Updates on the interactive chemistry and aerosols for E3SM

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E3SM Energy Exascale Earth System Model

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U.S. DEPARTMENT OF ENERGY

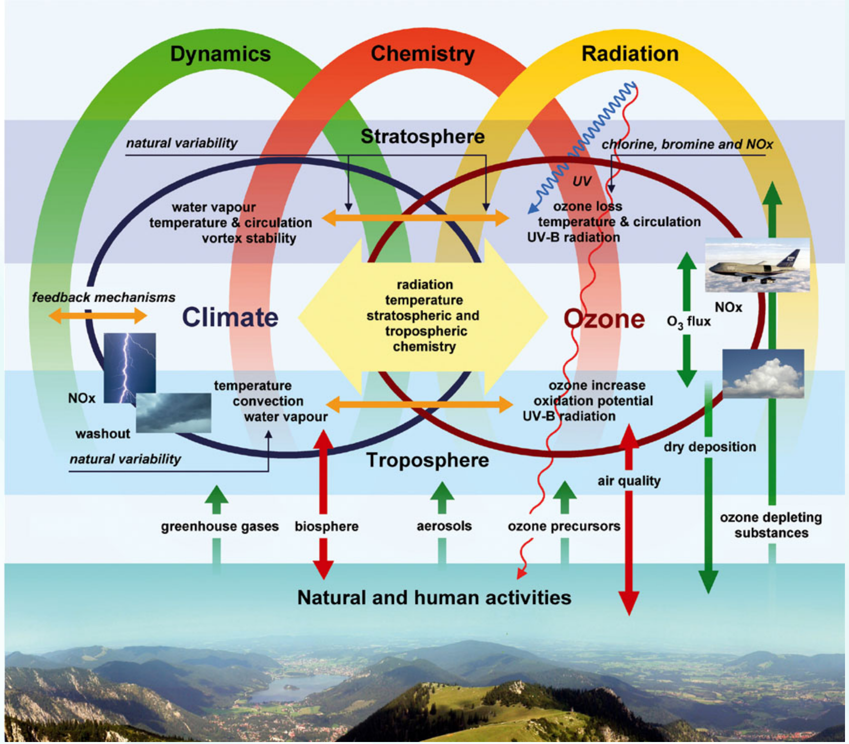
Overview

- Interactive chemistry developments
  - Troposphere and stratosphere
  - Radiation (Fast-JX, inline photolysis rates)
- Aerosol developments and coupling with chemistry
  - Representation of nitrate using MOSAIC-MAM4
  - Prognostic stratospheric sulfate for volcanic eruption (MAM7S)
  - More explicit treatment of the formation and sink of SOA
  - New dust emission scheme and optical properties
  - Currently coupled with (modified) MOZART chemistry

Interactive chemistry: Goals and current status

Goals

- Establish an interactive strat+trop gas-phase chemistry for E3SM v3/4
- Support aerosol chemistry and BGC including short-lived climate forcers



(https://earth.esa.int/image/image_gallery?img_id=391652)

