July, 2026

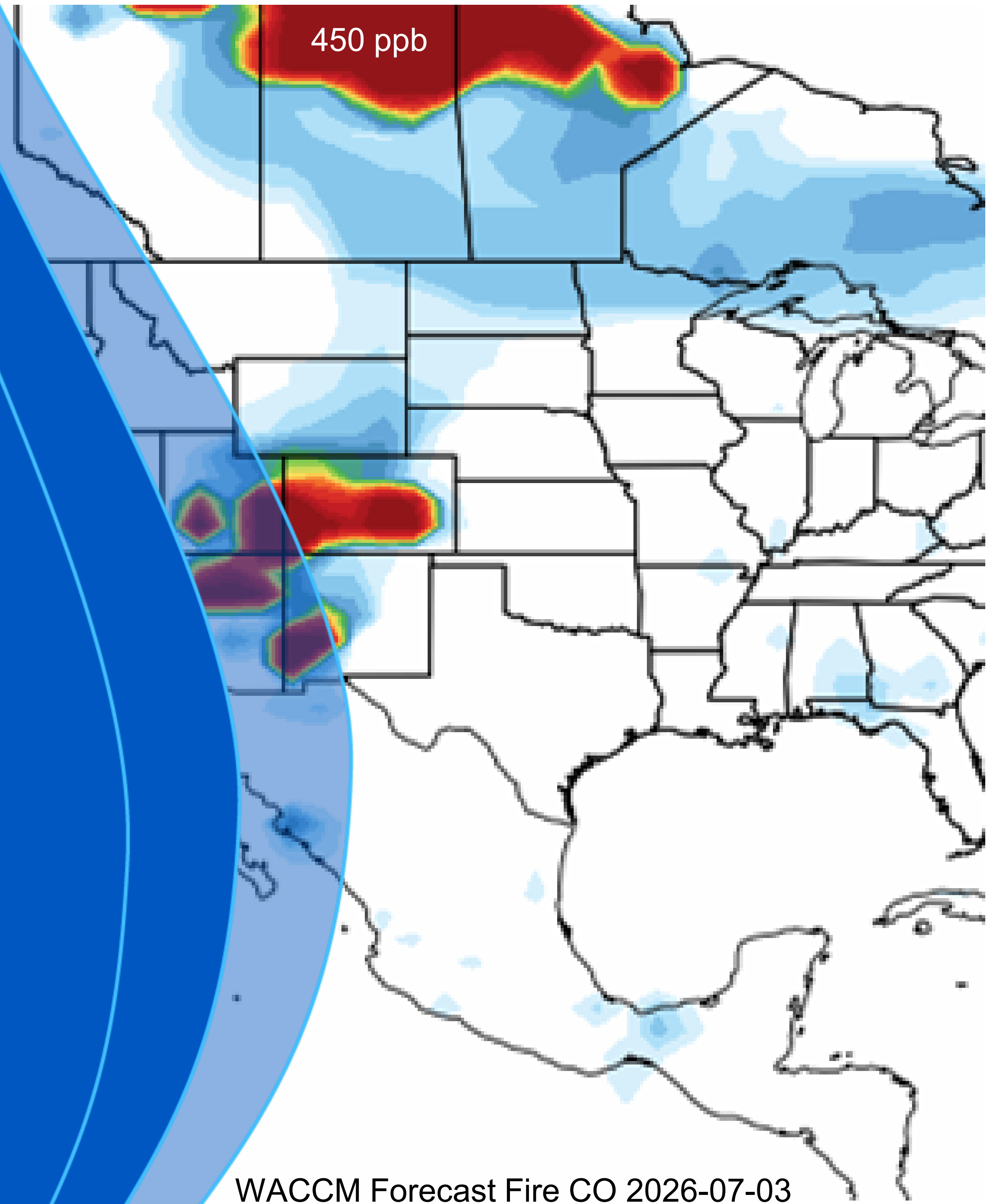
Modeling Atmospheric Chemistry and Aerosols

Presented by: **Rebecca R. Buchholz** Scientist V

Atmospheric Chemistry Observations and Modeling (ACOM) Laboratory,

Slide Content Contributions:

Simone Tilmes, Shawn Honomichl, Mike Mills, Louisa Emmons, Doug Kinnison, Kelley Barsanti, Wenfu Tang, Peter Lawrence, Peter Lauritzen, Danny Leung, Jun Zhang, Ben Gaubert



WACCM Forecast Fire CO 2026-07-03

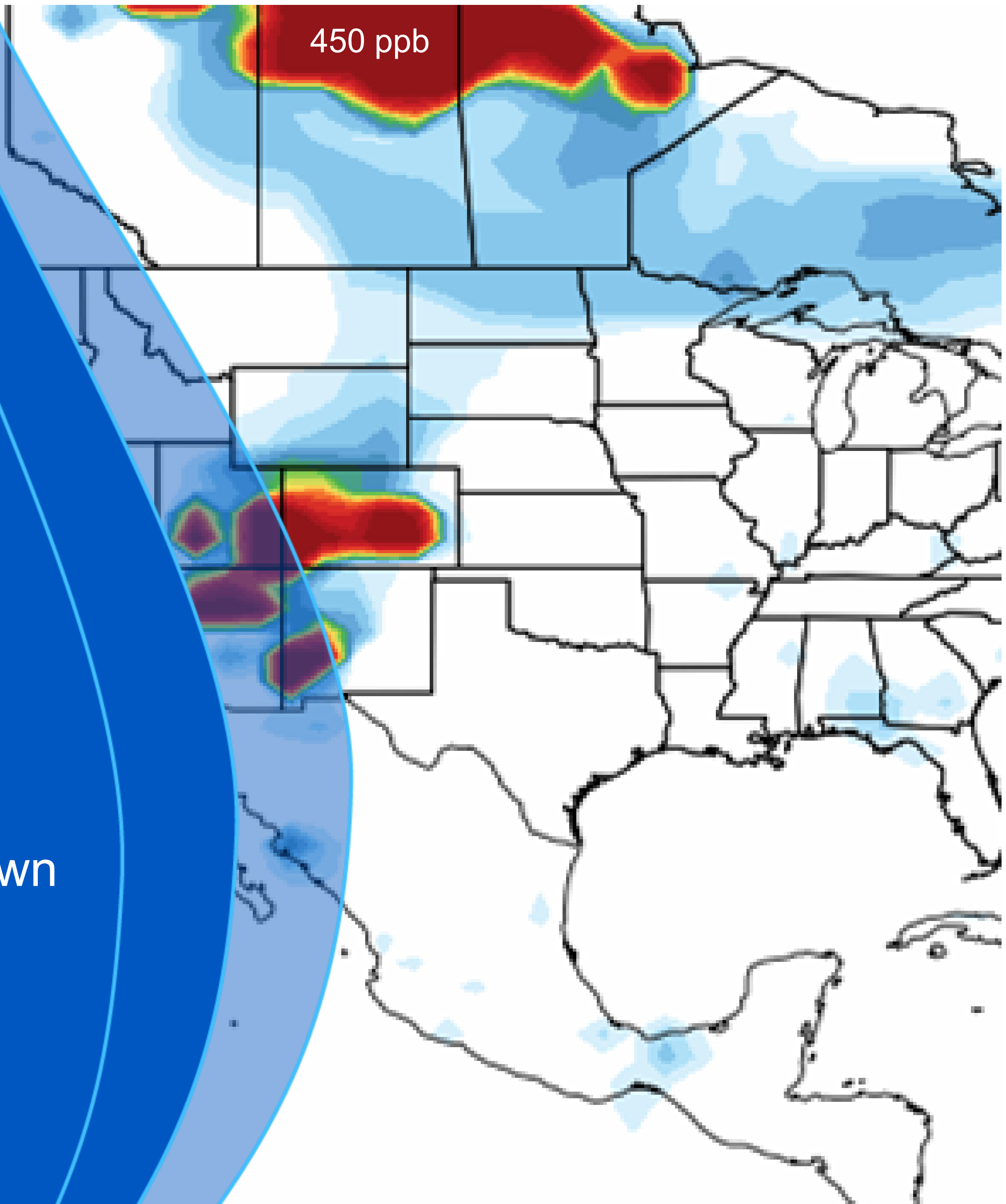
This material is based upon work supported by the NSF National Center for Atmospheric Research, a major facility sponsored by the U.S. National Science Foundation and managed by the University Corporation for Atmospheric Research. Any opinions, findings and conclusions or recommendations expressed in this material do not necessarily reflect the views of NSF.

Chemistry - Aerosol Working Group (CAWG)

CAWG Co-Chairs: Simone Tilmes
Rafael Fernandez

Software Engineer: Francis Vitt

CAWG Liaisons: Rebecca Buchholz
Shawn Honomichl



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Atmospheric Chemistry: Why is it important – Health

Ozone pollution (NOx, CO, VOC, CH4):

- Damages tissues, causes inflammation
- Coughing, chest tightness and worsening of asthma

Particulate Matter: PM2.5 and PM10 diameter < 2.5 or 10 µm (SO2, VOC, NH3, BC, OC, fine dust):

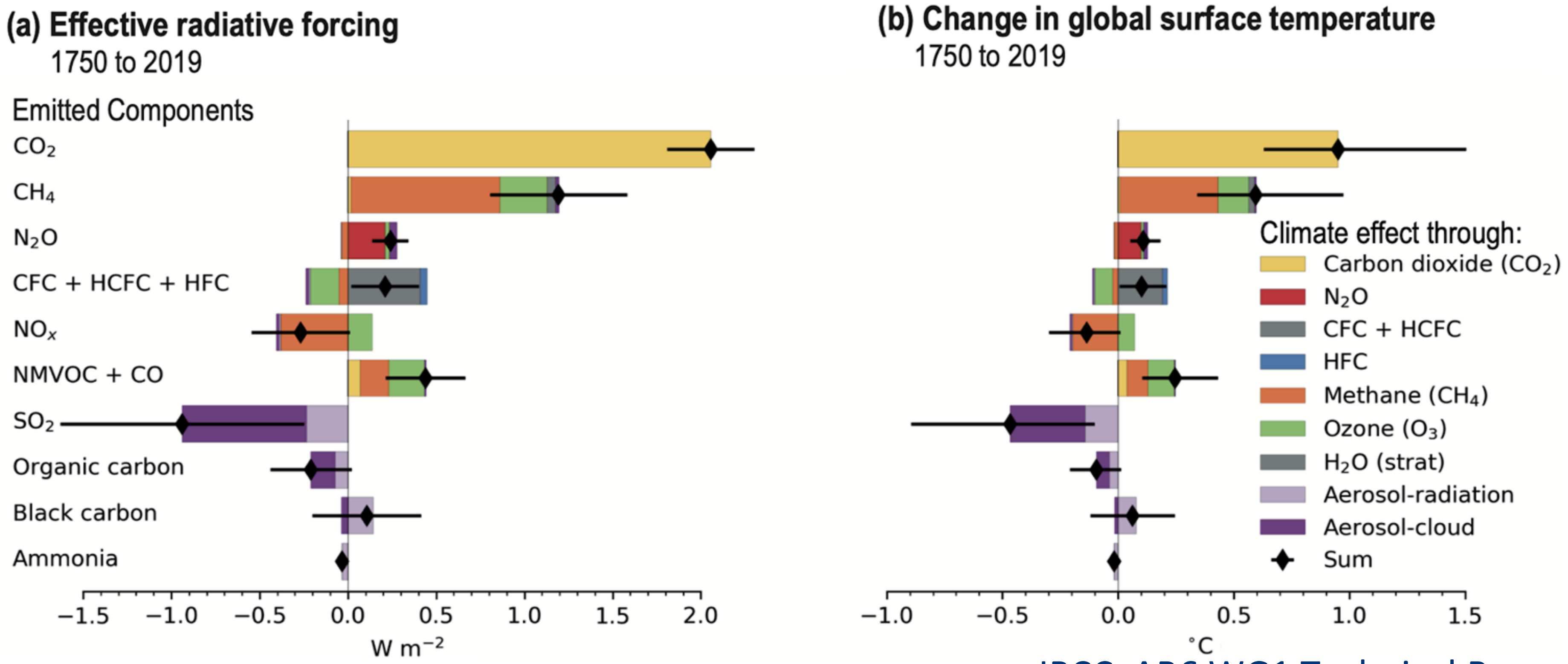
- Cardiovascular impacts (lungs and heart), mortality

