# Modeling IV, Chemistry and Aerosols presented by Simone Tilmes, ACOM

**Chemistry-Climate Working Group (CCWG)**

- **Chemistry-Climate WG Co-Chairs: Simone Tilmes, Rafael Fernandez**
- **Software Engineers: Francis Vitt**
- **CAMChem Liaison: Rebecca Buchholz**

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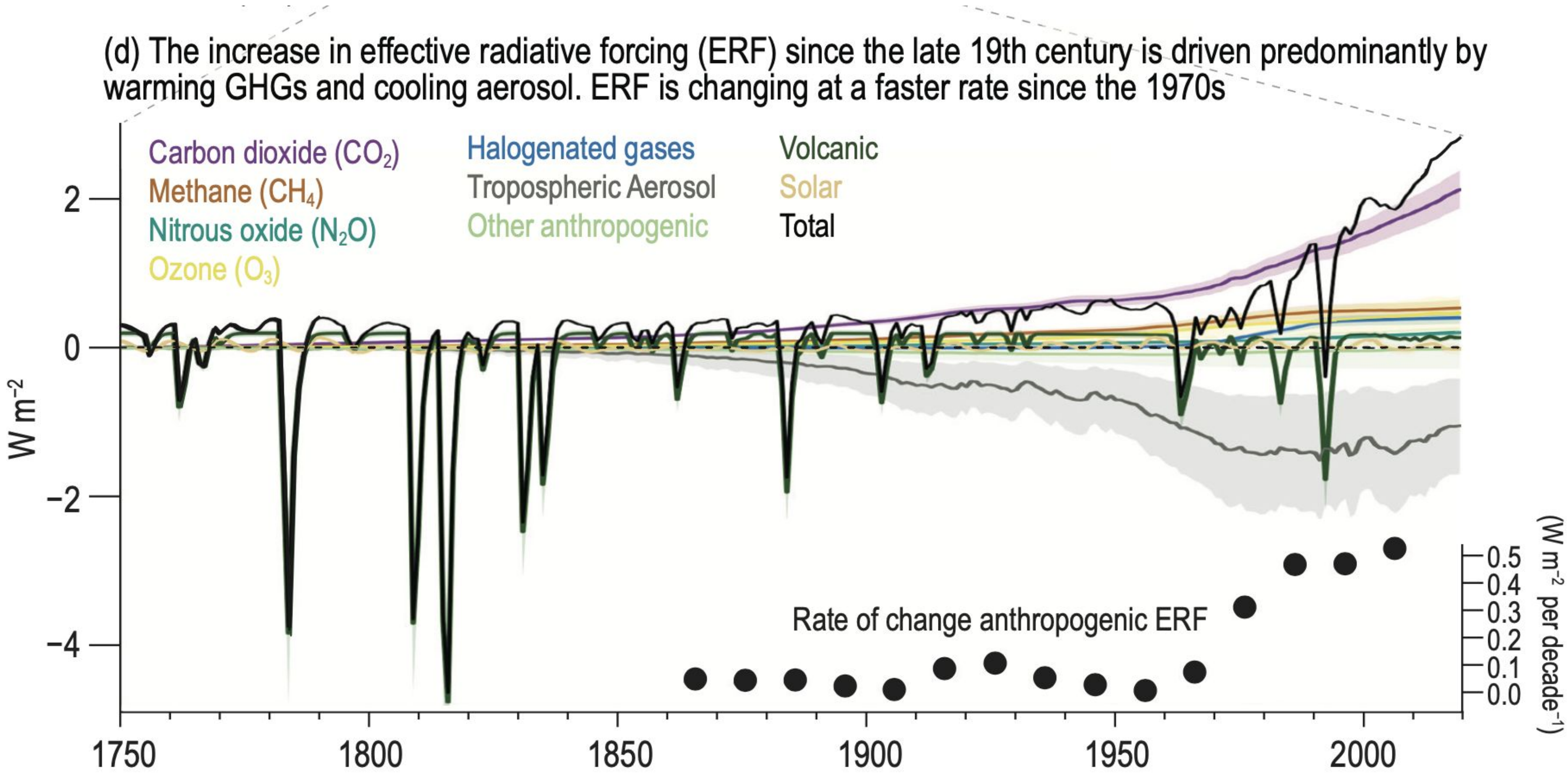
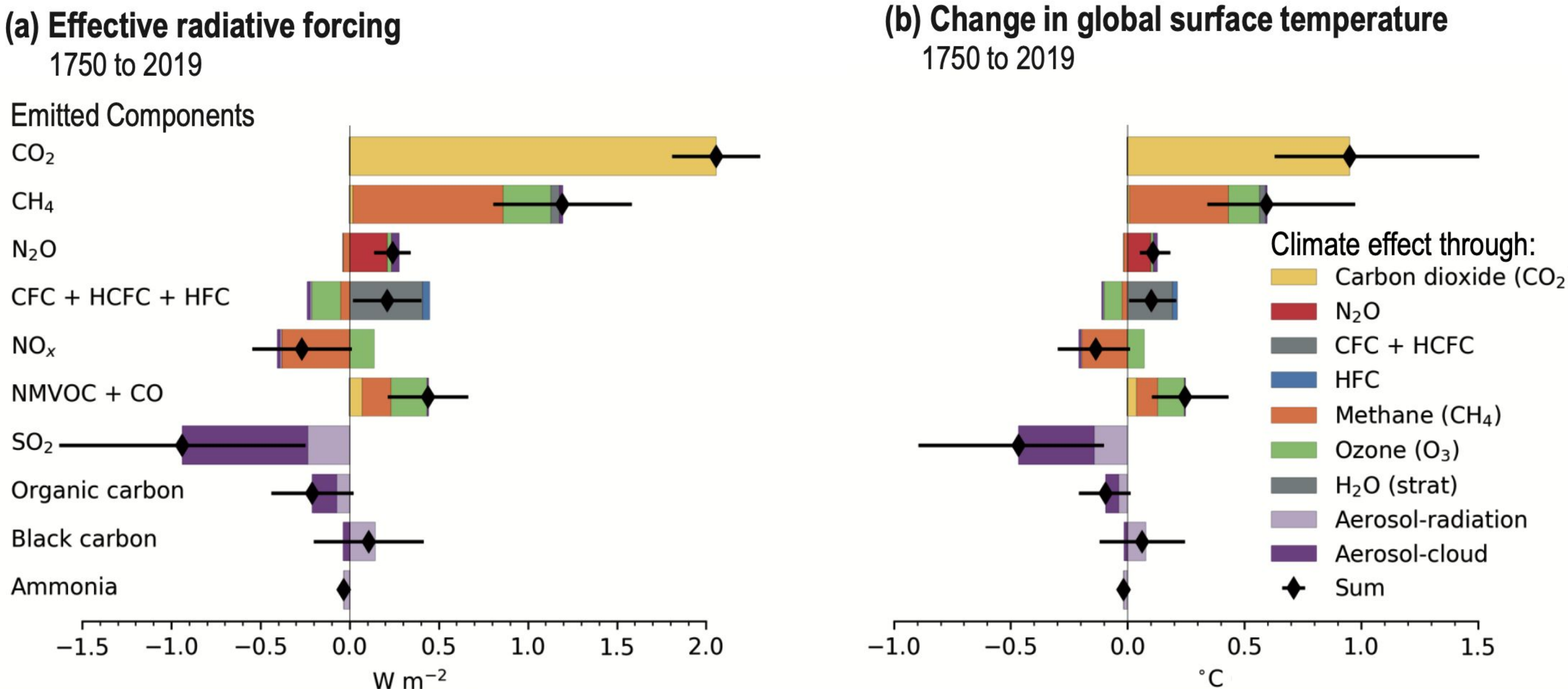
# Importance of Chemistry and Aerosols for Climate