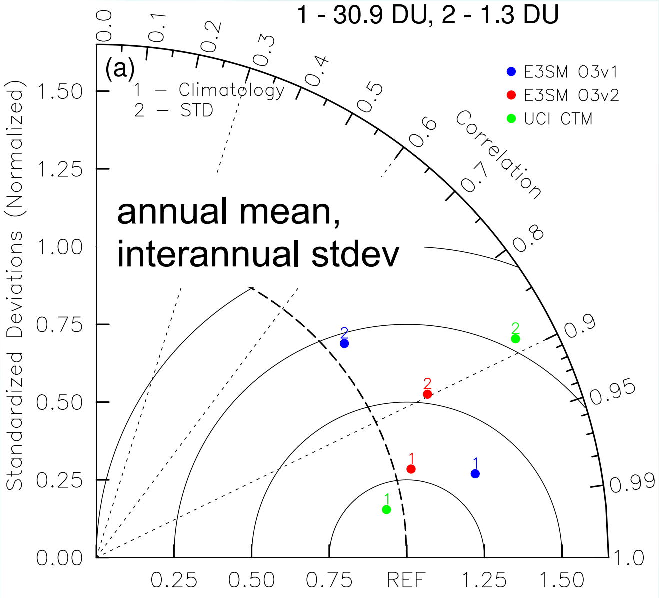
Current Status

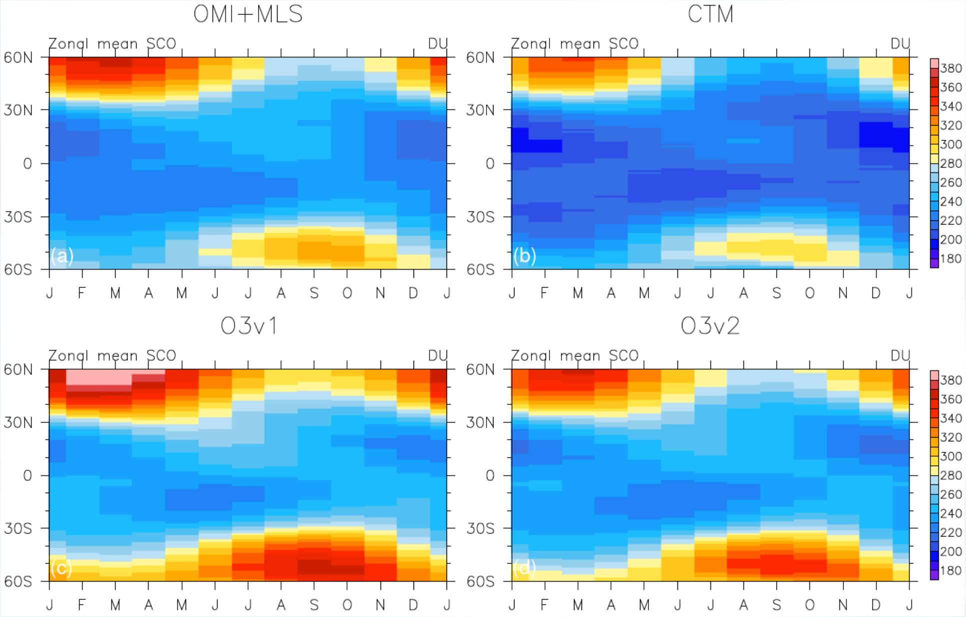
- The O3v2 paper under review in GMD
- The 3rd Solar-J paper under review in JAMES
- Rewrote UCI tropospheric chemistry mechanism and implemented it in E3SM
- Updated to Linoz v3 for the stratospheric chemistry
- Completed first decadal long test run with the UCI chemistry. Initial results look reasonable. Ready to couple with other NGD tasks.
- Implemented Fast-J in E3SM and coupled it with other components.