Sources:

- Fires
- Traffic / Industry & Private (anthropogenic)
- Farmland / Agriculture
- Vegetation
- PM: Dust storms
- PM: Volcanoes

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

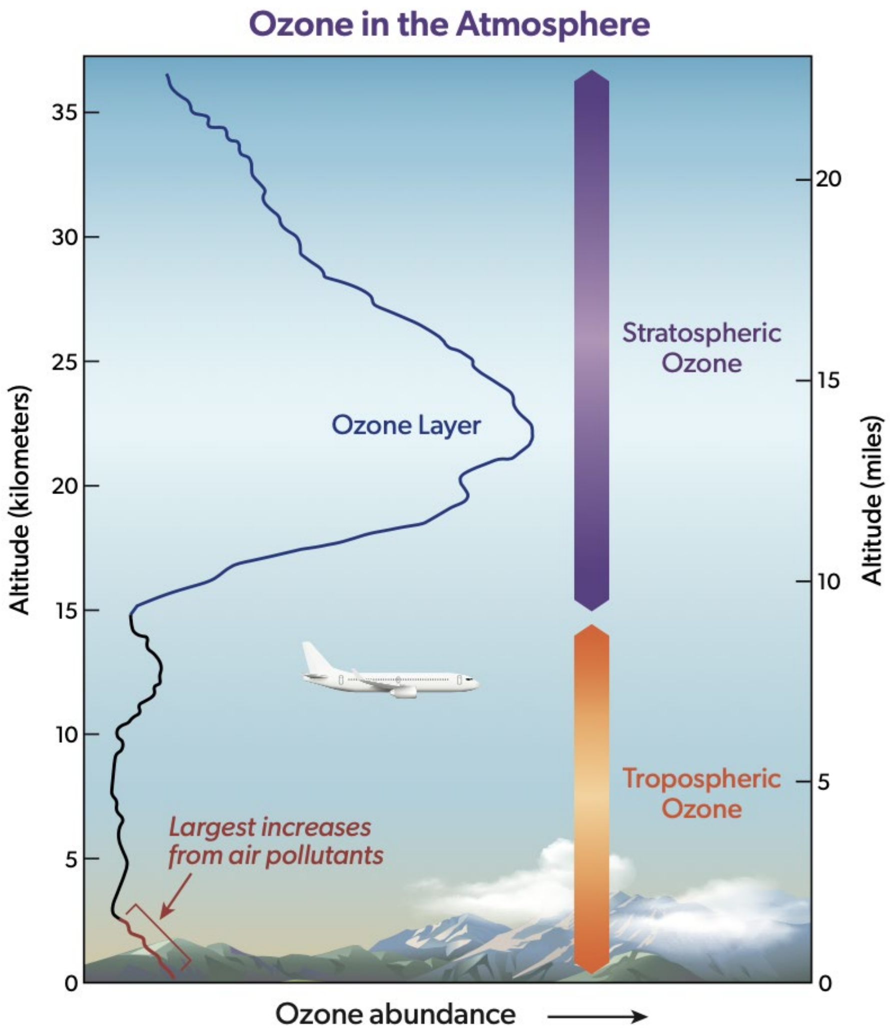
Atmospheric Chemistry:
Why is it important – Climate

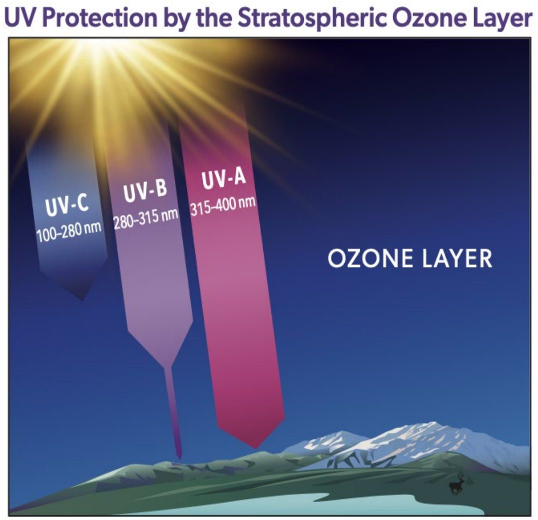


IPCC AR6 WG1 Technical Report, Figure TS15

- Chemistry and aerosols interact with weather and the climate
- Importance of describing ozone and aerosol precursors
- Importance of aerosol-cloud interactions in models

Atmospheric Chemistry:
Why is it important – Stratospheric Ozone



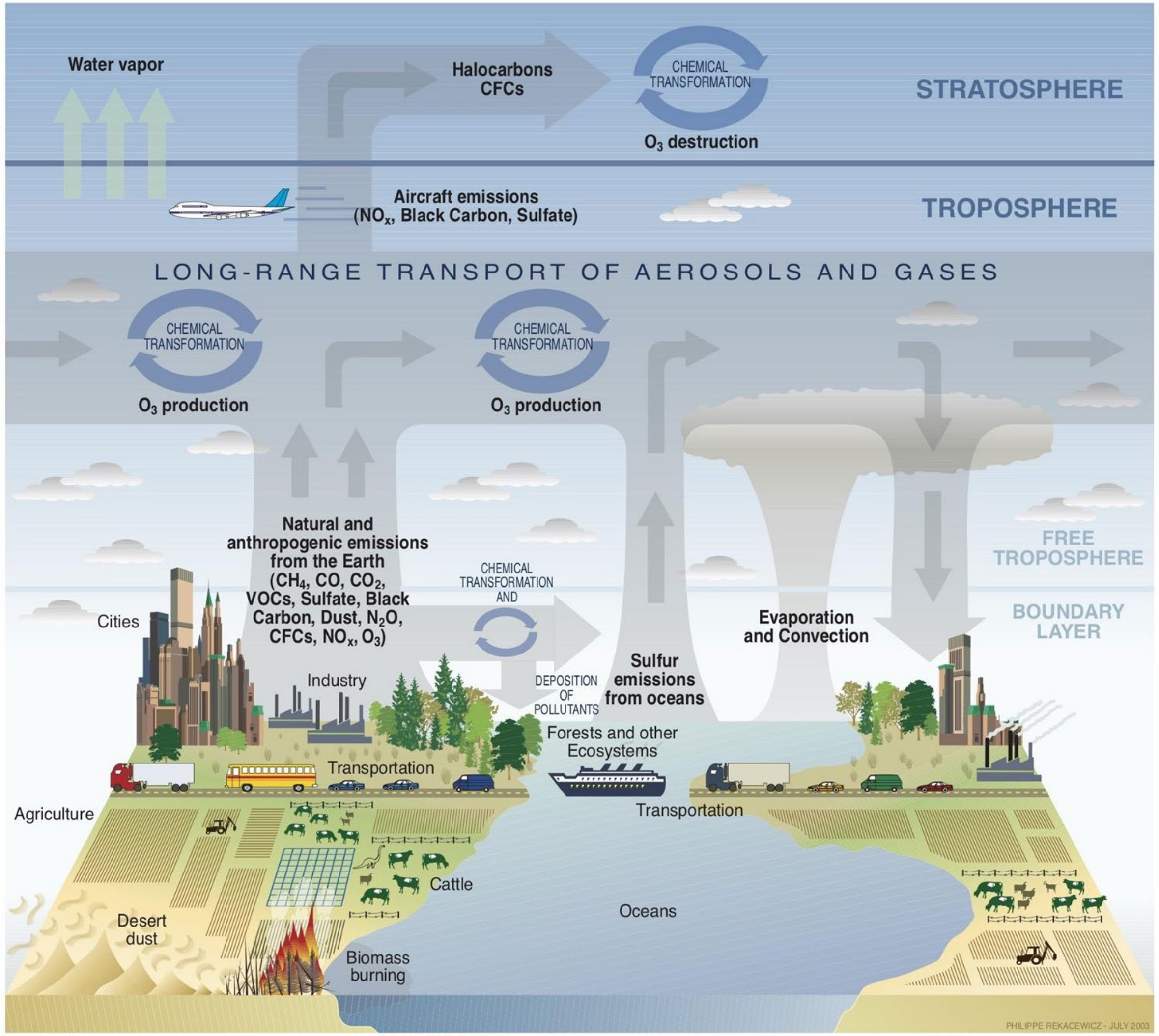


The ozone layer in the stratosphere protects life from harmful UV, through photochemical reactions

Accurate modeling is required:

- Impact on tropospheric chemistry
- Ozone hole recovery (CFCs)
  - e.g. cause of a slowing trend

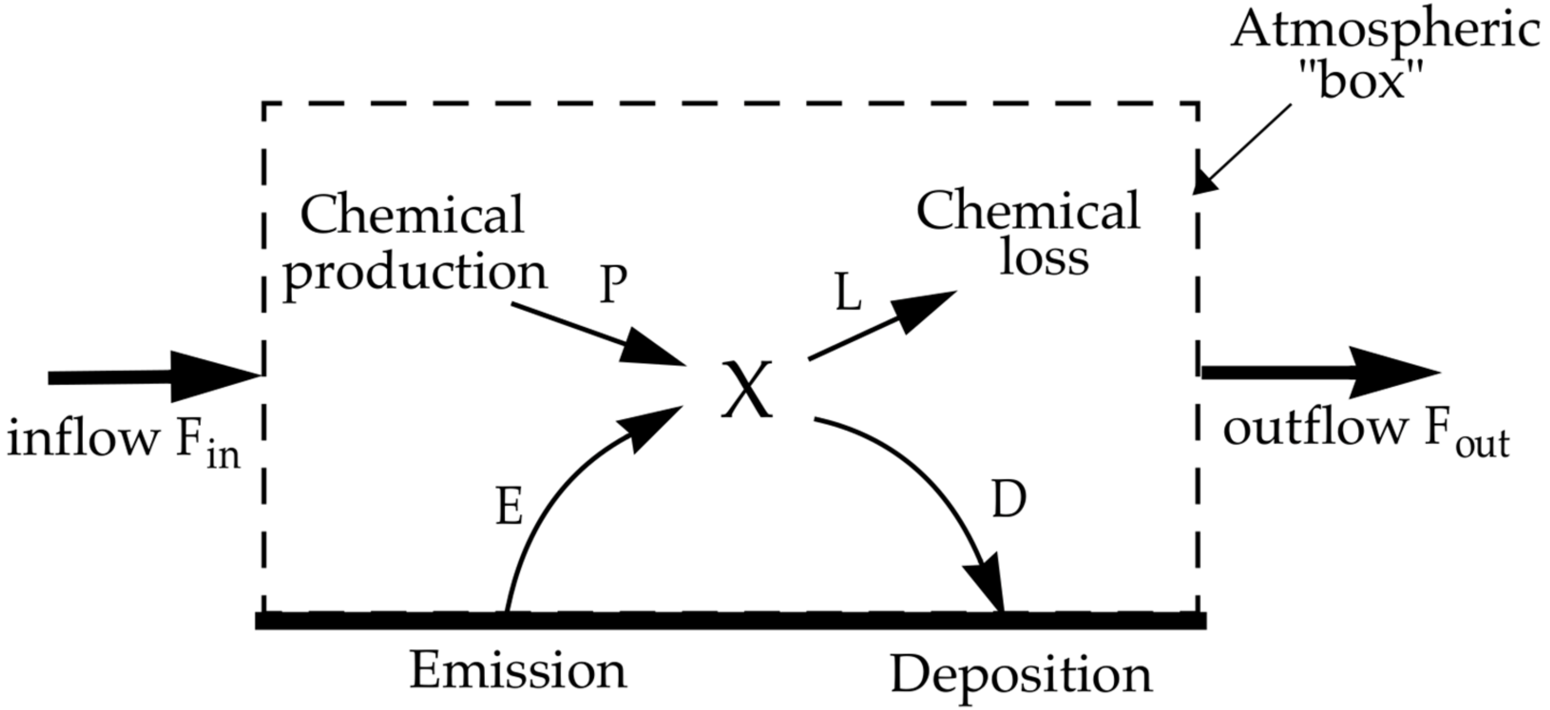
Atmospheric Chemistry in CESM3



- Modeled processes
  - Emissions
  - Chemical mechanism
  - Aerosol model and cloud interactions
  - Wet Deposition
  - Dry Deposition
- Support