IPCC AR6 WG1 Technical Report, Figure TS9

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

# Importance of Chemistry and Aerosols for Climate




IPCC AR6 WG1 Technical Report, Figure TS15

- **Importance of describing ozone and aerosol precursors**
- **Importance of aerosol-cloud interactions in models**

# Importance of Chemistry and Aerosols for Air Quality

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

- Traffic / Industry (use of fossil fuels)
- Private (use of fossil fuels)
- Farmland

-> Ozone can damage the tissues of the respiratory tract, causing inflammation and irritation, and result in symptoms such as coughing, chest tightness and worsening of asthma symptoms

**Particle Matter Pollution pm2.5 and pm10: particle diameter less than 2.5 or 10 micrometer (SO2, VOC, NH3, BC, OC, fine dust)**

- Traffic /Industry (use of fossil fuels)
- Farmland
- Fires (worsen with climate change)
- Dust storms (worsen with climate change)
- Volcanoes

Exposure to such particles can affect both your lungs and your heart, premature deaths, especially for people with heart or lung diseases

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

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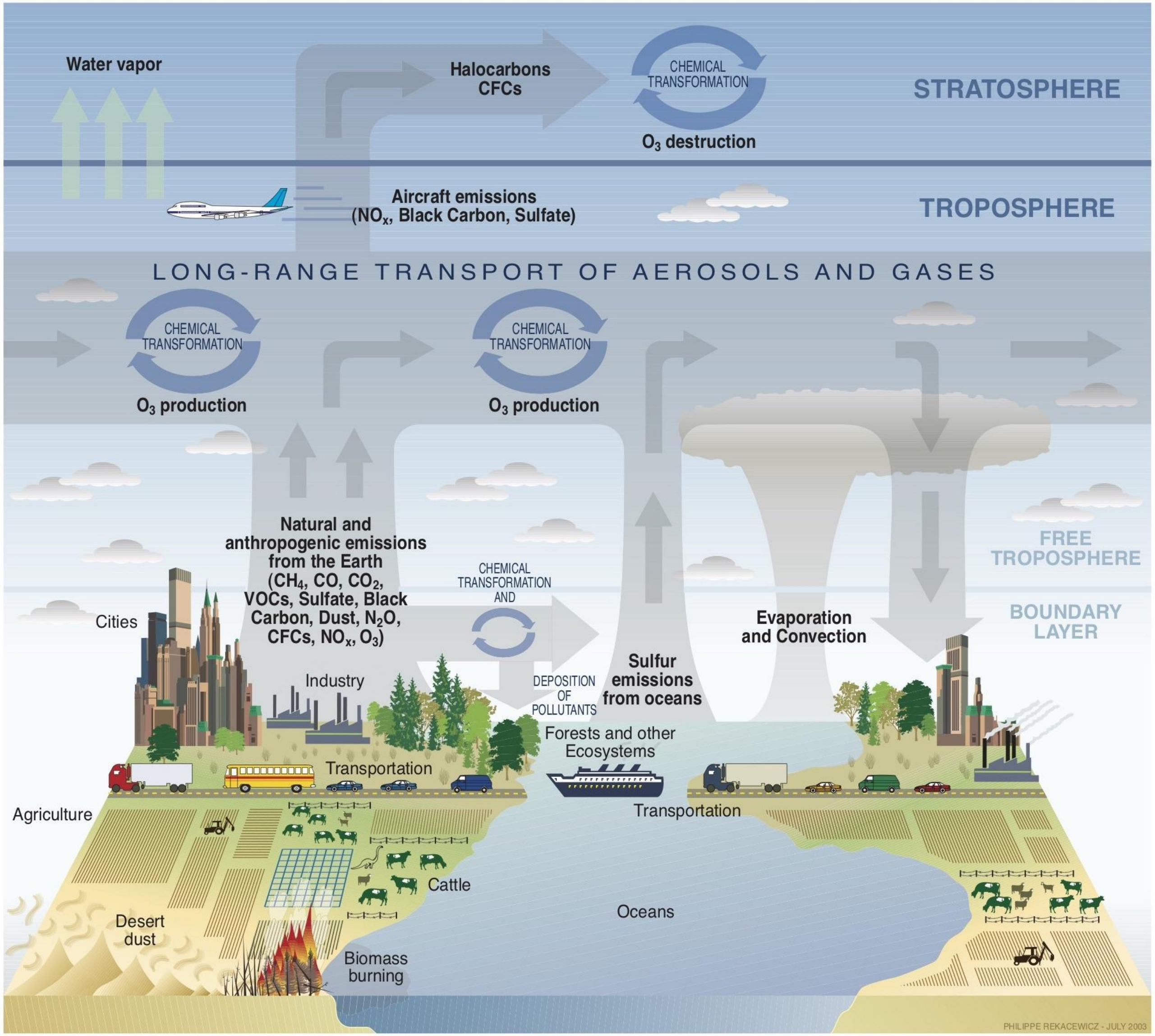
# Simulation of Atmospheric Composition

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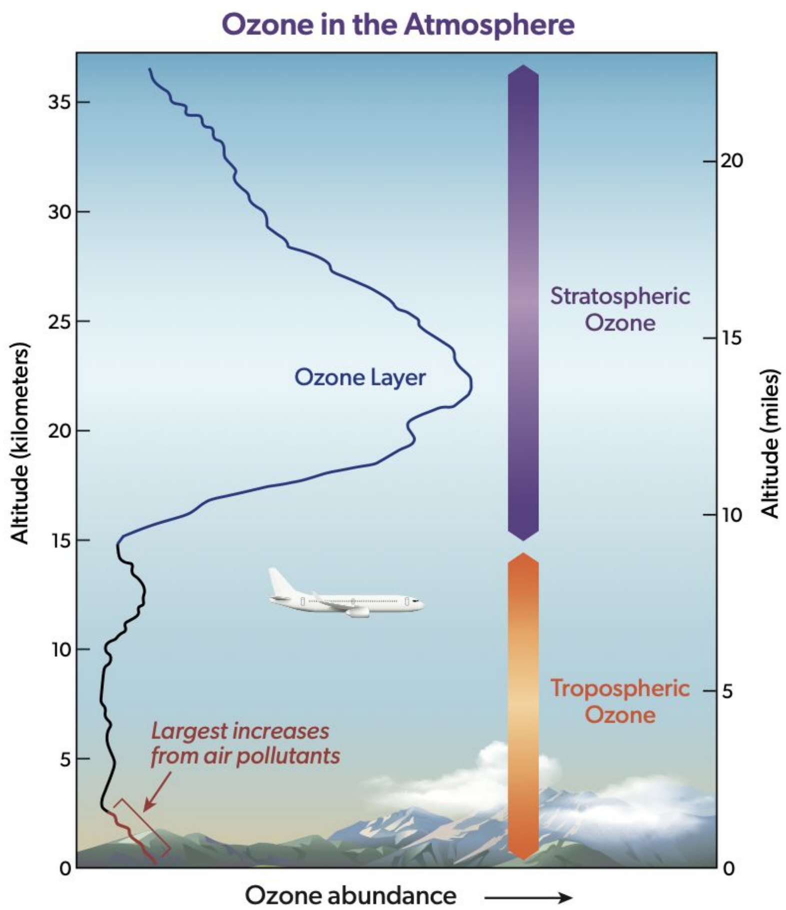
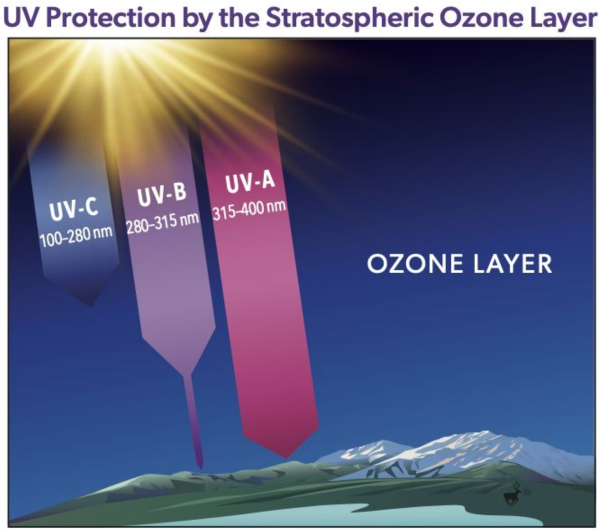
# Simulation of Stratospheric Ozone




