emissions
-> strongly dependent on MEGAN emissions

VBS Budgets 1995-2010

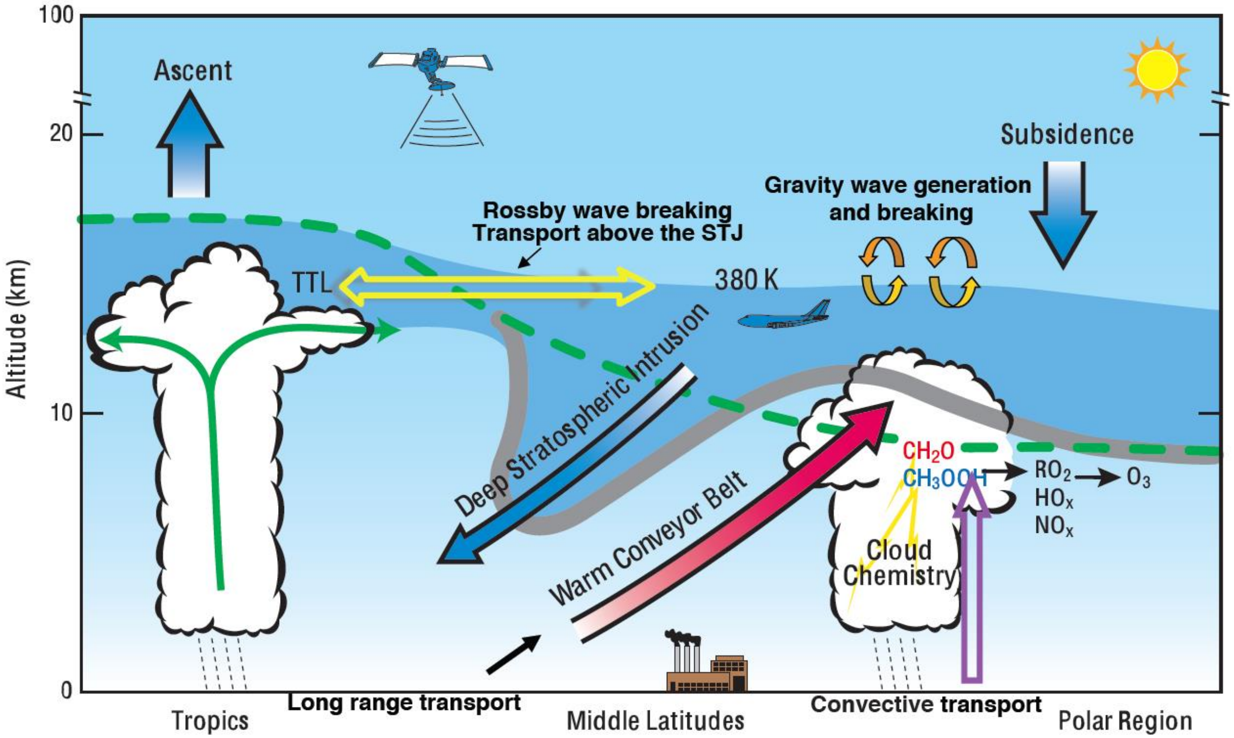
Biogenic, anthropogenic and biomass burning VOC, SIVOC

Lifetime: 4.5 years



Values very close to observational estimates!

Stratosphere-Troposphere Exchange



- Gases and aerosols are transported in stratosphere-troposphere exchange
- Impact of halogen loading on stratospheric ozone (ozone hole)
- Impact on climate (importance of very short-lived species)

-> local changes on short time scales are important