Models solve the following for each chemical (χ)

$$\frac{\partial \chi(i)}{\partial t} = \mathrm{Sources(i)} - \mathrm{Sinks(i)} = \mathrm{E_i} + \mathrm{C_i} + \mathrm{A_i} + \mathrm{T_i} - \mathrm{W_i} - \mathrm{D_i}$$



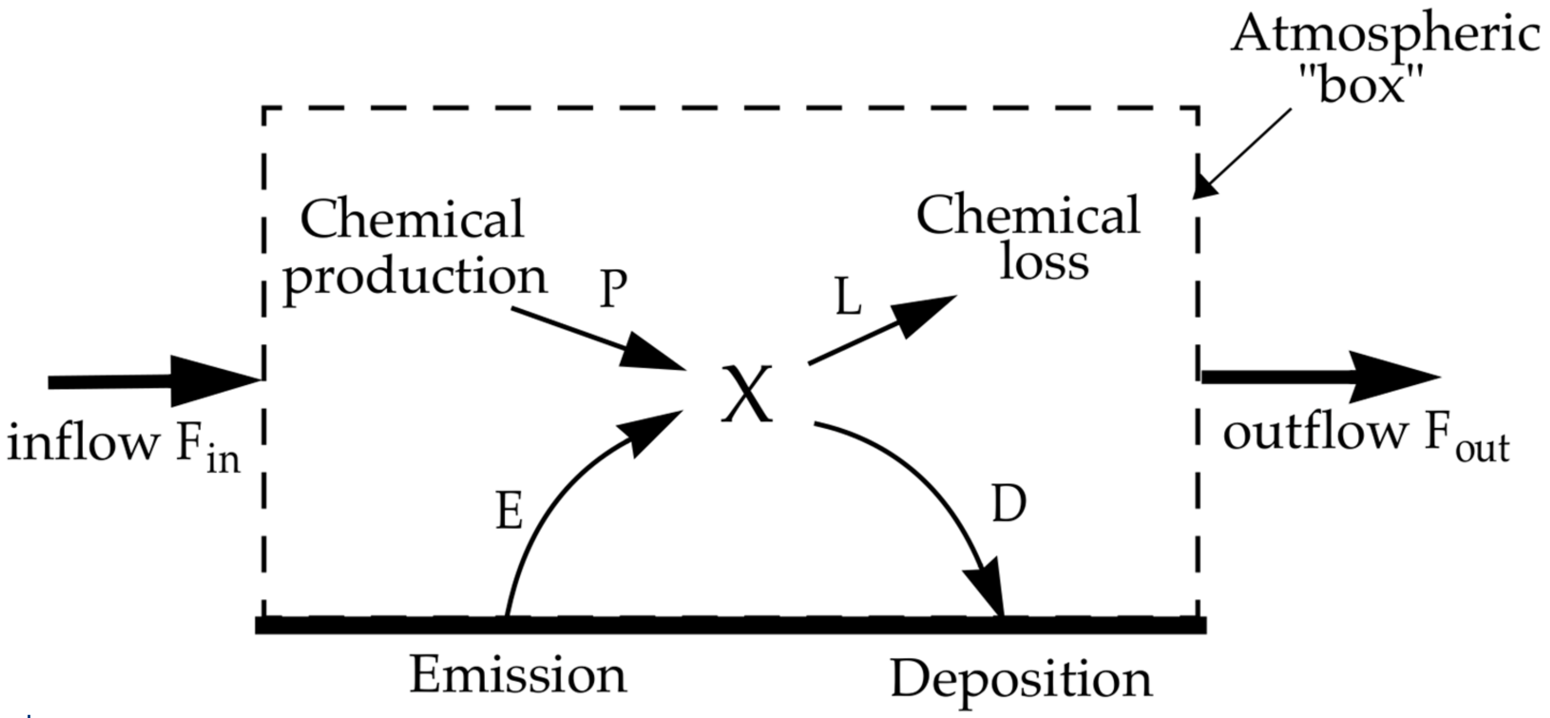
E_i Emissions
C_i Gas-phase-Chemistry
A_i Aerosol-processes (Gas-aerosol exchange, het chem.)
T_i Advection + Diffusion
W_i Cloud-processes (wet deposition)
D_i Dry deposition

Introduction to Atmospheric Chemistry, Daniel J. Jacob

Models solve the following for each chemical (χ)

it can get expensive very fast! $$$

$$\frac{\partial \chi(i)}{\partial t} = \mathrm{Sources(i)} - \mathrm{Sinks(i)} = \mathrm{E_i} + \mathrm{C_i} + \mathrm{A_i} + \mathrm{T_i} - \mathrm{W_i} - \mathrm{D_i}$$



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[Introduction to Atmospheric Chemistry](), Daniel J. Jacob

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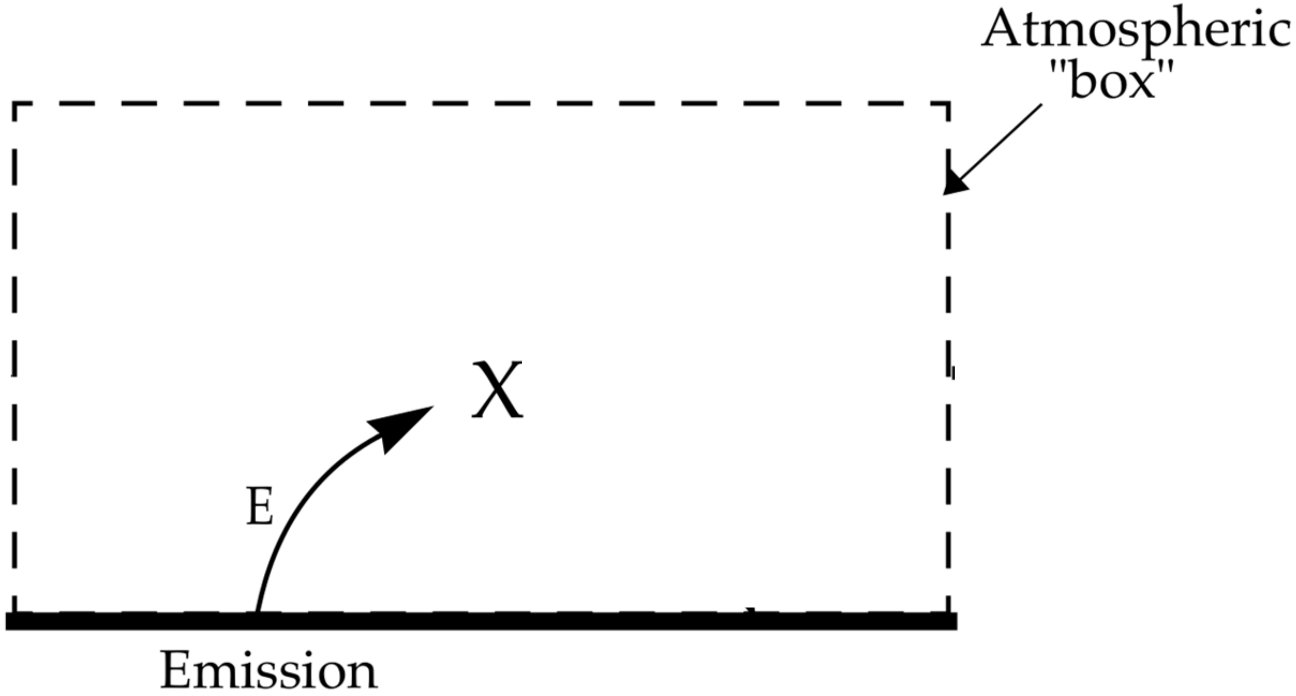


E_i Emissions

[Introduction to Atmospheric Chemistry](), Daniel J. Jacob

Emissions in CESM: 4 main “types”

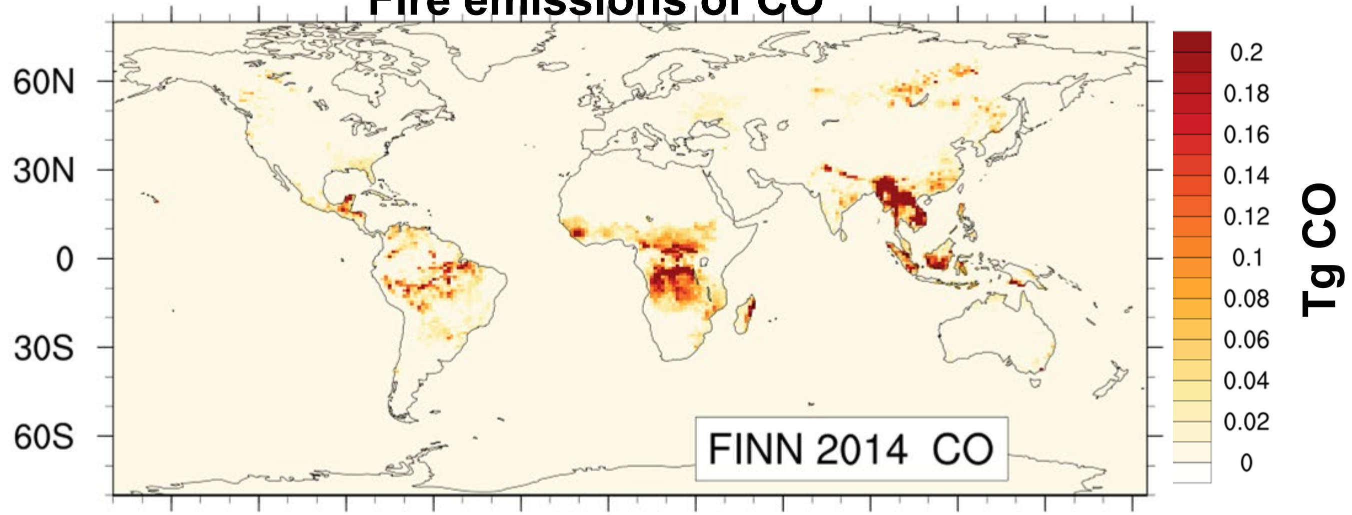
Emissions

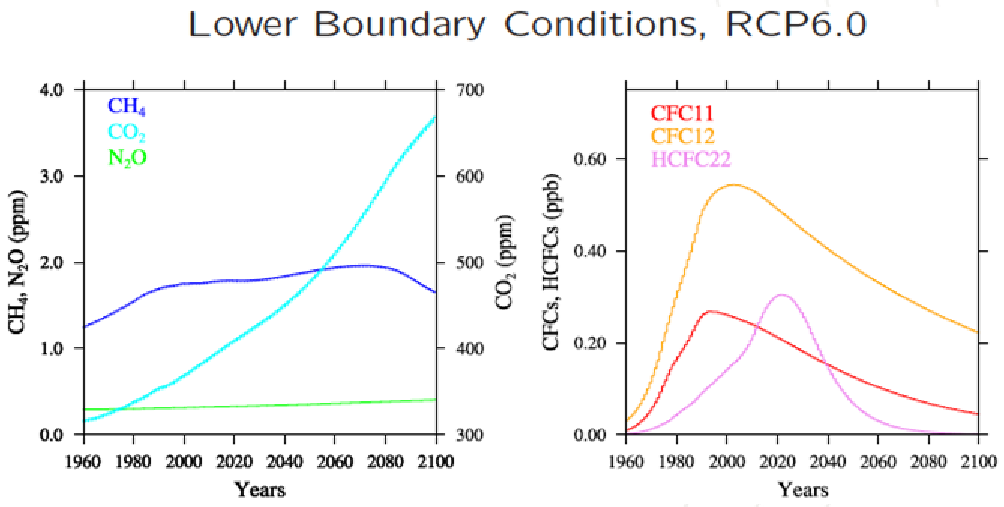
- Surface emissions: anthropogenic, biogenic, biomass burning (fire), ocean, soil
- Vertical emissions: (external forcings): aircraft, volcanoes, power plants, (fire optional)
- Interactive: Dust, biogenic, sea salt, lightning NOX, (fire optional/experimental)

Surface concentrations

- Lower boundary conditions (greenhouse gases CO2, CH4, O3, N2O and, long-lived gases CFCs). Can vary latitudinally.