UV-C (very dangerous) mostly filtered out by ozone

UV-B only partially filtered by ozone.

UV-B and $UV_{ERY}$ changes are directly related to skin cancer and cataract

- Societal impacts, Effect terrestrial and aquatic systems, Impact on tropospheric chemistry, Vitamin D production

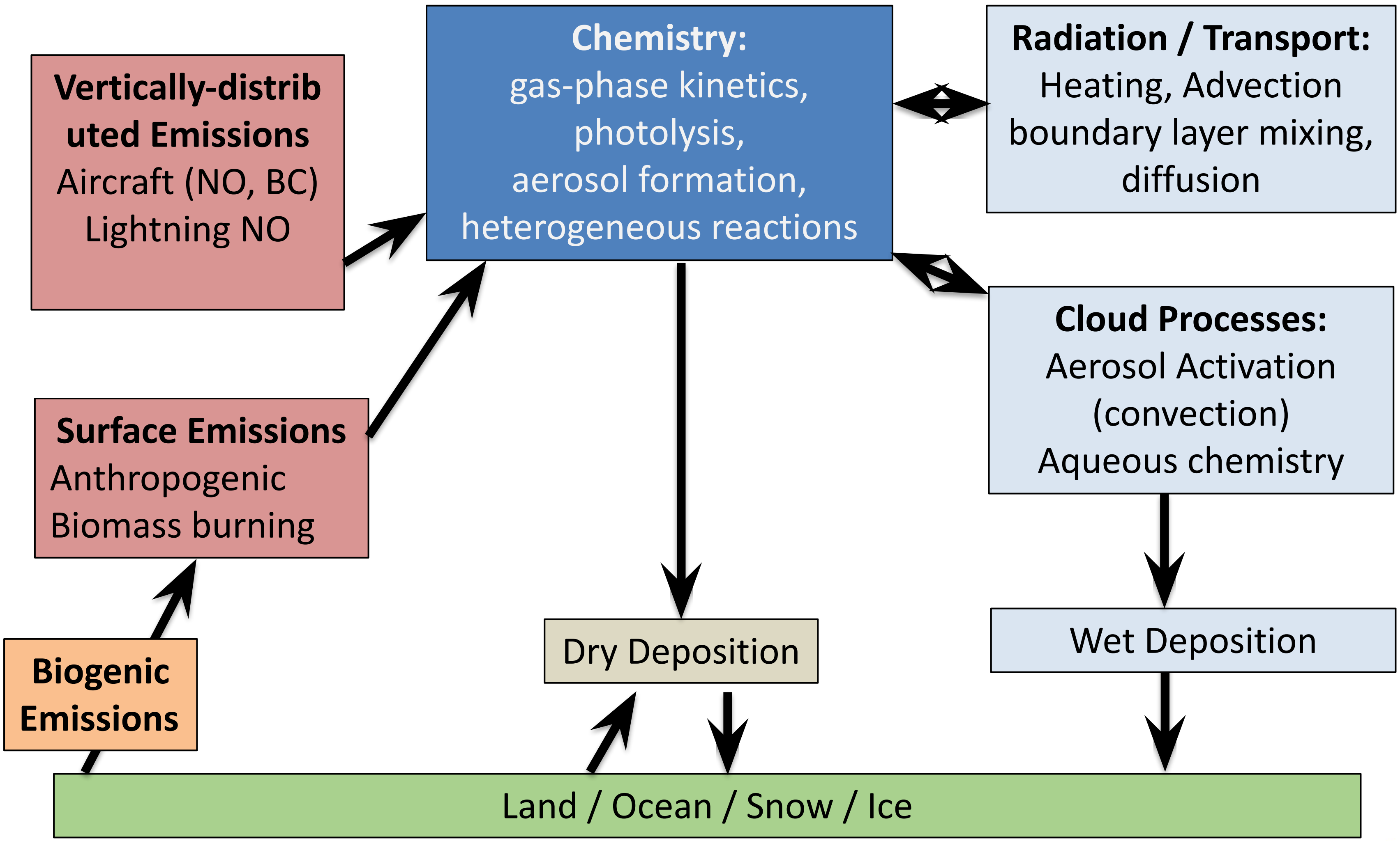
# Solution for each Chemical Species *i*

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

- 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 (Gas-aerosol exchange, het chem.)
  - $T_i$: Advection + Diffusion
  - $W_i$: Cloud-processes (wet deposition)
  - $D_i$: Dry deposition

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

# Lifecyle of Atmospheric Constituencies



# Chemistry-Climate Components in CESM2

- **Surface emissions and concentrations**
- Chemical mechanism
- Aerosol model and cloud interactions
- Dry Deposition
- Wet Deposition