Updated to O3v2 in the stratosphere for E3SMv2

Tang et al., GMDD 2020 also see poster

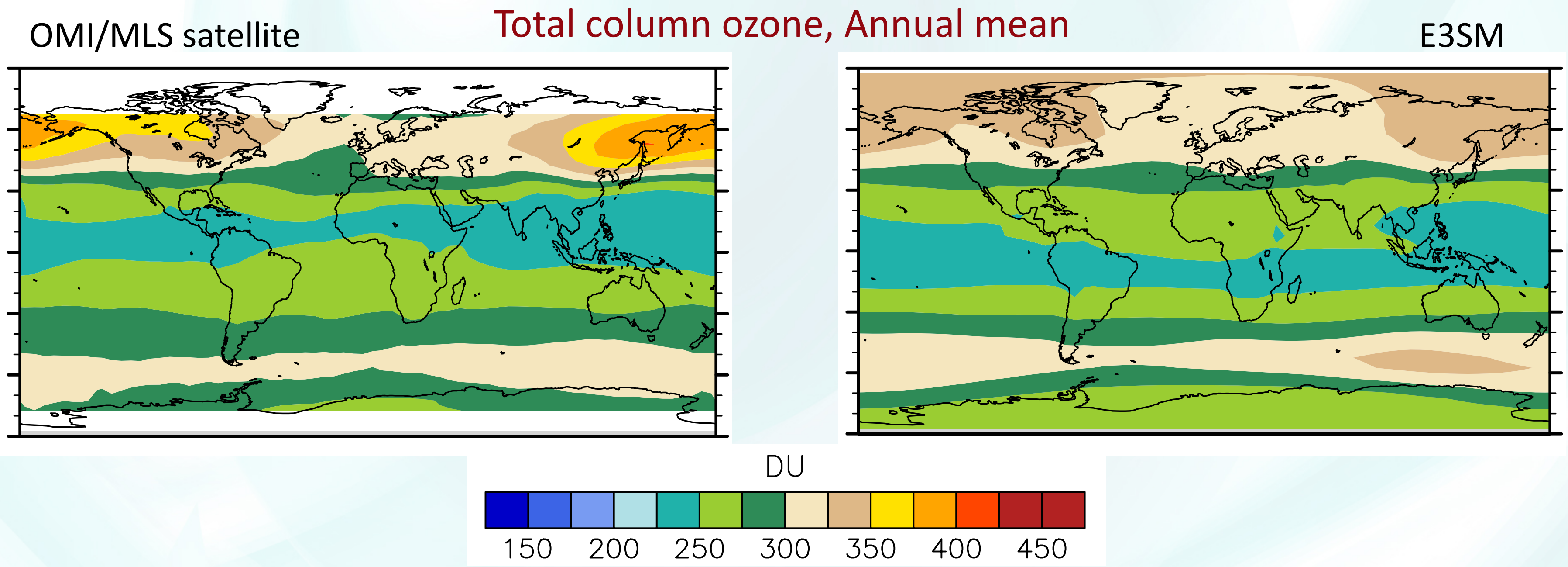
- E3SMv1 chemistry (O3v1) is incompatible with any interactive chemistry.
- Updated to O3v2 to be compatible with chemUCI and improved the simulated O3.





- Taylor diagram for zonal mean stratospheric column ozone (SCO) comparing O3v2, previous O3v1, and UCI CTM. O3v2 shows improvements over O3v1.

First chemUCI (full chemistry) results are encouraging



- Annual mean geographic patterns of the total column ozone are somewhat reasonable, but we need to reduce the low biases.
- Signals are mainly from the stratospheric Linoz.

First chemUCI results are encouraging vs aircraft obs

- Initial 15-year test results are reasonable compared to observations.
- Code on git branch (tangq/atm/UCI-chem), ready to be coupled with aerosols and BGC.

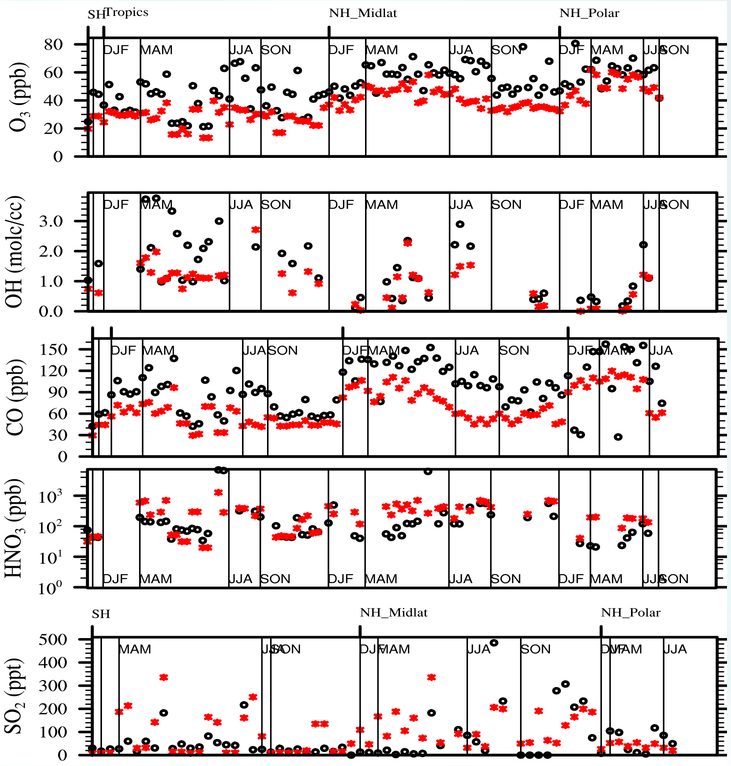
O_3

OH

CO

HNO_3

SO_2



2-7 km

E3SM vs Aircraft

(historical missions)

First-order spatio-temporal variability is acceptable for key tracers in this first quicklook at the details of the chemistry.