Fire emissions of CO





Interactive emissions: Dust

$$F_{dustemis} = F_{dustemis}(u_*, w)$$

horizontal wind/friction

soil moisture

becomes

$$F_{dustemis} = F_{dustemis}(u_*, w, \underbrace{z_{0,rock}, \mathrm{LAI}}, \sigma_{\tilde{u}})$$

(Leung et al., 2024)

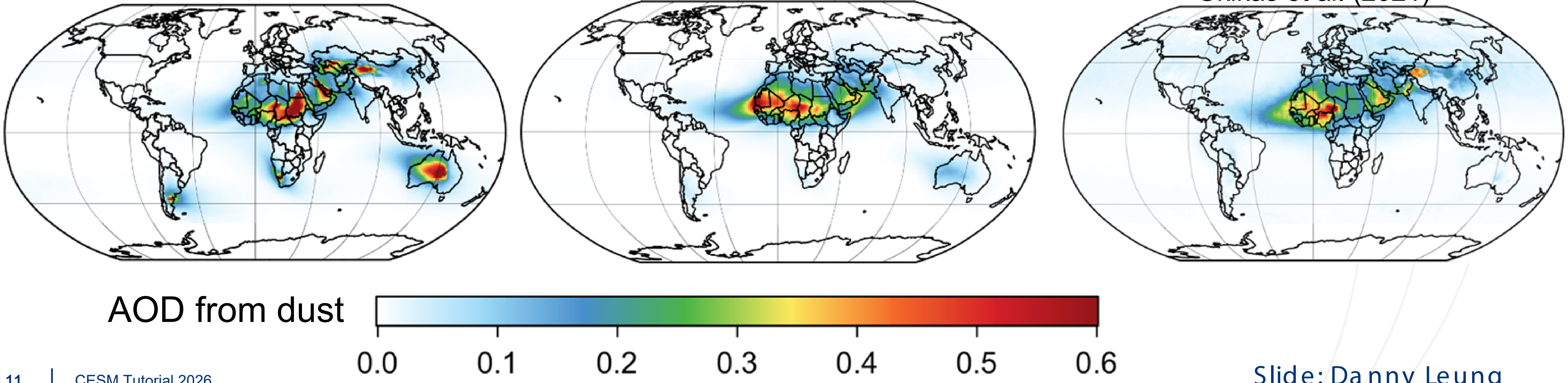
Drag partition due to surface roughness

Subtimestep wind following the similarity theory

Charlie Zender et al. (2003; DEAD)
CESM2/CAM6

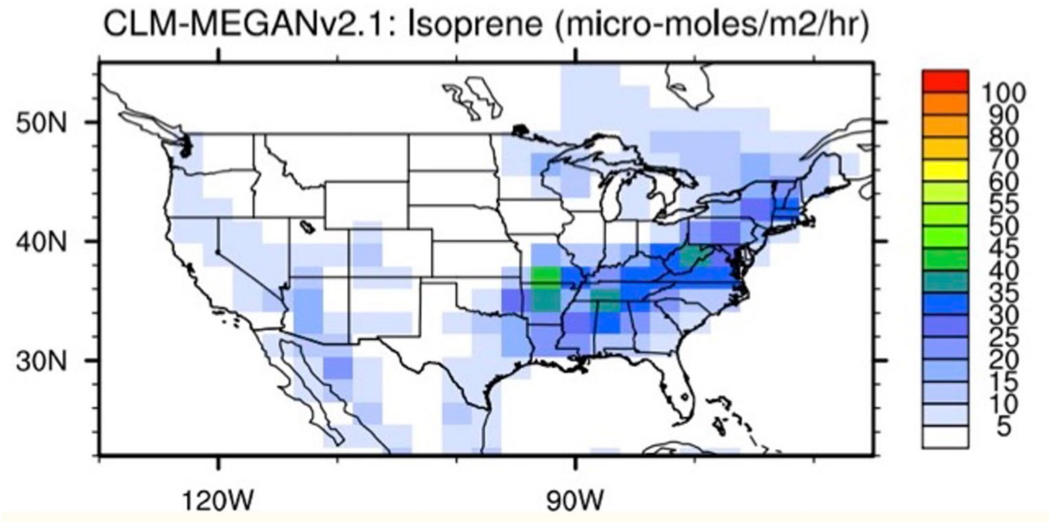
Danny Leung et al. (2024; L23)
CESM3/CAM7 (**default**)

MIDAS (MODIS/Aqua) dust
Gkikas et al. (2021)



Slide: Danny Leung

Interactive emissions: Biogenic



Guenther et al., GMD, 2012

The MEGAN - v2.1 algorithm

Emissions for species i:

$$F_i = \gamma_i \; \Sigma \varepsilon_{i,j} \, \chi_j$$

where

- γ_i : emission activity factor, depends on leaf area index (LAI), meteorology (T, solar radiation), leaf age, soil moisture, with separate light-dependent and light-independent factors
- $\varepsilon_{i,j}$: emission factor at standard conditions for vegetation type (PFT) j
- χ_j : fractional area of PFT j

Slide: Louisa Emmons

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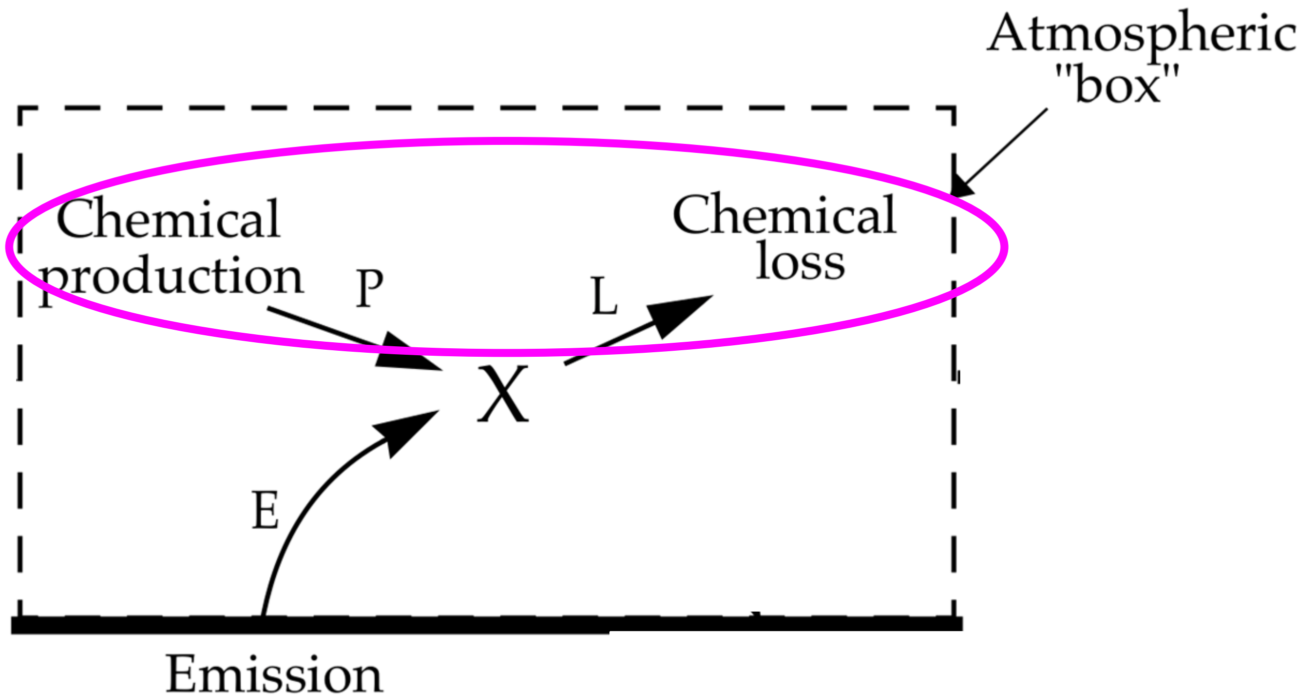
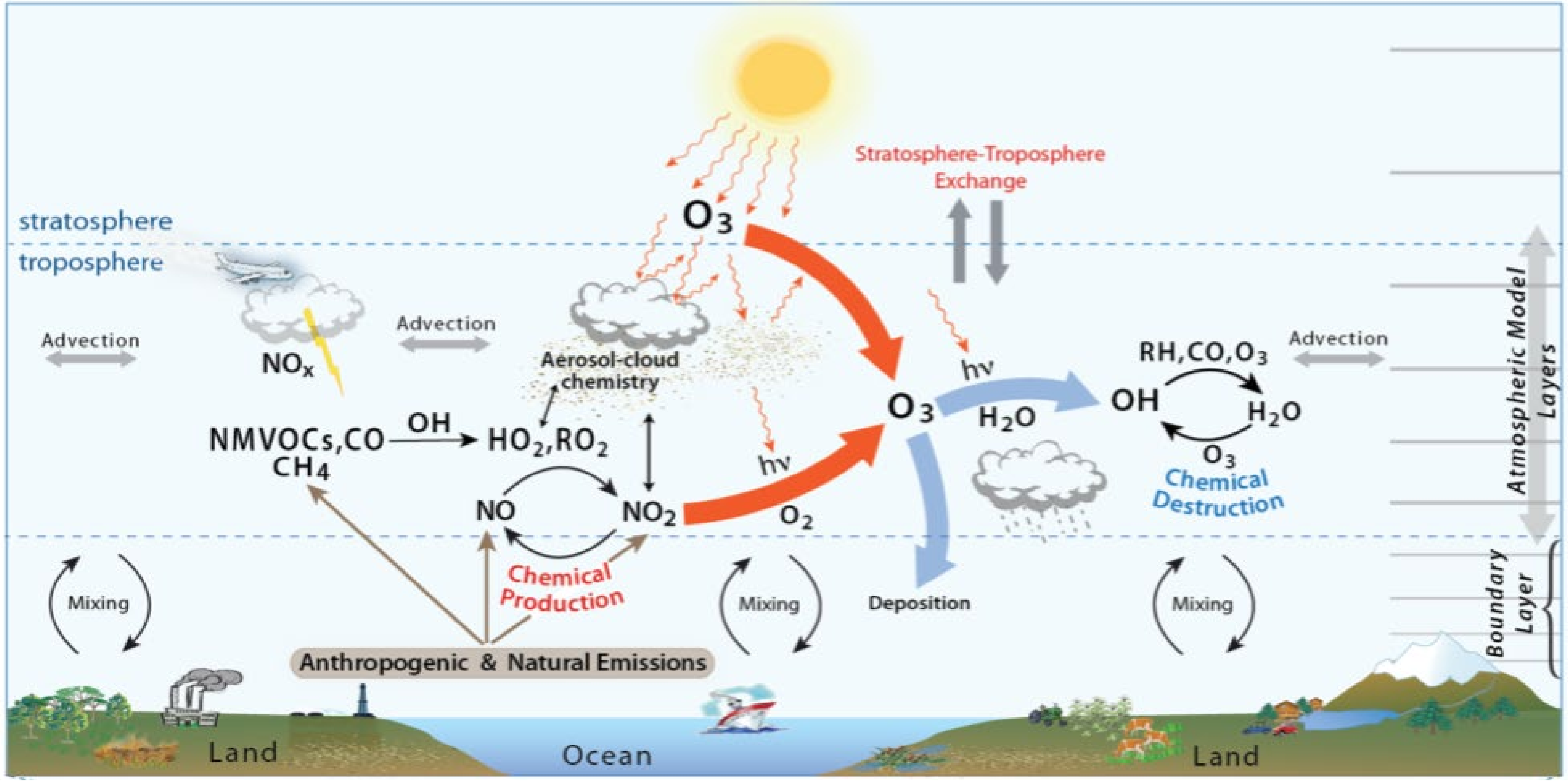


E_i Emissions
C_i Gas-phase-Chemistry
A_i Aerosol-processes (Gas-aerosol exchange, het chem.)