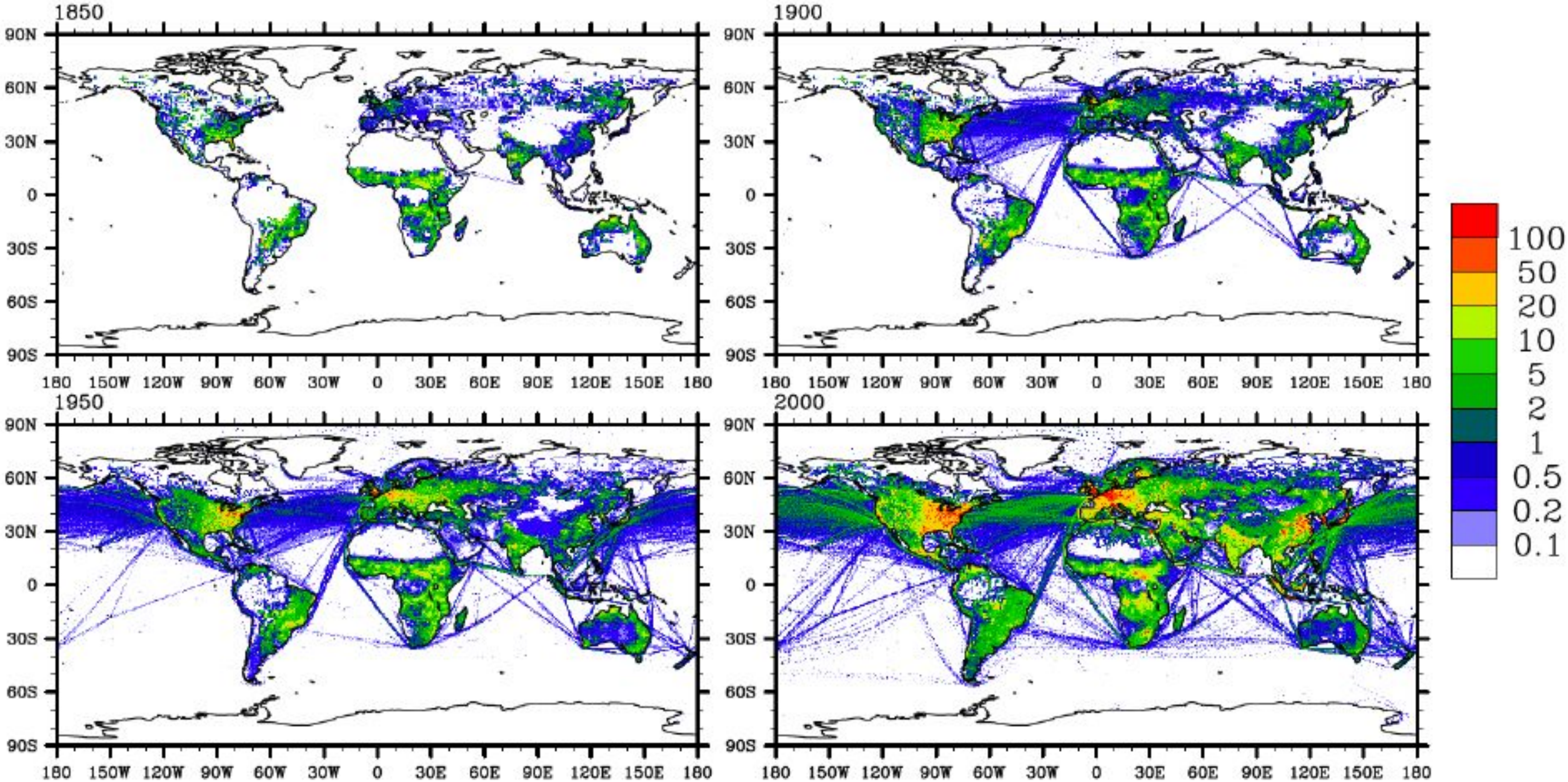
# Chemistry-Climate Components in CESM2

## Surface emissions and concentrations

- **Emissions**
  - Surface emissions:  anthropogenic, biogenic, biomass burning, ocean, soil
  - Vertical emissions (external forcings): aircraft, volcanoes, power plants

- **Surface concentrations**
  - Lower boundary conditions (greenhouse gases, long-lived gases)

# Example of NOx Surface Emissions

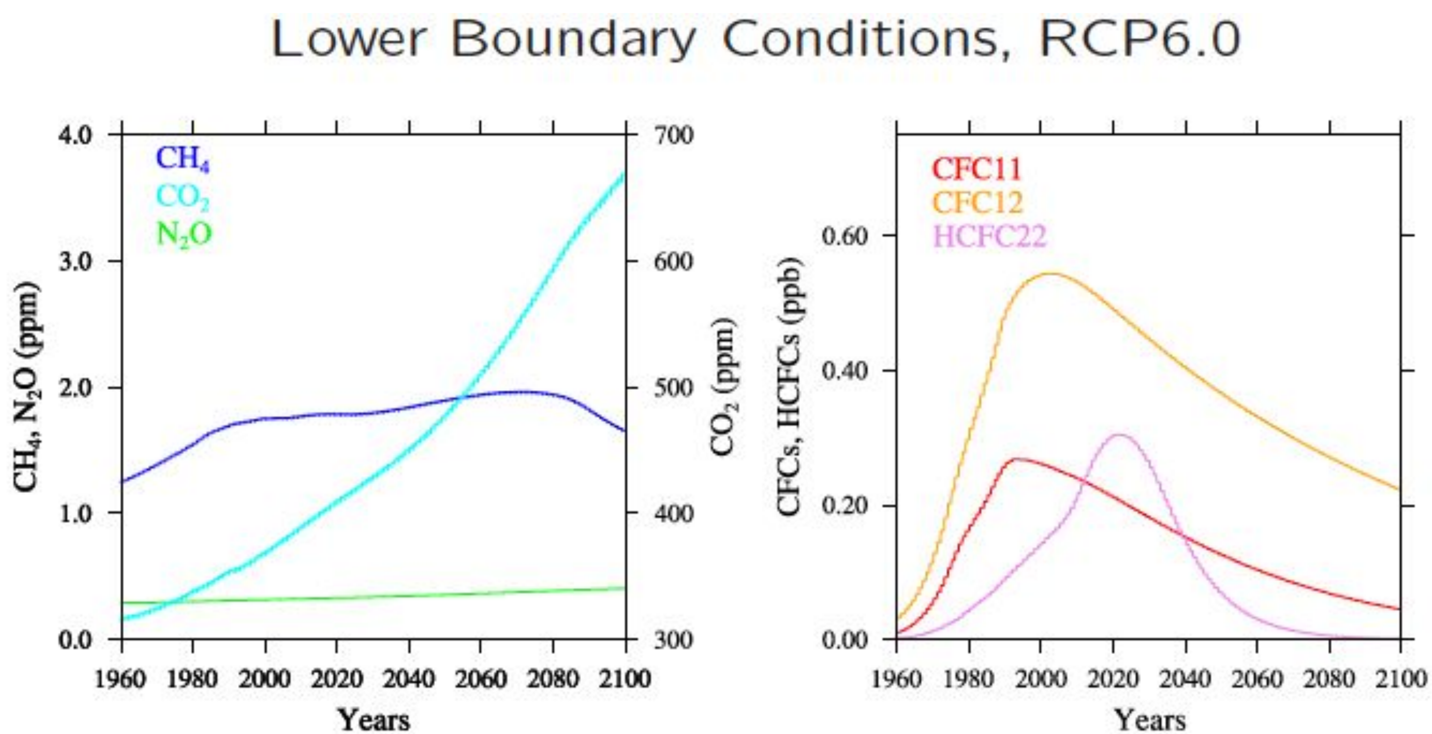



*Lamarque et al., 2010*

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

# Example of Lower Boundary Conditions

- Greenhouse gases are prescribed as 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.
- Can vary with latitude