Fast-J implemented and coupled to photochemistry

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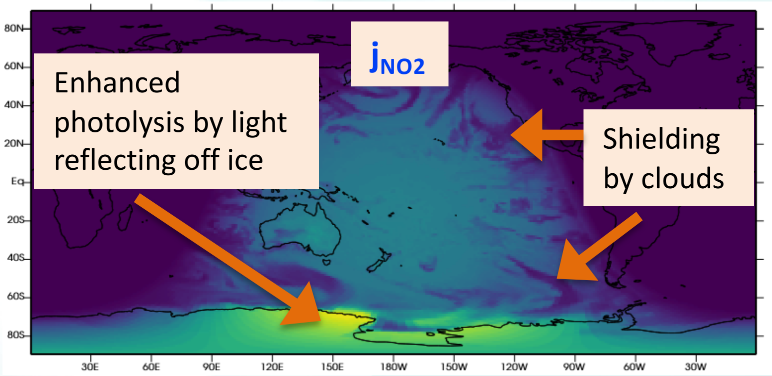
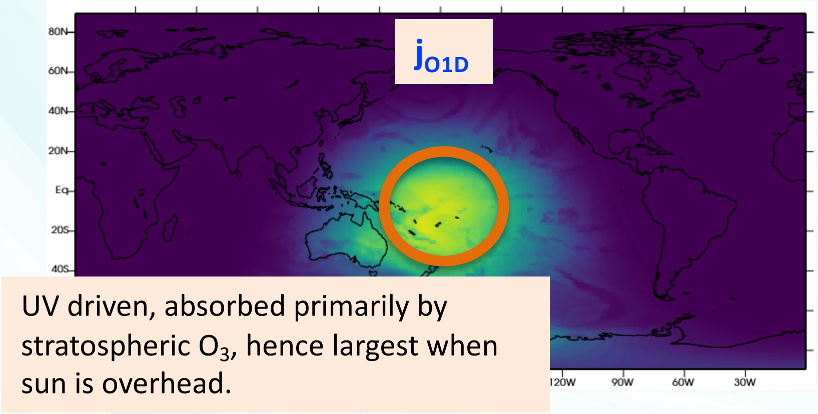




Fast-J is a huge improvement over lookup table.

- Removes lookup table biases in E3SM (Superfast chemistry)
- Consistent treatment with options for overlapping clouds
- Aerosol absorption and scattering
- Spherical geometry of atmosphere (Prather & Hsu, 2019)
- Multi-angle scattering:
  - Enhanced photolysis above clouds and in top of clouds.
  - Realistic diffuse PAR incident on ocean and biosphere
- Updated and updatable laboratory data tables
- Supported for global community by UC Irvine

See Cameron-Smith et al. poster

Solar-J development completed with JAMES paper

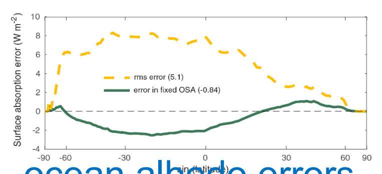
Assessing Uncertainties and Approximations in Solar Heating of the Climate System

Juno Hsu & Michael Prather (UC Irvine), revised 08/2020

Evaluates a wide range of well-known errors & uncertainties in solar heating codes used for climate simulations ***within a single, realistic climate framework*** with 25 variants of Solar-J