Introduction to Atmospheric Chemistry, Daniel J. Jacob

Tropospheric Chemistry

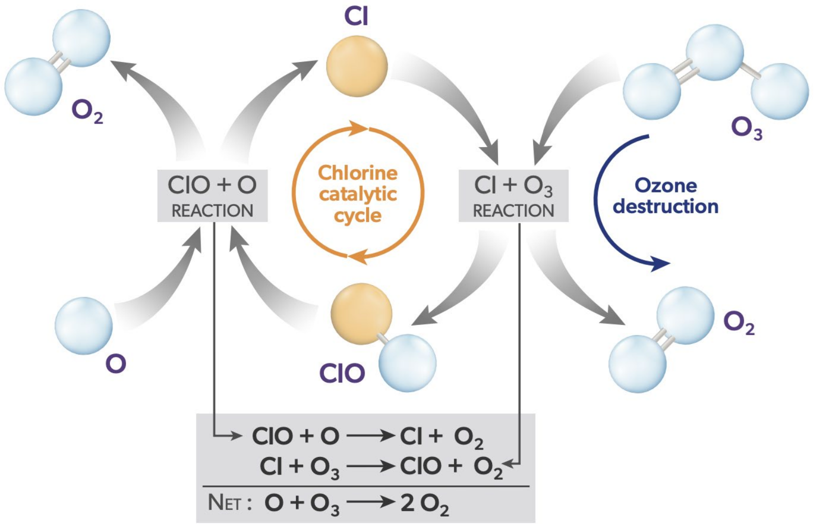


Young et al., 2018, https://doi.org/10.1525/elementa.265

- Photochemistry
- Gas-phase chemistry
- Heterogeneous chemistry
- Aqueous phase chemistry
- Gas-to-aerosol Exchange

Stratospheric Chemistry

Ozone Destruction Cycle 1 : Upper Stratosphere



Ozone Destruction Cycles 2 and 3 : Polar Regions

WMO2022

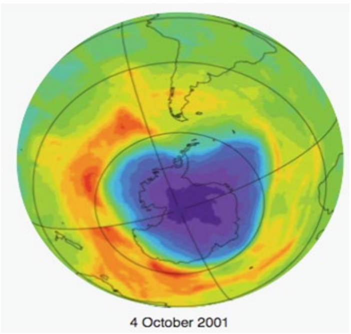
CYCLE 2 :

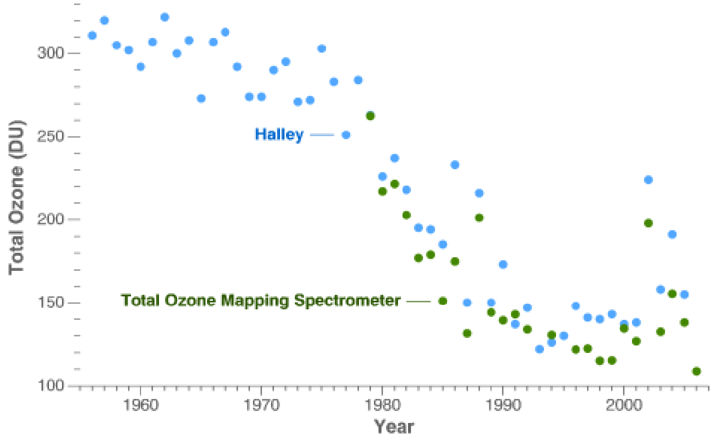
$$ClO + ClO \rightarrow (ClO)_2$$
$$(ClO)_2 + \textit{sunlight} \rightarrow ClOO + Cl$$
$$ClOO \rightarrow Cl + O_2$$
$$2(Cl + O_3 \rightarrow ClO + O_2)$$
$$\text{NET: } 2O_3 \rightarrow 3O_2$$

CYCLE 3 :

$$ClO + BrO \rightarrow Cl + Br + O_2$$

or
$$\left(\begin{array}{l} ClO + BrO \rightarrow BrCl + O_2 \\ BrCl + \textit{sunlight} \rightarrow Cl + Br \end{array} \right)$$
$$Cl + O_3 \rightarrow ClO + O_2$$
$$Br + O_3 \rightarrow BrO + O_2$$
$$\text{NET: } 2O_3 \rightarrow 3O_2$$



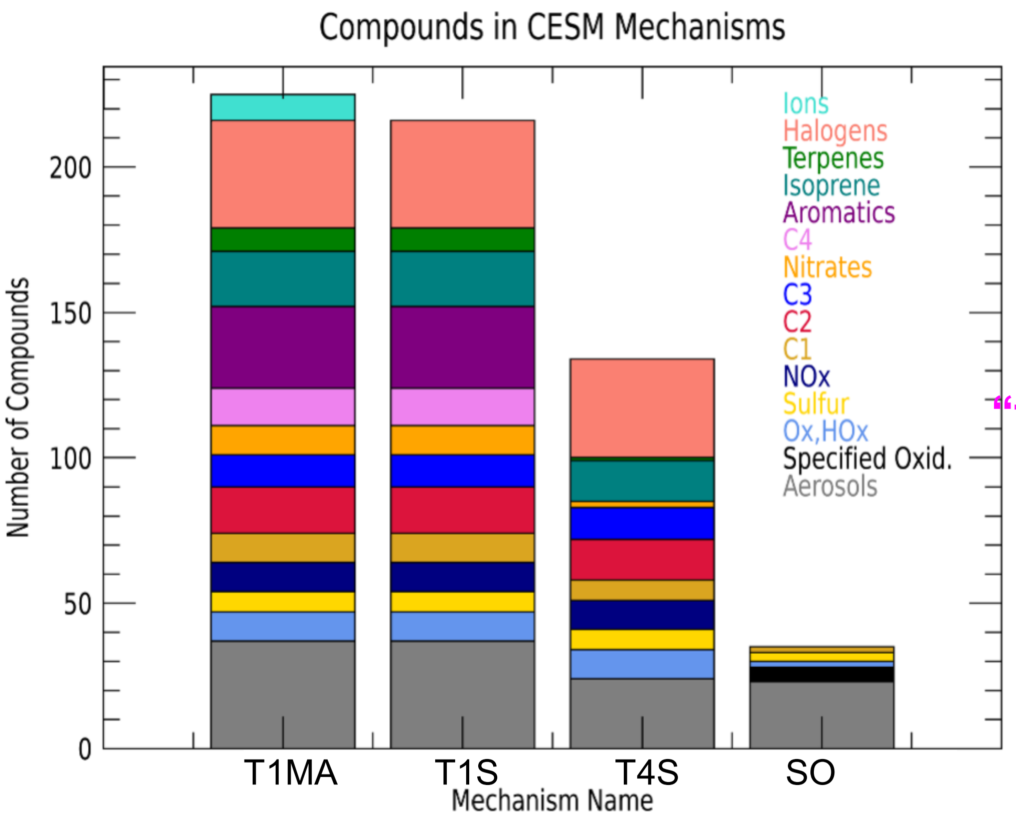


Comprehensive Stratospheric Chemistry

- Heterogeneous reactions
- Catalytic Cycles

Atmospheric chemistry mechanisms in CESM3

Chemistry mechanism descriptions: https://www2.acom.ucar.edu/gcm/mozart



T1S = default “full-chemistry” Troposphere and Stratosphere

Name	Description	# species
T1	Comprehensive tropospheric chemistry; for air quality simulations	179
T2	T1 with detailed terpene chemistry	265
T4	Simpler tropospheric chemistry suitable for climate simulations	97
T1S	T1 with comprehensive stratospheric chemistry	216
T1MA (TSMLT)	T1 with stratosphere, mesosphere, lower thermosphere chemistry	225
T4S	T4 with comprehensive stratospheric chemistry	134
SO	Specified Oxidants, with GHGs	33

Slide: Louisa Emmons

CESM3 Configurations with Chemistry

WACCM

TSMLT->T1MA
234 tracers

Middle Atmosphere (MA)
100 tracers

Specified chemistry -> Prescribed Oxidants
31 tracers

Provides Upper Boundary Conditions

Air Quality Chemistry

T1S: 231 tracers
T3S: 278 tracers
T5S (halogen chemistry): 277 tracers

MOSAIC/CARMA

oxidants, ozone, strat. aerosol

Trop4 / Strat Chemistry

T4S: 141 tracers
30% cheaper than TS1

As TS1 but cheaper tropospheric chemistry for climate

Specified Oxidant Chemistry

31 tracers
prescribed ozone, oxidants, aerosol
interactive GHGs and tropospheric aerosol

140 km

WACCM (High Top Model) 135L

80 km

Workhorse Model 93L

40 km

Low Top Model 58L

Fully coupled simulations with chemistry are required to inform GHG chemistry runs

CAM7 (Specified Oxidants, SO) vs Full Chemistry

Same atmosphere, physics, resolution
Different chemistry and aerosols -> emissions and coupling

CAM7: Aerosols are calculated, using simple chemistry (with “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 are derived using chemistry - climate simulations

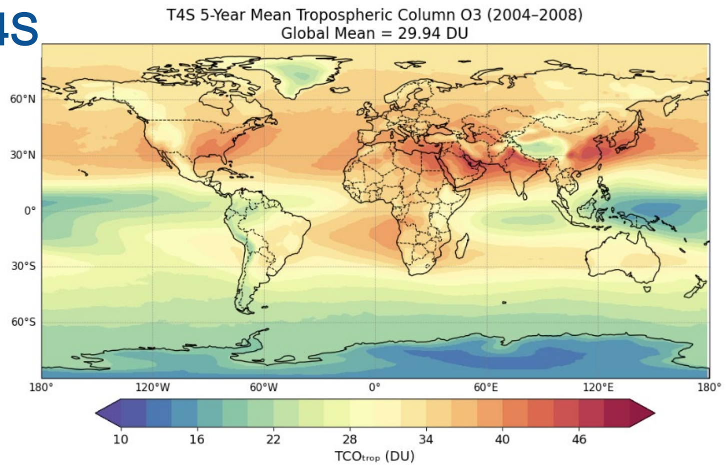
- Prescribed ozone is used for radiative calculations
- Prescribed oxidants is used for aerosol formation
- Prescribed methane oxidation rates
- Prescribed stratospheric aerosols
- Prescribed nitrogen deposition
- Simplified secondary organic aerosol description

*** New in CAM7 compared to CAM6: GHG chemistry (oxidation, photolysis) as opposed to fixed values, interactive SOAG production from biogenic emissions.