# Chemistry-Climate Components in CESM2

- Surface emissions and concentrations
- **Chemical mechanism**
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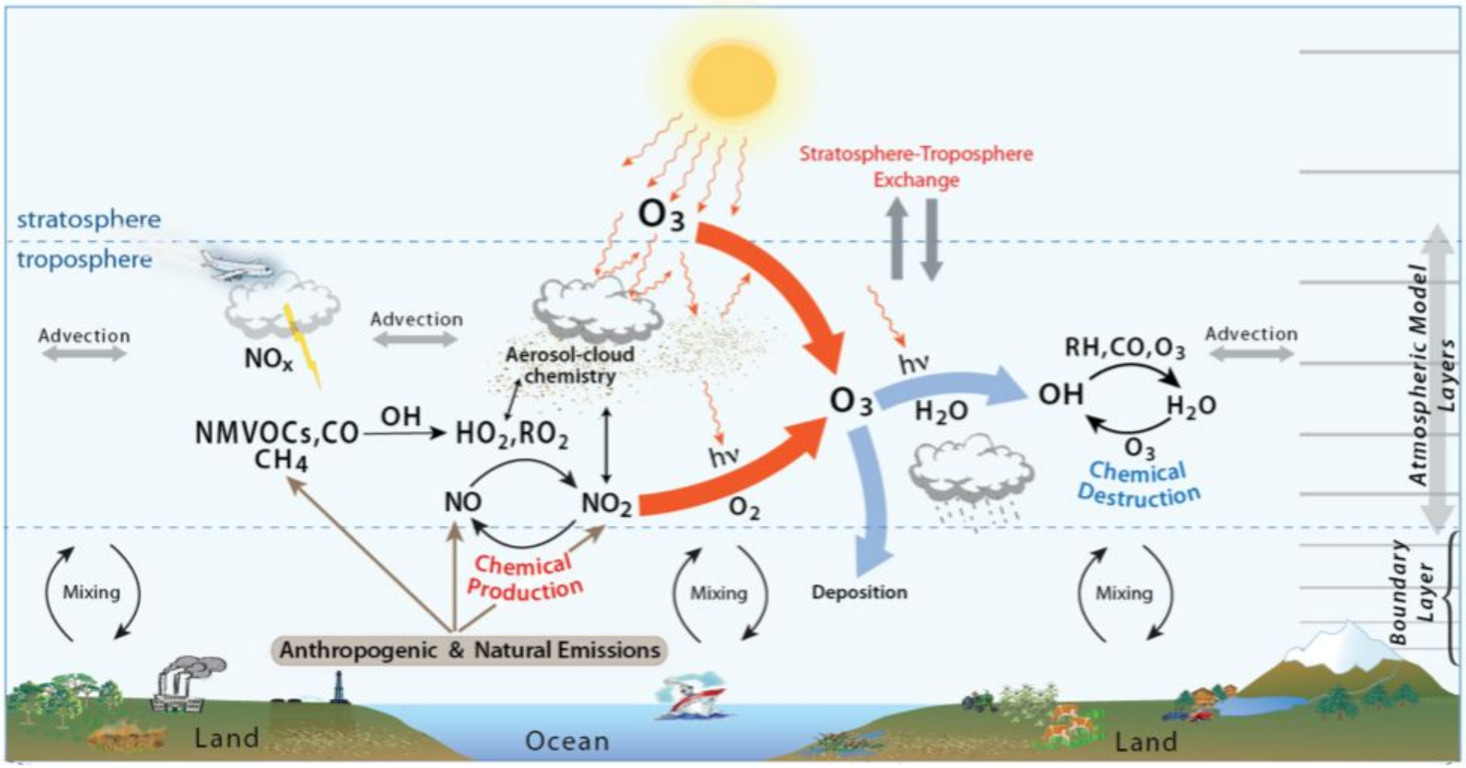
# Tropospheric Chemistry in CESM



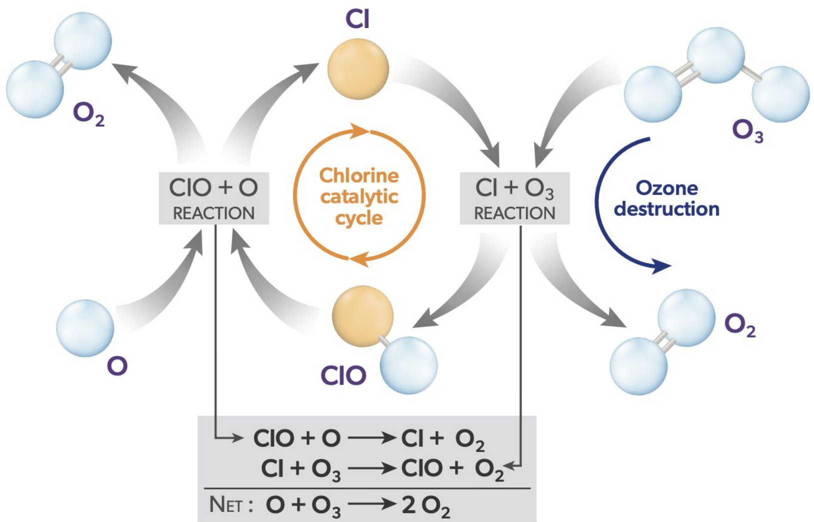

*Young et al., 2017*

- Photo-chemistry
- Gas-phase chemistry
- Heterogeneous chemistry
- Aqueous phase chemistry,
- Gas-to-aerosol Exchange

# Stratospheric Chemistry in CESM

*WMO2022*

### Ozone Destruction Cycle 1 : Upper Stratosphere




### Ozone Destruction Cycles 2 and 3 : Polar Regions

**Cycle 2 :**

$$ClO + ClO \rightarrow (ClO)_2$$
$$(ClO)_2 + sunlight \rightarrow ClOO + Cl$$
$$ClOO \rightarrow Cl + O_2$$
$$2(Cl + O_3 \rightarrow ClO + O_2)$$

Net: $2O_3 \rightarrow 3O_2$

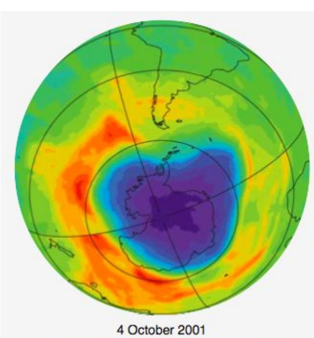
**Cycle 3 :**

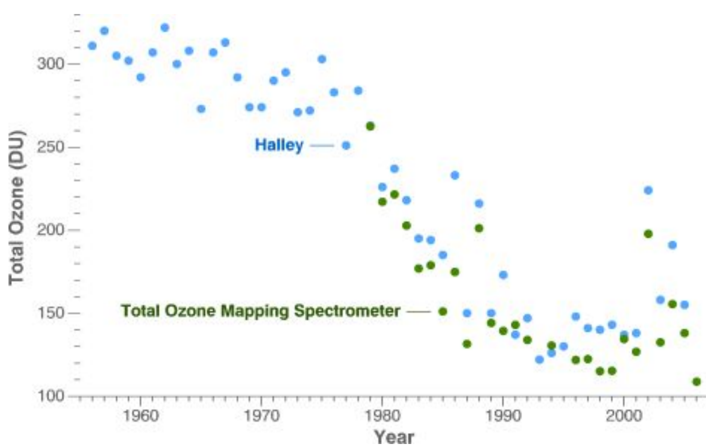
$$ClO + BrO \rightarrow Cl + Br + O_2$$

*or*
$$\left( \begin{array}{l} ClO + BrO \rightarrow BrCl + O_2 \\ BrCl + sunlight \rightarrow Cl + Br \end{array} \right)$$