Class 1 errors (***1-3 W m^{-2}***, *clearly fixable but some w/cost)*

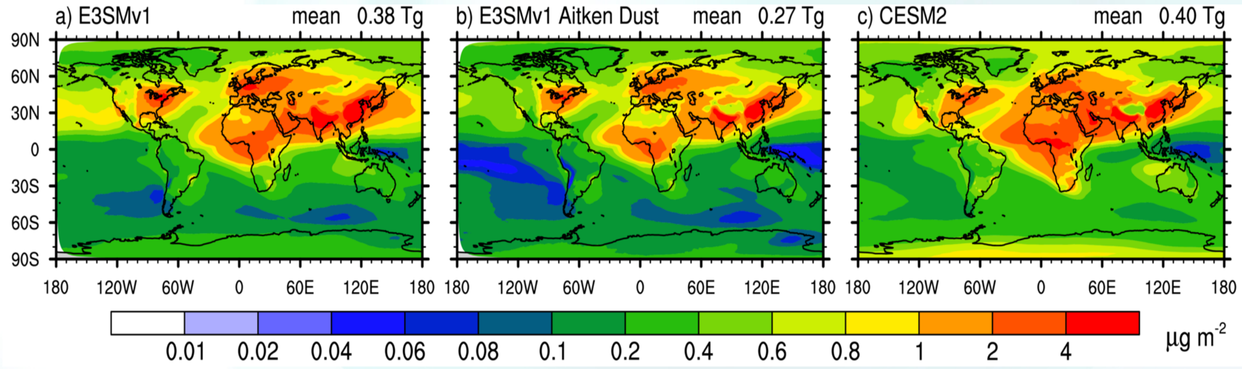
- Spherical, refracting atmosphere instead of flat.
- Resolve cloud spectral absorption instead of RTM broad bands.
- Multi-stream scattering instead of 2-stream (no δ-scaling).
- Ocean surface albedo resolved by zenith angle.
- Monte Carlo noise in atmospheric heating rates.



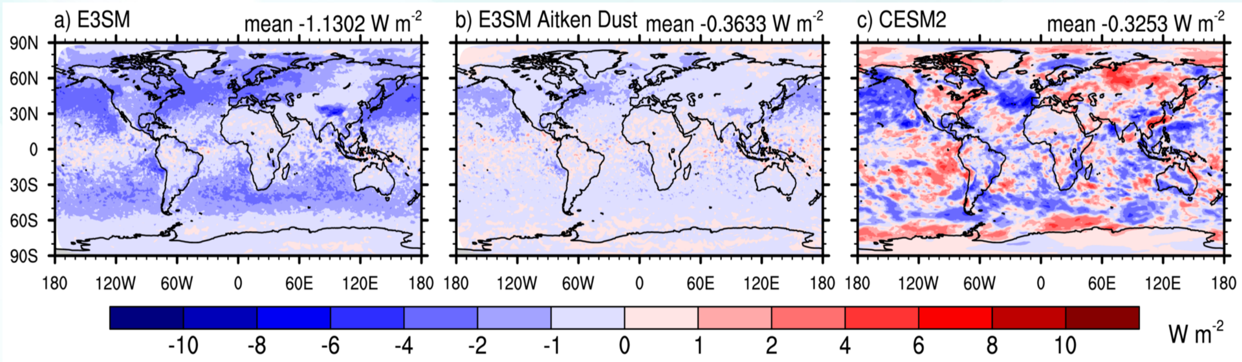
ocean albedo errors

While clear uncertainties with similar error levels remain (3D effects), it seems prudent to push ahead on these Class 1 errors for short-term climate simulations

Representation of nitrate and its impact in E3SMv1



Nitrate burden ($\mu g\ m^{-2}$) simulated in E3SMv1 (without and with Aitken mode dust) and in CESM2