Simplified T4S Chemistry: Climate Simulations

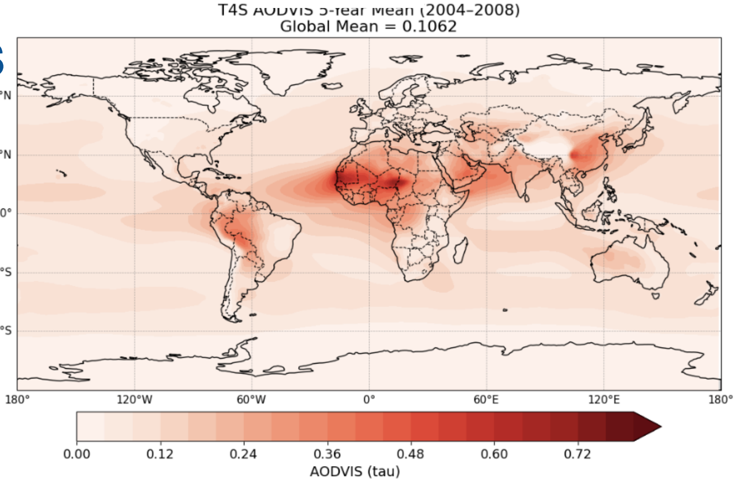
Tropospheric Column Ozone

T4S

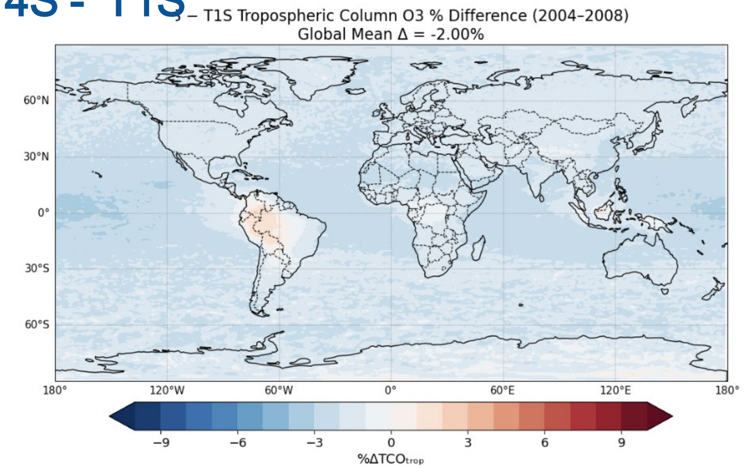


AODVIS

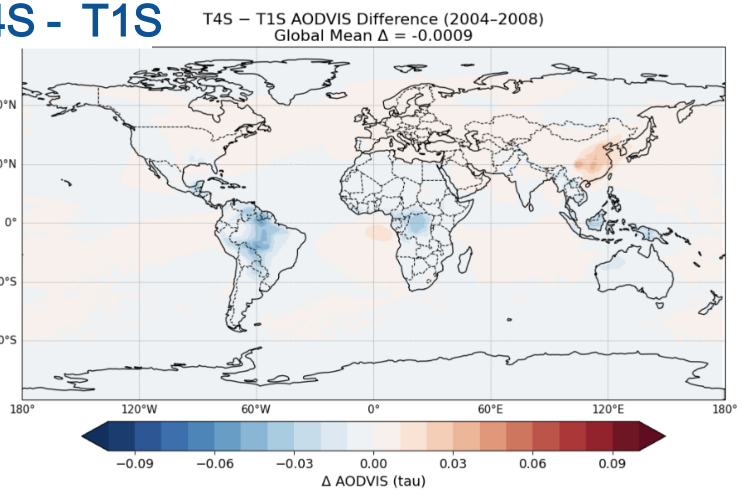
T4S



T4S - T1S



T4S - T1S



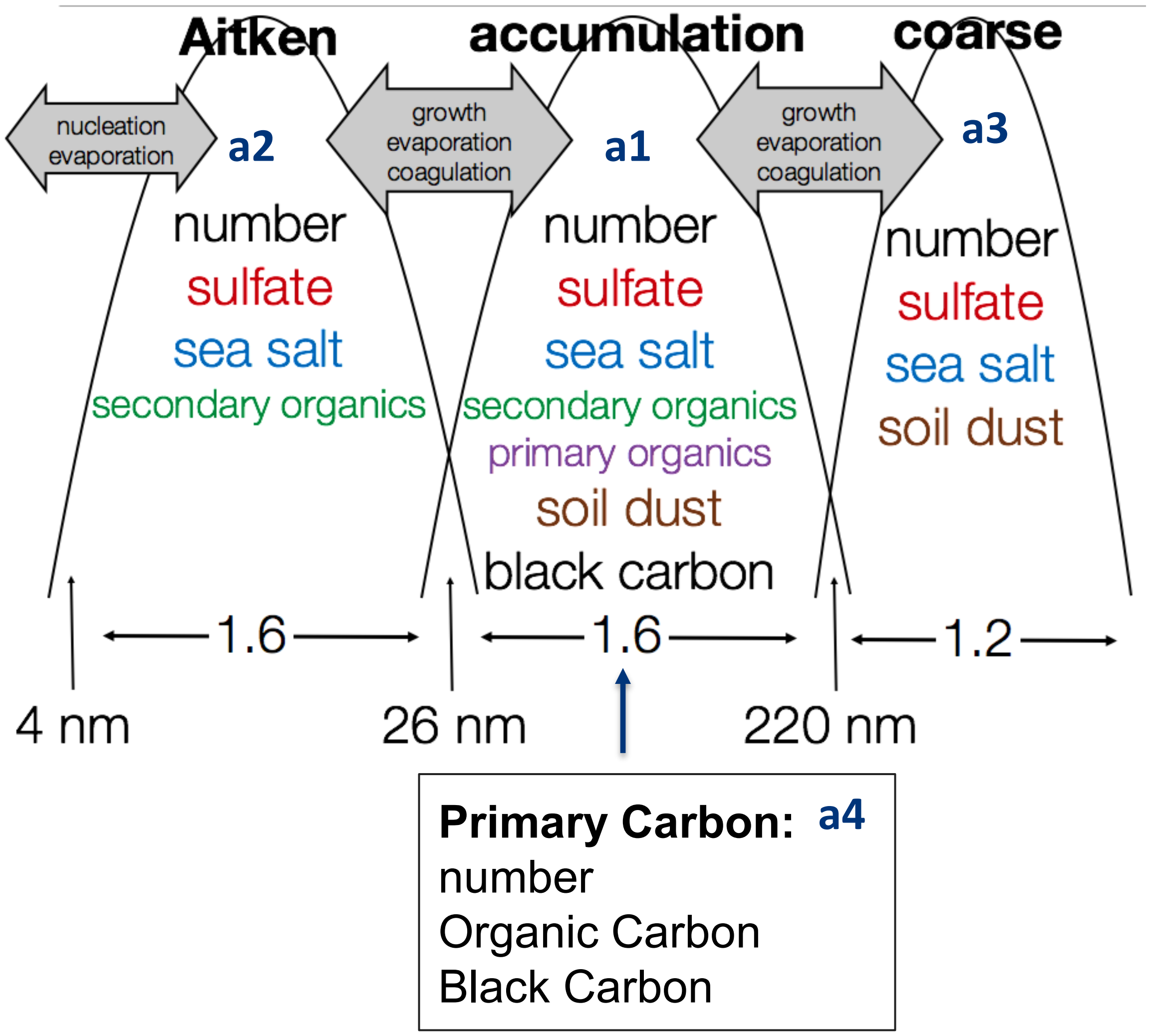
T4S substantially reduces computational cost (30%) compared to T1S, while retaining interactive tropospheric chemistry

Interactive biogenic emission for secondary organic aerosol production.

Small differences in Tropospheric Ozone and AOD compared to T1S chemistry.

Slide: Jun Zhang

Default Modal Aerosol Model (MAM4)

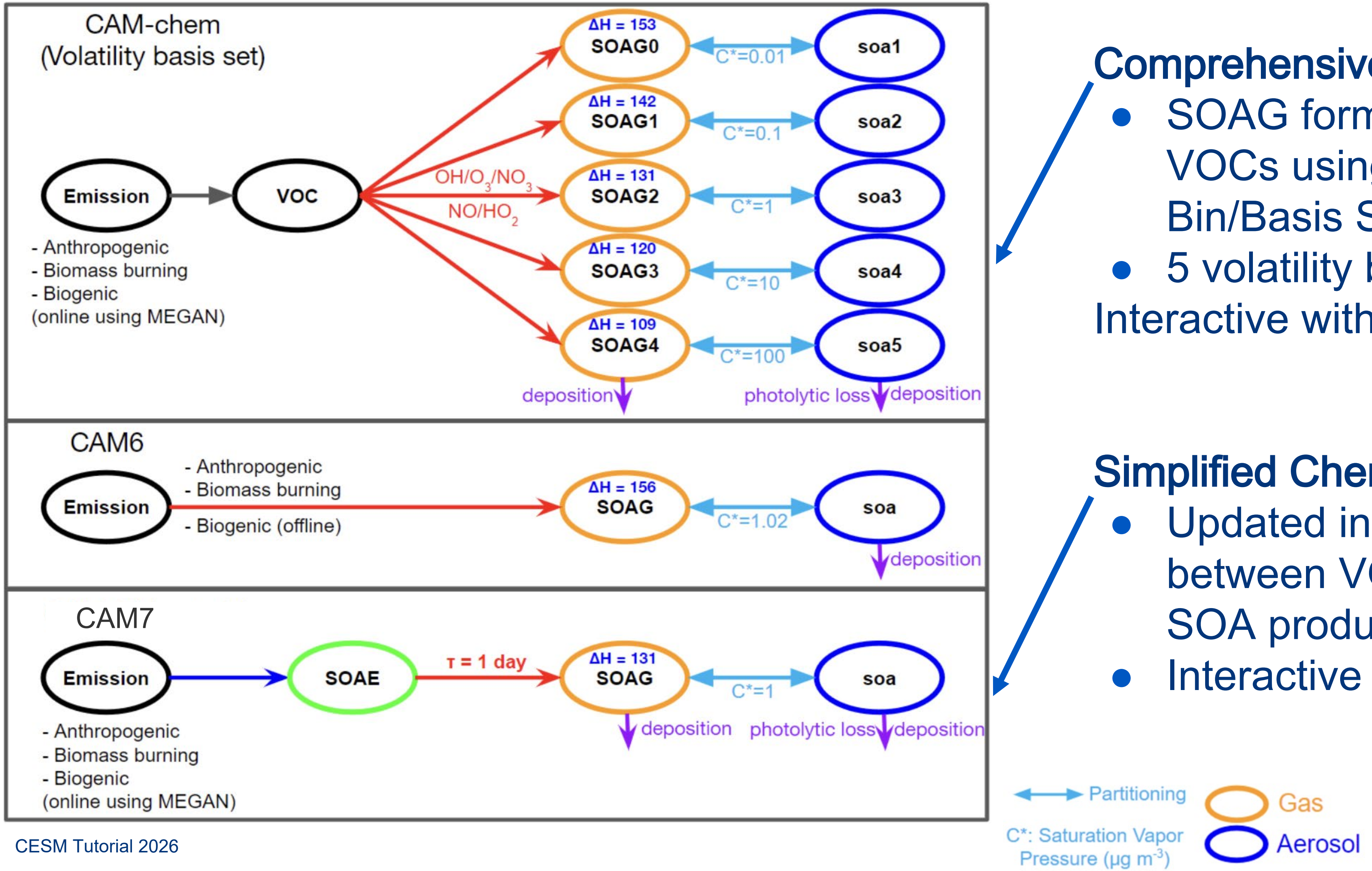


Representation of
Sulfates,
Black Carbon
Organic Carbon, Organic Matter (OC, SOA),
Mineral Dust and Sea - Salt

MAM5 : + Stratospheric sulfate mode

Slide: Mike MIlls

Secondary Organic Aerosol Description



Comprehensive Chemistry:

- SOAG formation derived from VOCs using Volatility Bin/Basis Set (VBS)
- 5 volatility bins

Interactive with land emissions

Simplified Chemistry (CAM7)

- Updated interactions between VOC emissions and SOA production
- Interactive with land

Jo et al., 2023, GMD

Models solve the following for each chemical (χ)

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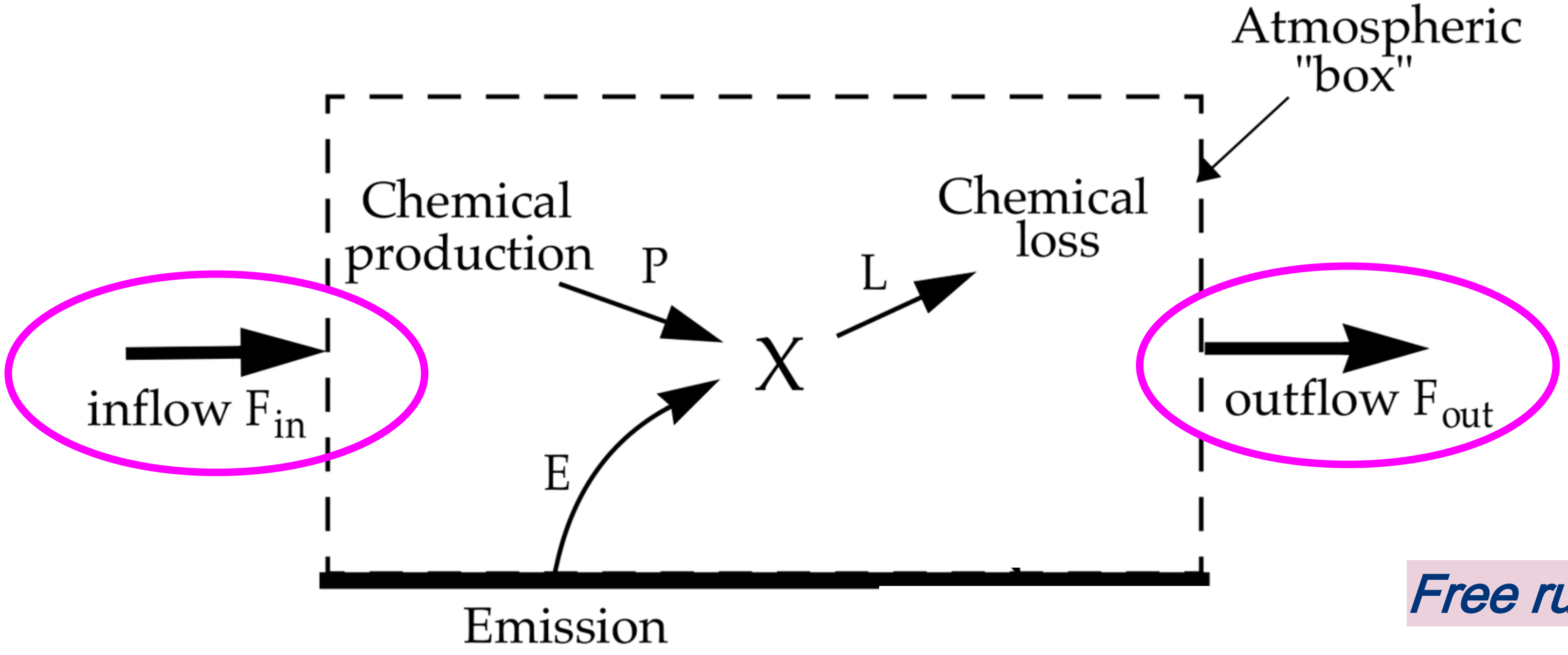