$$Cl + O_3 \rightarrow ClO + O_2$$
$$Br + O_3 \rightarrow BrO + O_2$$

Net: $2O_3 \rightarrow 3O_2$




Comprehensive Stratospheric Chemistry

- Heterogeneous reactions
- Catalytic Cycles

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# Available Chemical Mechanisms

| 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) |

# 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

# Chemistry-Climate Components in CESM2

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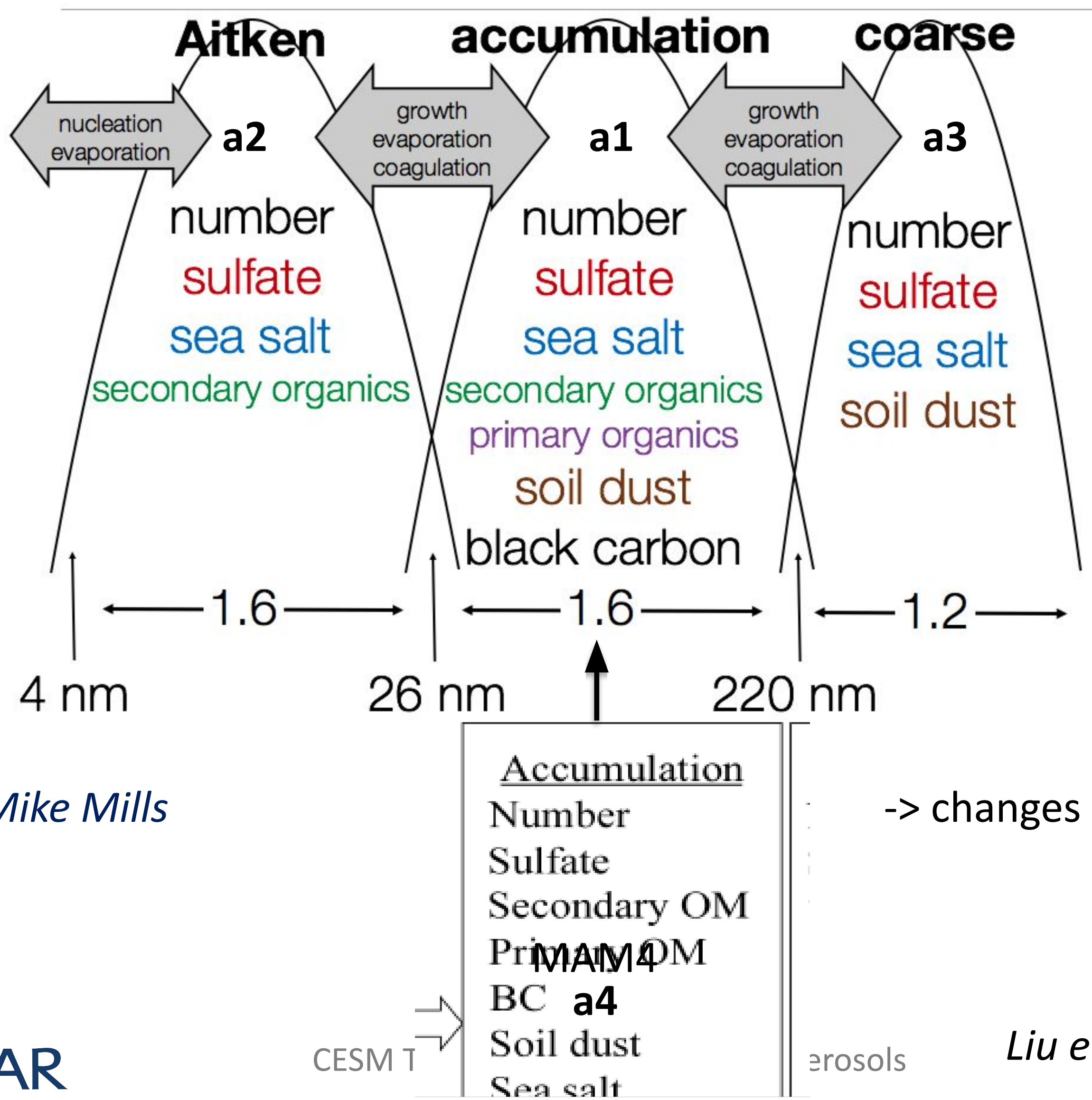
- **Aerosol model and cloud interactions**
- Dry Deposition
- Wet Deposition

# Default Modal Aerosol Model (MAM)



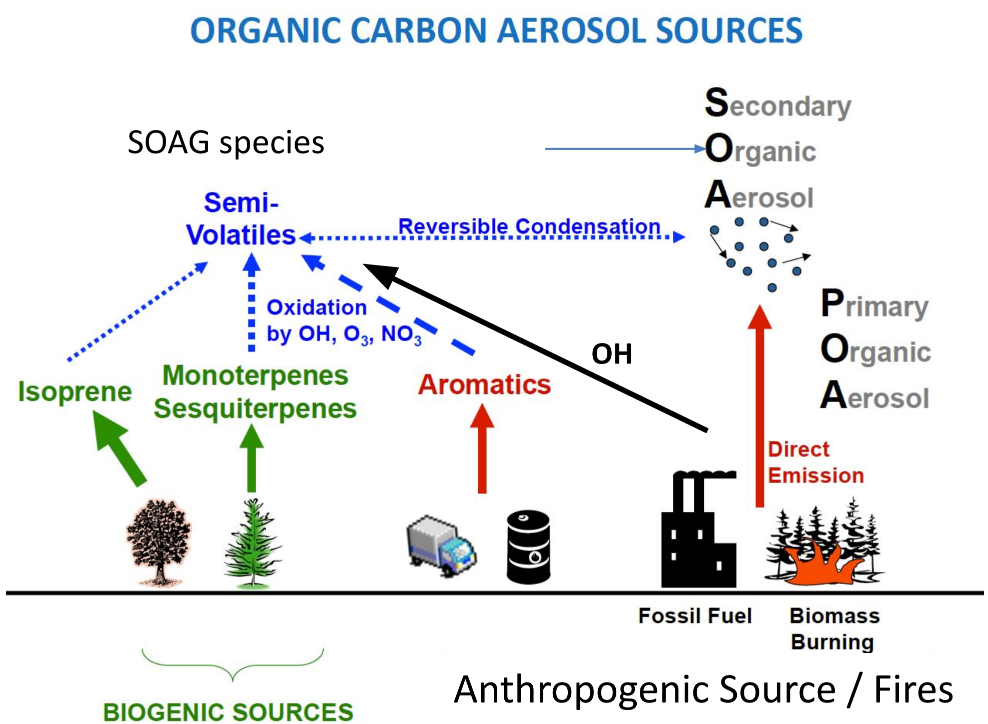

Representation of
- Sulfates,
- Black Carbon
- Organic Carbon, Organic Matter (OC, SOA),
- Mineral Dust and Sea-Salt