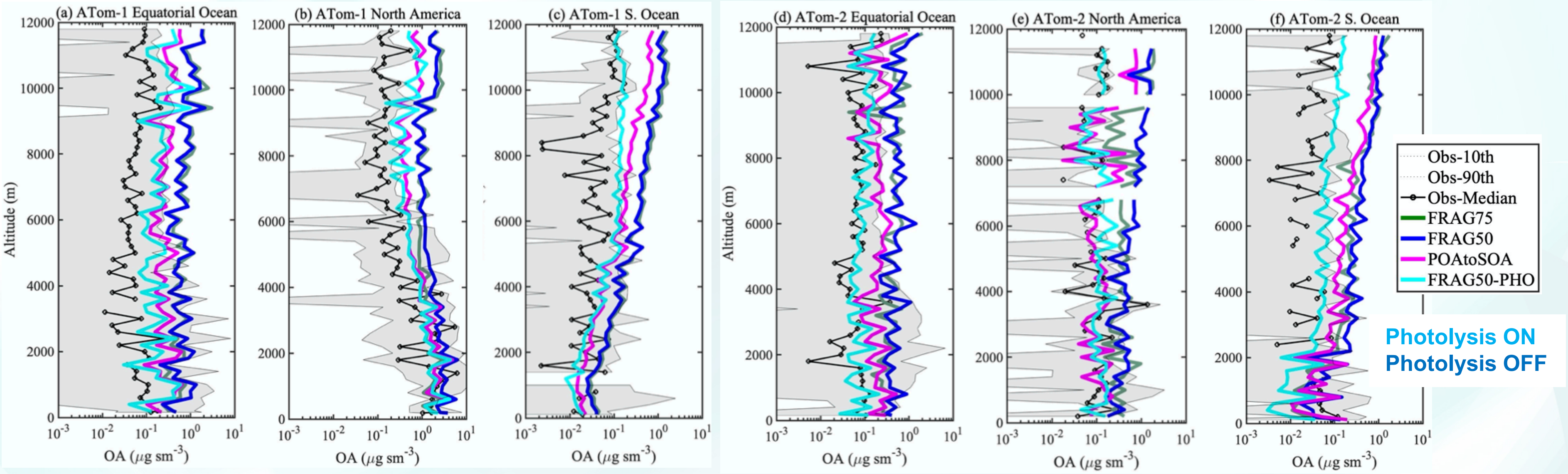


Change in cloud radiative forcing ($W\ m^{-2}$) due to nitrate aerosol for E3SM and CESM2

- MOSAIC has been implemented in E3SMv1 and coupled with MOZART chemistry and a modified MAM4 (e.g., NO_3, NH_4, Ca, CO_3, Na, Cl, and Aitken-mode dust)
- E3SMv1 produces less nitrate than CESM2, especially over ocean, and even less when Aitken-mode dust is treated as part of the MOSAIC and MAM4 coupling
- The magnitude of change in cloud radiative forcing by nitrate is significantly reduced when Aitken-mode dust is treated, becoming comparable to that in CESM2

See Wu et al. poster (PS2-Atmosphere)

Strong production and sinks govern atmospheric SOA distributions and radiative forcing



- A detailed treatment of SOA precursor gas chemistry including multigenerational aging via fragmentation and functionalization reactions, particle-phase oligomerization, and particle-phase loss by photolysis
- Including photolysis improves simulated SOA vertical profiles significantly compared to ATom aircraft measurements
- Different SOA chemistry treatments cause a factor of 3 in SOA lifetime; PD-PI RFari (SOA) decreases from -0.42 to -0.08 W m^{-2} when photolysis is included as a sink of SOA

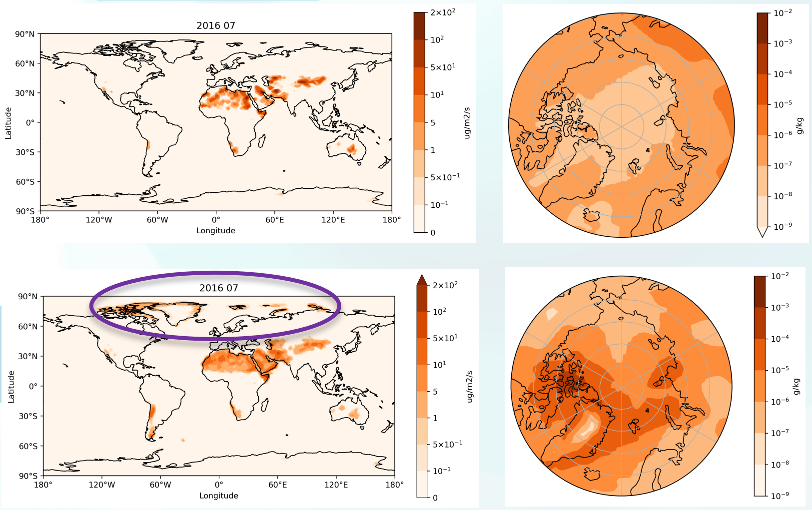
Lou, Shrivastava et al. (Submitted, JAMES)