E_i Emissions
C_i Gas-phase-Chemistry
A_i Aerosol-processes (Gas-aerosol exchange, het chem.)
T_i Advection + Diffusion

Free running versus nudged (T, U, V)

Introduction to Atmospheric Chemistry, Daniel J. Jacob

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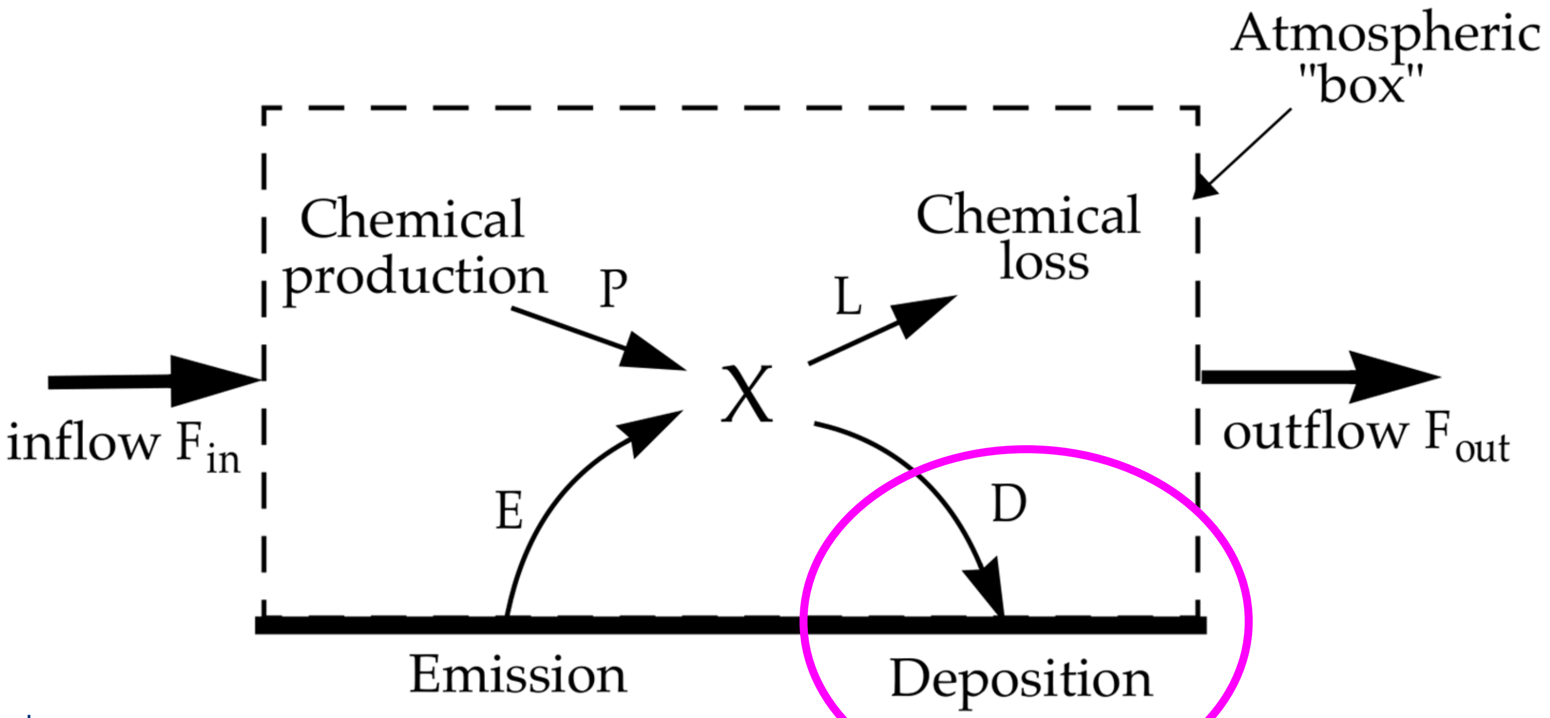

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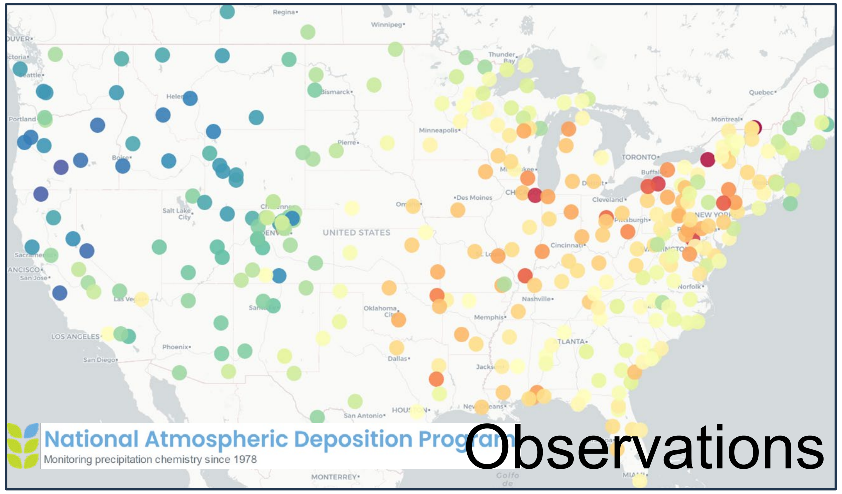
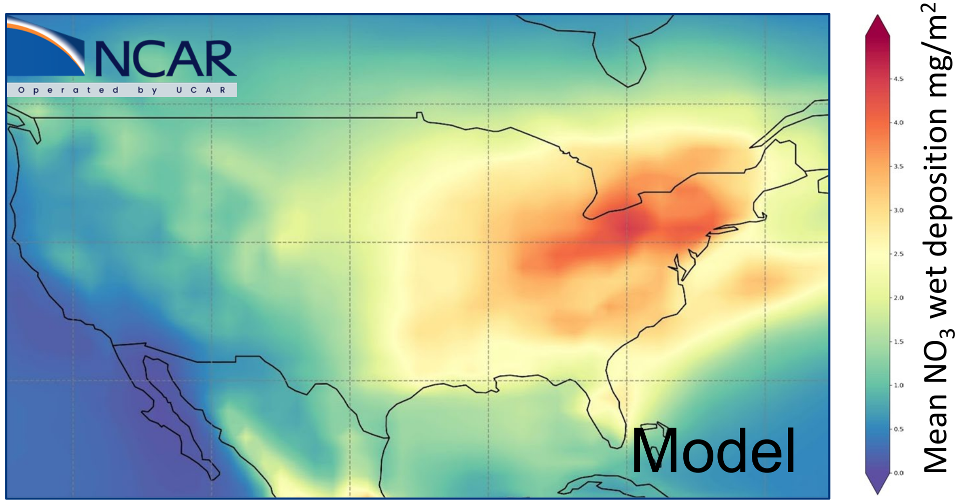
W_i Cloud-processes (wet deposition)
D_i Dry deposition

Introduction to Atmospheric Chemistry, Daniel J. Jacob

Wet Deposition





Images: Deni Murray

Large - scale and convective precipitation:
uptake of chemical constituents in rain or ice

Considers in - cloud and below - cloud scavenging rates and solubility factors of aerosol and chemical species

A first - order loss process:

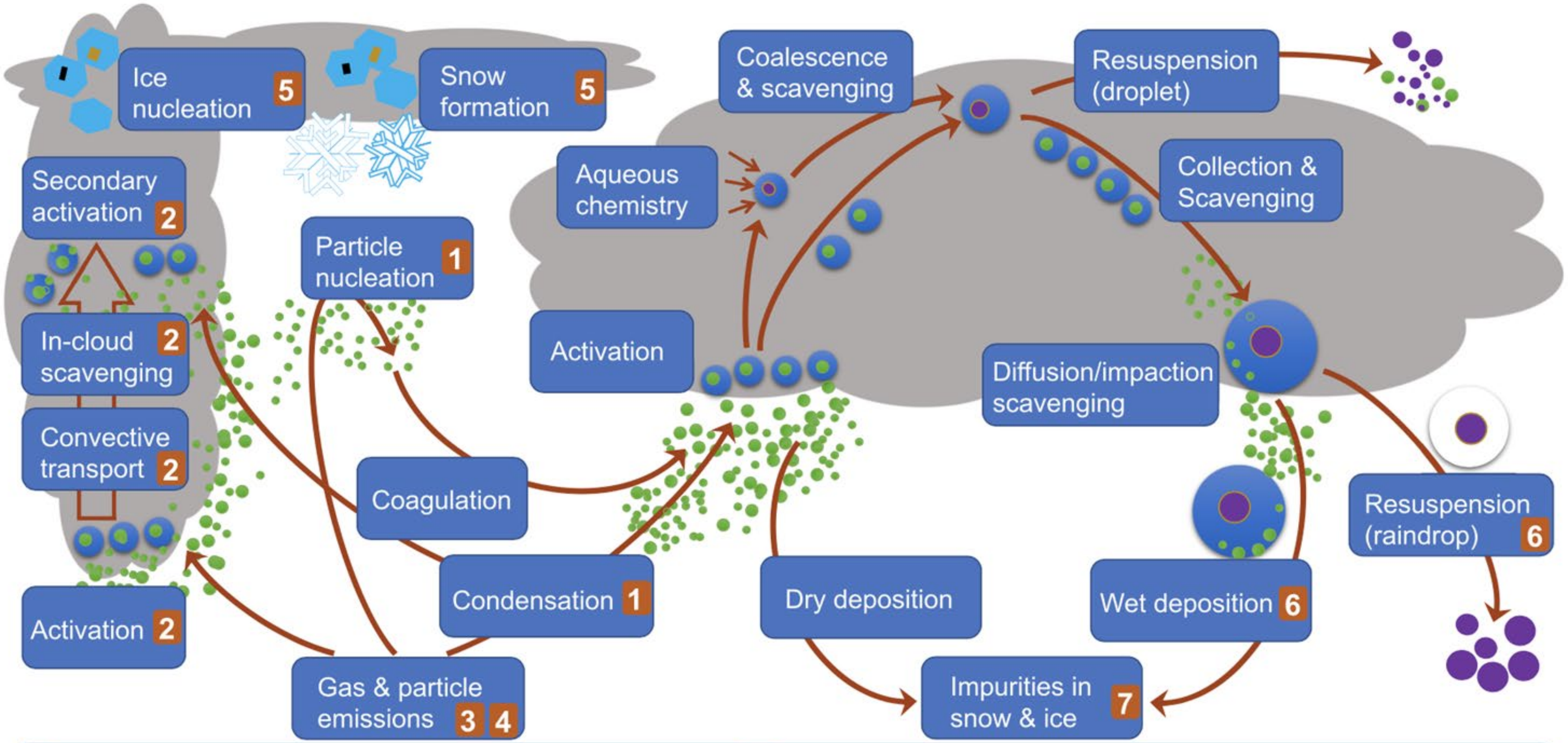
$$\chi_{iscav} = \chi_i \times F \times (1 - \exp(-\lambda \Delta t))$$

where

X_{iscav}	scavenged species (kg)
X_i	species
F	fraction of the grid box from which tracer is being removed
λ	is the loss rate

References: (Barth et al., 2000, Neu and Prather 2012, Lamarque et al., 2012)