*Curtesy Mike Mills*

-> changes the lifetime of BC

*Liu et al., 2016*

# Secondary Organic Aerosol Description in WACCM and CAM-chem




*Modified after C. Heald, MIT Cambridge*

**Simplified Chemistry (CAM6):**

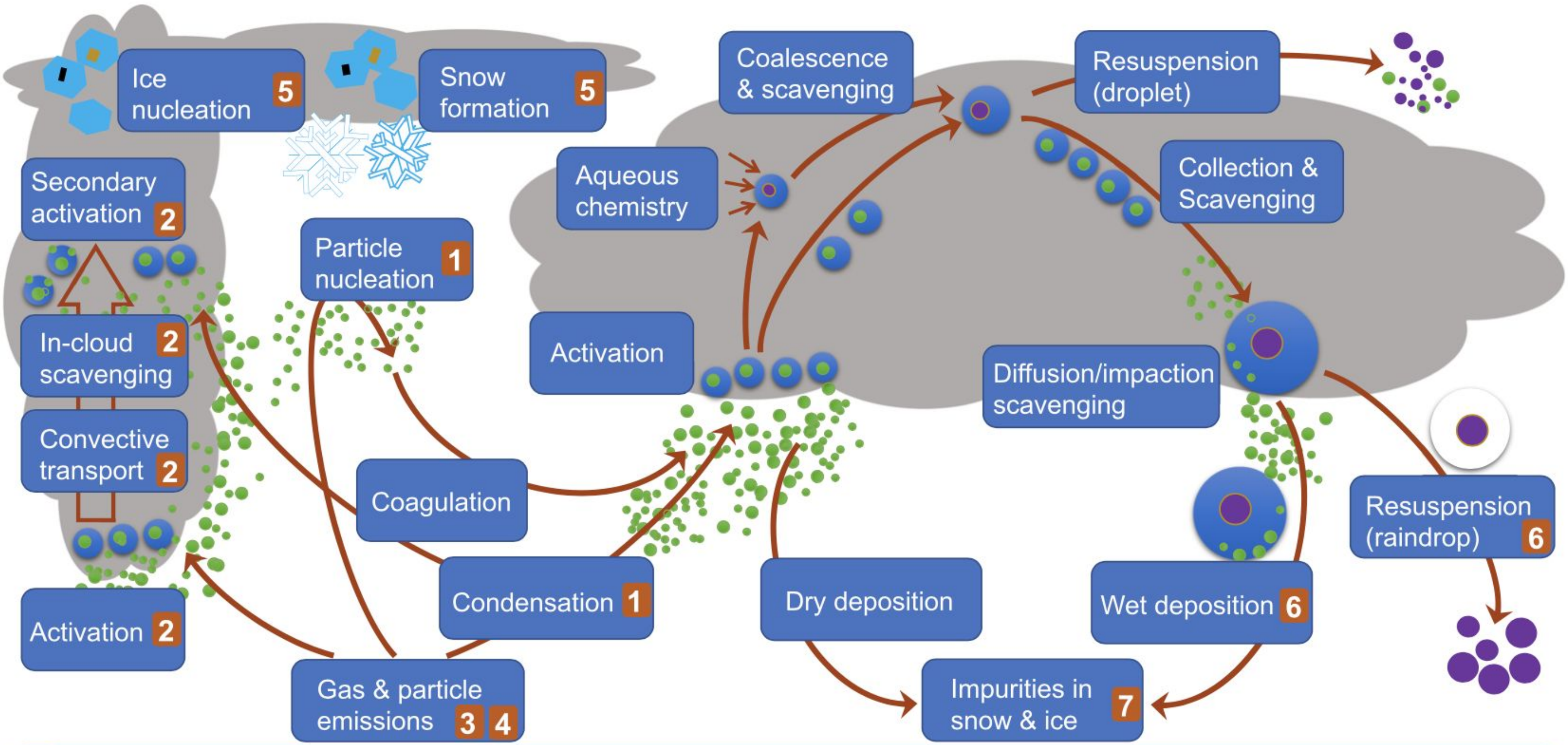
- SOAG (oxygenated VOCs) derived from fixed mass yields
- no interactions with land

**Comprehensive Chemistry:**

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

-> more physical approach

# 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)*

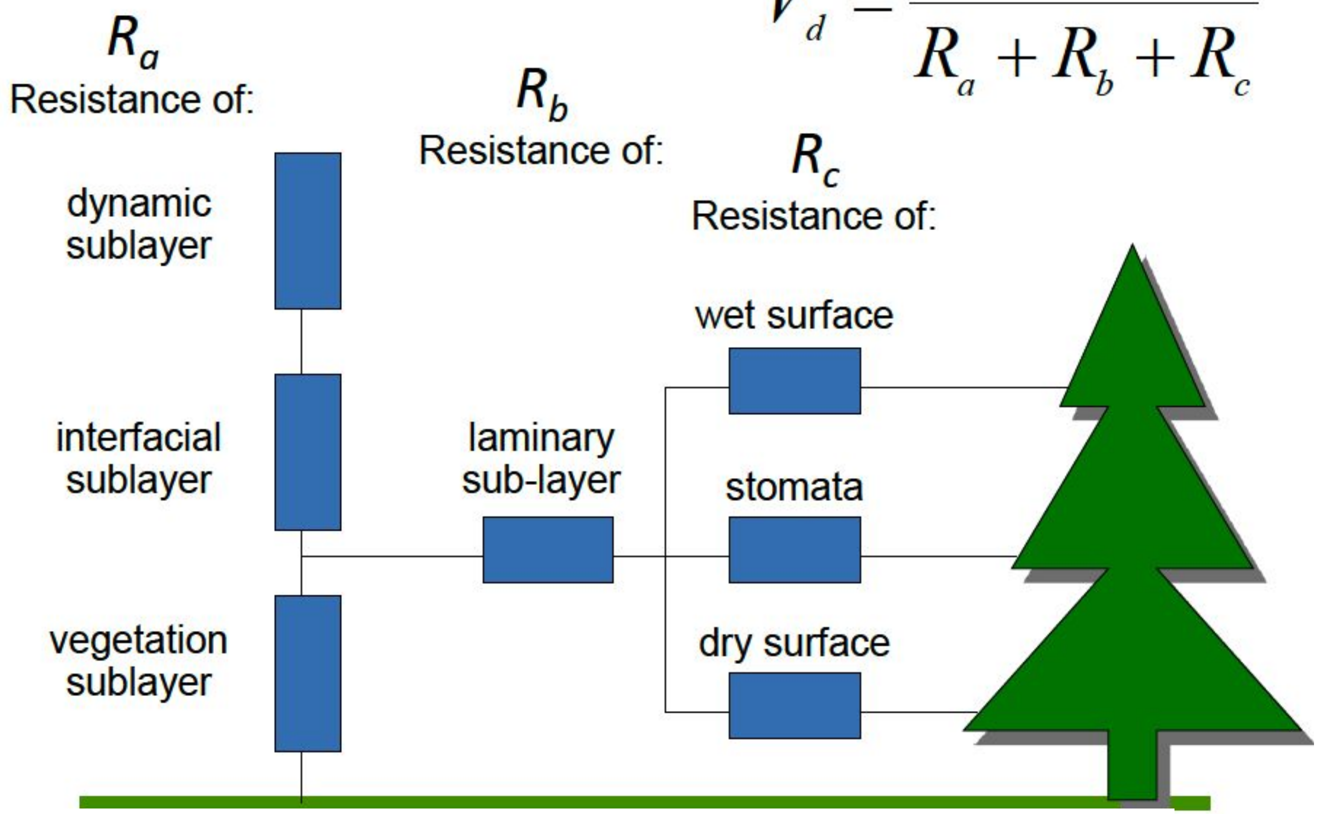
# Chemistry-Climate Components in CESM2

- Surface emissions and concentrations
- Chemical mechanism
- Aerosol model and cloud interactions
- **Dry Deposition**
- **Wet Deposition**

# Dry Deposition Velocity Calculation

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

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




Deposition flux: $F = -v_d C$

C: concentration of species in 10m

# Wet Deposition

**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
- $X_{iscav}$ 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.