New dust emission scheme to account for time-varying soil properties and high-latitude sources

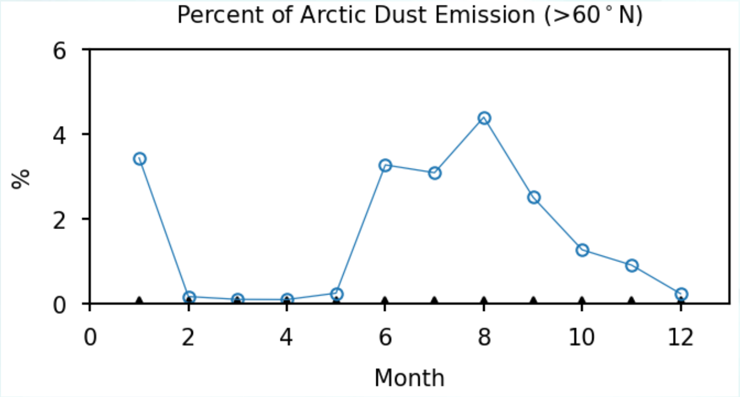
Dust Emission | Surface Concentration

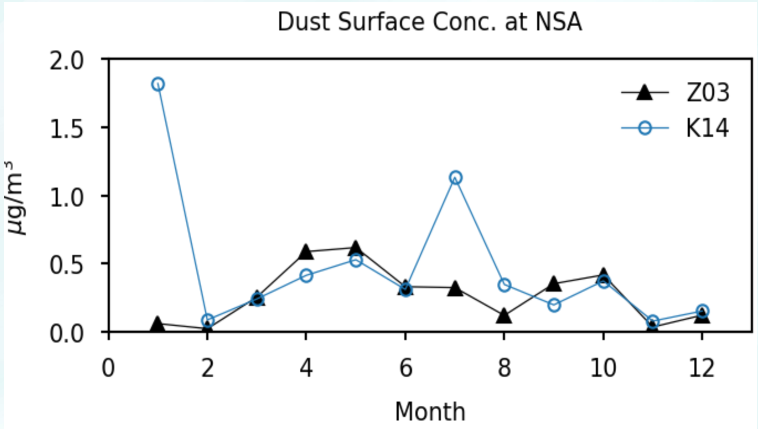
Zender scheme (E3SMv1)

Kok scheme



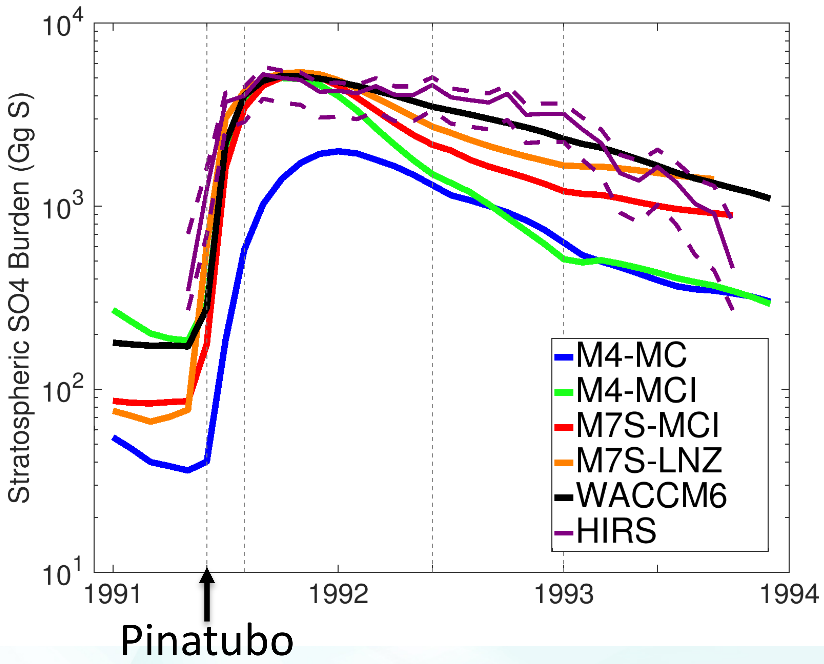
- Zender scheme produces nearly zero emission beyond 60N, while the Kok scheme predicts 2% of the global dust emission from 60-90N with a seasonal cycle, leading to an increase in surface concentrations; Arctic dust can be an important source for cloud nucleation and iron
- Dust surface concentrations agree better with the long-term surface observations at NSA (Barrow, Alaska)