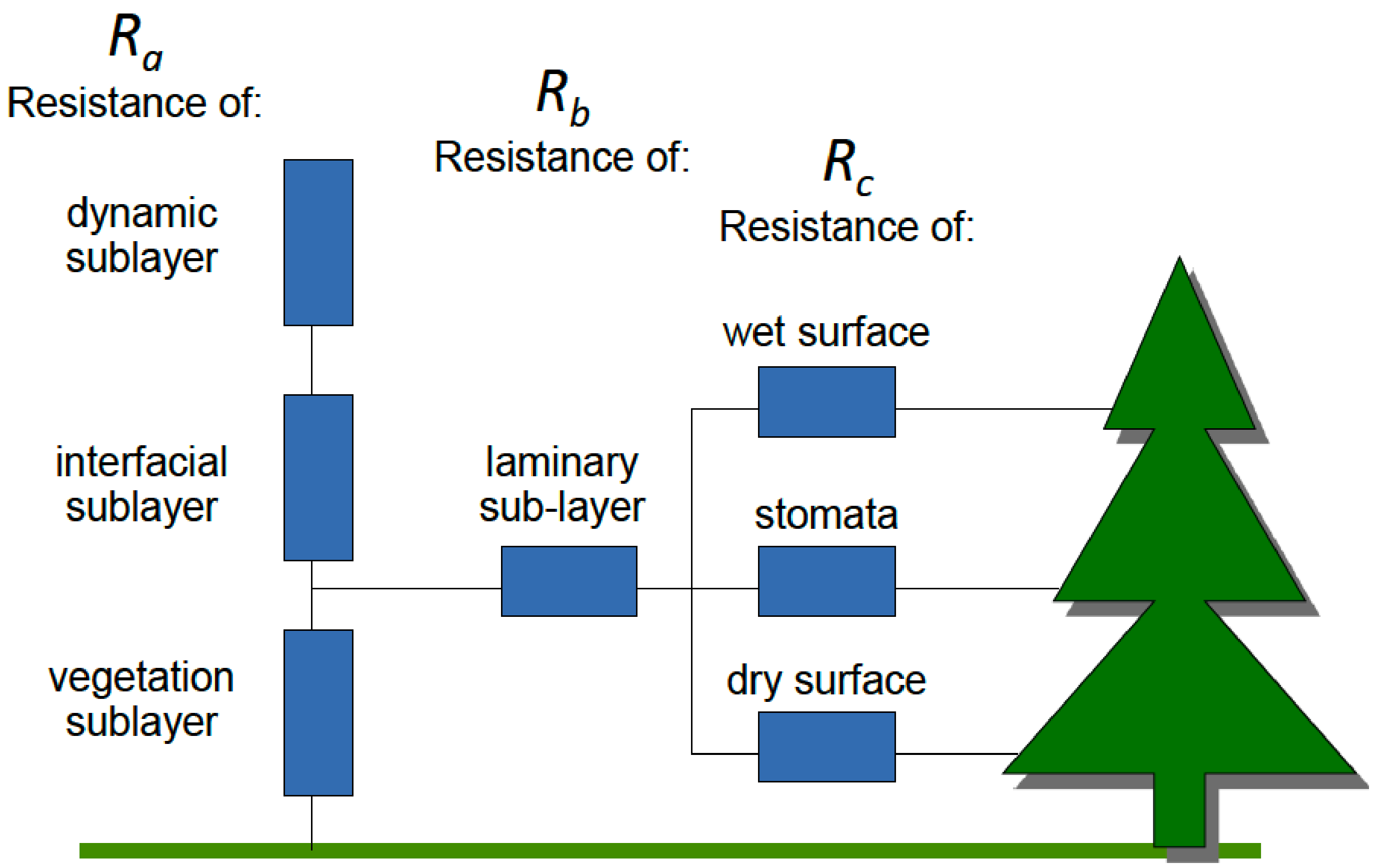
Aerosol – Cloud Interactions



1. H_2SO_4 vapor production and loss (NewH2SO4)
2. Convective transport and wet removal (NewConvTran)
3. SOA precursor gas emission (NewSOA)
4. Representation of marine organic aerosol (NewMOA)
5. Ice nucleation and ice-to-snow conversion (NewIceNuc)
6. Resuspension of aerosol from evaporated raindrops (NewResusp)
7. Light-absorbing particles in snow and ice (NewInSnow)

E3SM: Wang et al., 2020 (JAMES)

Dry Deposition Velocity Calculation



Resistance model:

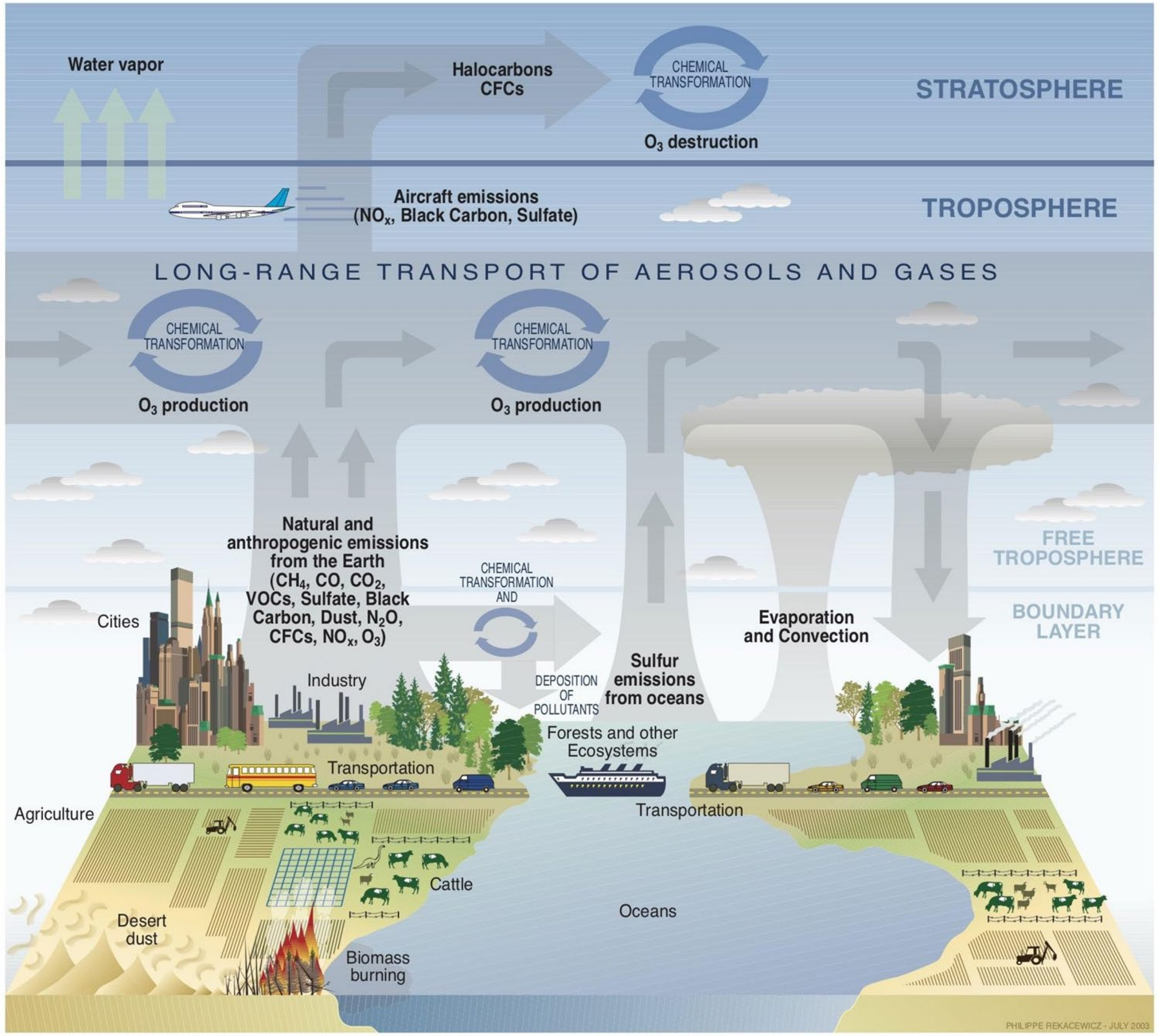
$$V_d = \frac{1}{R_a + R_b + R_c}$$

$$\boxed{F = -v_d C}$$

F = deposition flux
C = concentration of species in 10m surface layer

Uptake of chemical constituents by plants and soil (CLM), depends on land type, roughness of surface

Atmospheric Chemistry in CESM3



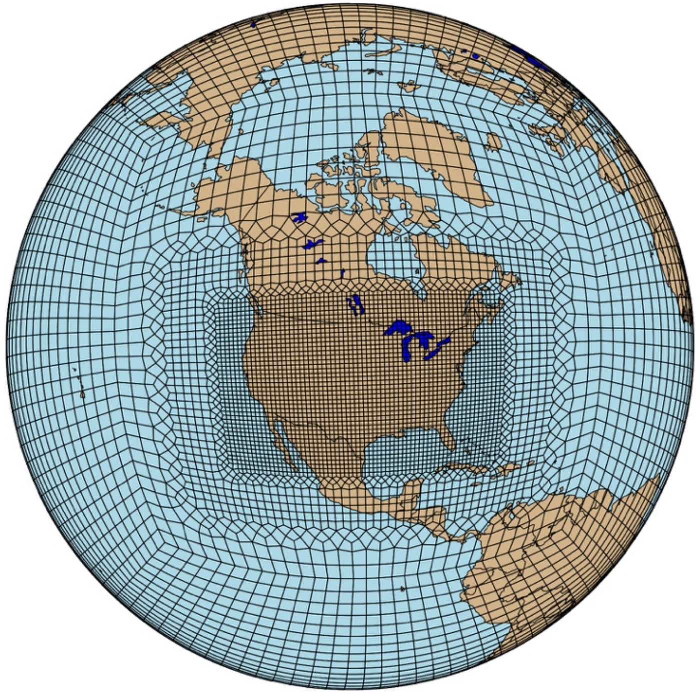
- Modeled processes
  - Emissions
  - Chemical mechanism
  - Aerosol model and cloud interactions
  - Wet Deposition
  - Dry Deposition
- Support

User Support for chemistry modeling in CESM

Wiki Page for Chemistry:
https://wiki.ucar.edu/display/camchem/Home

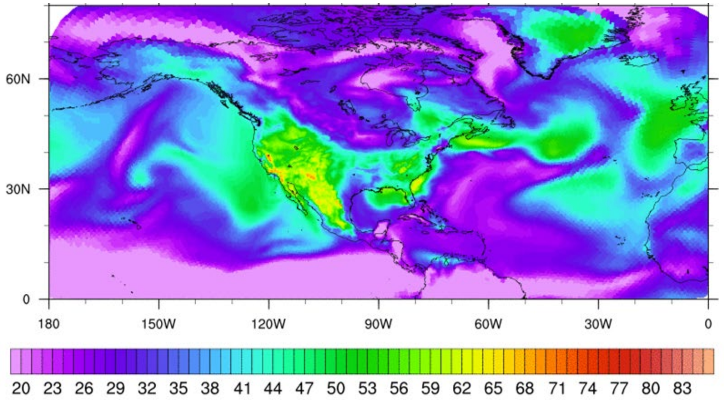
MUSICA: Regional Refinement WIki:
https://wiki.ucar.edu/display/MUSICA

Forum to search for and ask questions:
http://bb.cgd.ucar.edu/



MUSICA:
Multi-Scale Infrastructure for Chemistry and Aerosols

Regional Refined



Contact us:

Simone Tilmes
CAWG Co - chair
tilmes@ucar.edu

Rebecca Buchholz
CAWG Liaison
buchholz@ucar.edu

Shawn Honomichl
CAWG Liaison
shawnh@ucar.edu

Key takeaways

- Atmospheric chemistry is important in models due to the feedback into the earth system. It has **impacts on health, weather and climate**.
- Adding atmospheric chemistry processes into earth system models requires many **approximations and parametrizations**

$$\boxed{\frac{\partial \chi(i)}{\partial t} = \mathrm{Sources(i)} - \mathrm{Sinks(i)} = \mathrm{E_i} + \mathrm{C_i} + \mathrm{A_i} + \mathrm{T_i} - \mathrm{W_i} - \mathrm{D_i}}$$

  - Considerations include: Emissions, Chemical mechanism, Aerosol model and cloud interactions, Transport, Dry Deposition, Wet Deposition
- Models allow us to perform multiple experiments regarding our atmosphere. **Using the correct model** and model **configuration** is important to correctly answer your question.