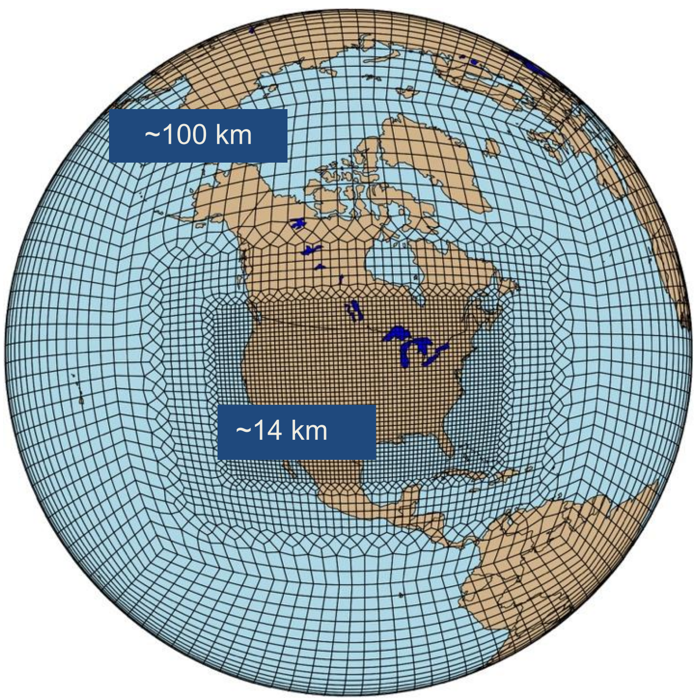
$$X_{\mathrm{iscav}} = X_i \times F \times (1 - \exp(-\lambda \ \Delta t))$$

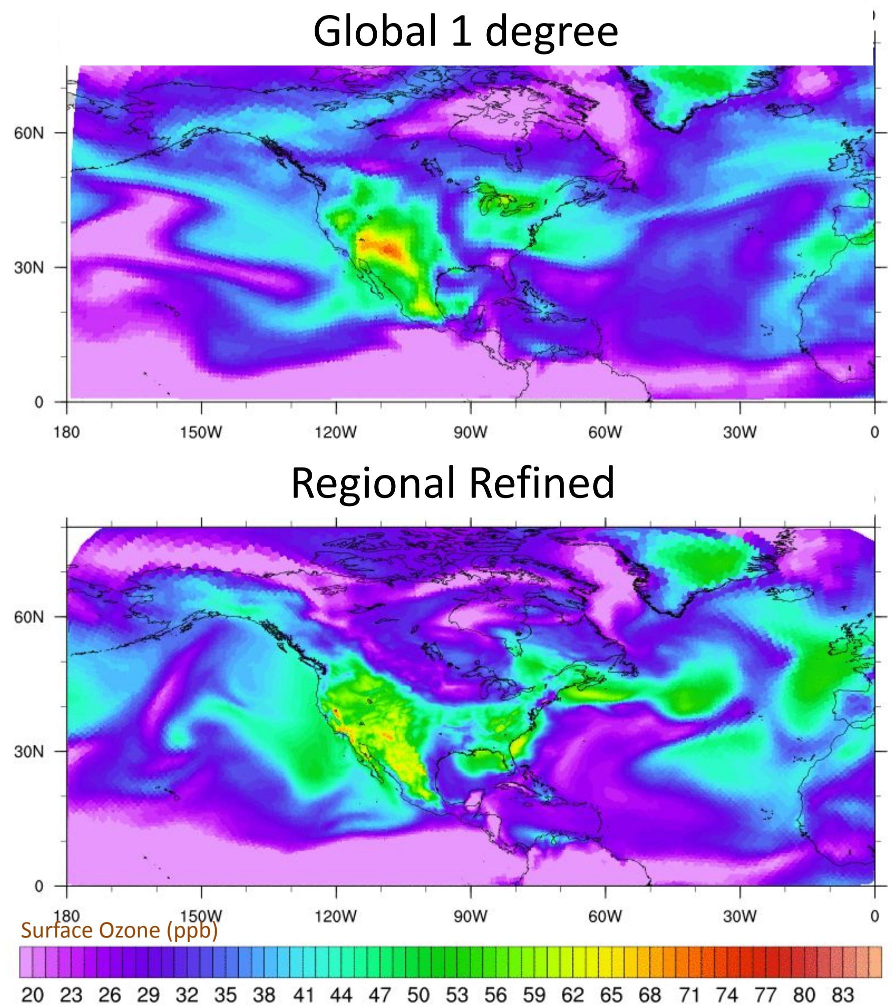
# CAM-cam (MUSICA-V0) Applications for Air quality

MUSICA-V0: **Multi-Scale Infrastructure for Chemistry and Aerosols**
CAM-chem-SE-RR - Community Atmosphere Model with Chemistry With Spectral Element (SE) dynamical core and Regional Refinement (RR)
**MUSICA-wiki: tutorials and support https://wiki.ucar.edu/display/MUSICA**

**Regional refinement for U.S. Air Quality**

- Exposure Relevant scales and Large scale feedbacks on and of air quality






Credits: Forrest Lacey (ACOM)

# User Support for CAM-Chem and WACCM

| | |
|---|---|
| **Advanced Changes** | • Updating Gas-phase Chemistry (including kinetics, deposition, aerosol uptake, etc.)<br>• Tagging CO and simple tracers<br>• CAM-chem with regional refinement: ***MUSICA***<br>• Physics-based nudging - creating regridded reanalyses (on model levels) |
| **Model Component Descriptions** | • Wet Deposition<br>• Dry Deposition<br>• Gas-phase Chemistry<br>• Emission Inventories<br>• HEMCO ***NEW!***<br>• Aerosols<br>• Data Assimilation |
| **Online Interactive Emissions** | • Biogenic Emissions from CLM-MEGAN<br>• Online Air-Sea Interface for Soluble Species (OASISS)<br>• Ammonia |
| **Use and Diagnostics** | • Boundary conditions for regional modeling<br>• Automated CESM diagnostic package<br>• Using CAM-chem output |
| **User Community** | • Current Users/Projects<br>• Contributions to Model Intercomparisons (MIPs)<br>• CAM-chem Forum<br>• Chemistry-Climate Working Group Publications<br>• CAM-chem Publications from NCAR<br>• CESM Publications |
| **Other links and documents** | • Recent Bug Fixes<br>• CAM Documentation (User and Scientific Guides)<br>• ACOM CAM-chem page<br>• CESM Chemistry Climate Working Group<br>• Join the CESM Chemistry WG mailing list<br>• Benchmarks and Production Experiment Diagnostics |

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

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