See Feng et al. poster (PS1-WC)

Evaluation of E3SMv1-MAM7S against observations for the major volcanic eruptions during 1991-1993

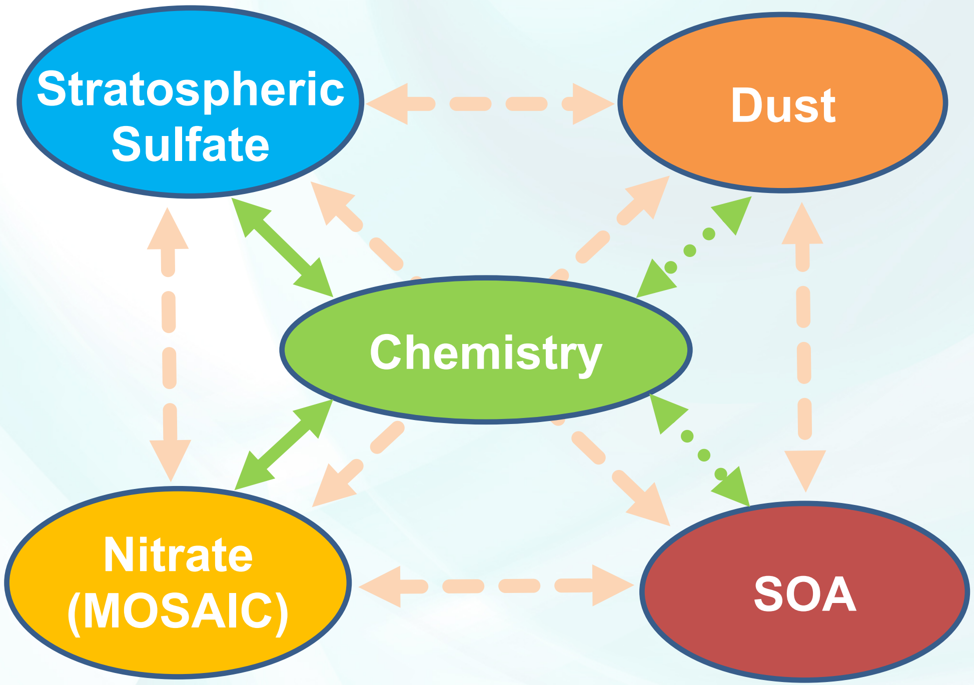


Name	Aerosol Module	Chemistry
M4-MC	MAM4	MOZART
M4-MCI	MAM4	Improved MOZART
M7S-MCI	MAM7S	Improved MOZART
M7S-LNZ	MAM7S	Linoz
WACCM6	MAM4	WACCM6

- Stratospheric sulfate burden simulated by MAM7S agrees well with observations and WACCM6 results
- Sulfate formation in MAM7S responds more rapidly to the Pinatubo eruption due to an improved HO2-OH chemistry in MOZART
- MAM7S maintains the stratospheric sulfate burden better than MAM4 in E3SM but worse than Linoz with prescribed OH
- Impact on stratospheric AOD, ozone and radiation will be assessed

See Ke et al. poster (PS2-Atmosphere)

Future work for coupling aerosols with chemUCI and integration with other new developments for v3/v4



- Complete the development and evaluation of the individual pieces
- Integrate the different new aerosol developments
  - Dynamic solver of gas-particle partitioning to use MOSAIC for SOA
  - Changes to MAM4 (MAM7S) and emissions
- Coupling of the MOSAIC and MAM7S with chemUCI will require additional chemical species and reactions
- Evaluate dust iron dissolution model in the coupled BGC modeling framework
- Integrate and evaluate the new treatments in v3/v4