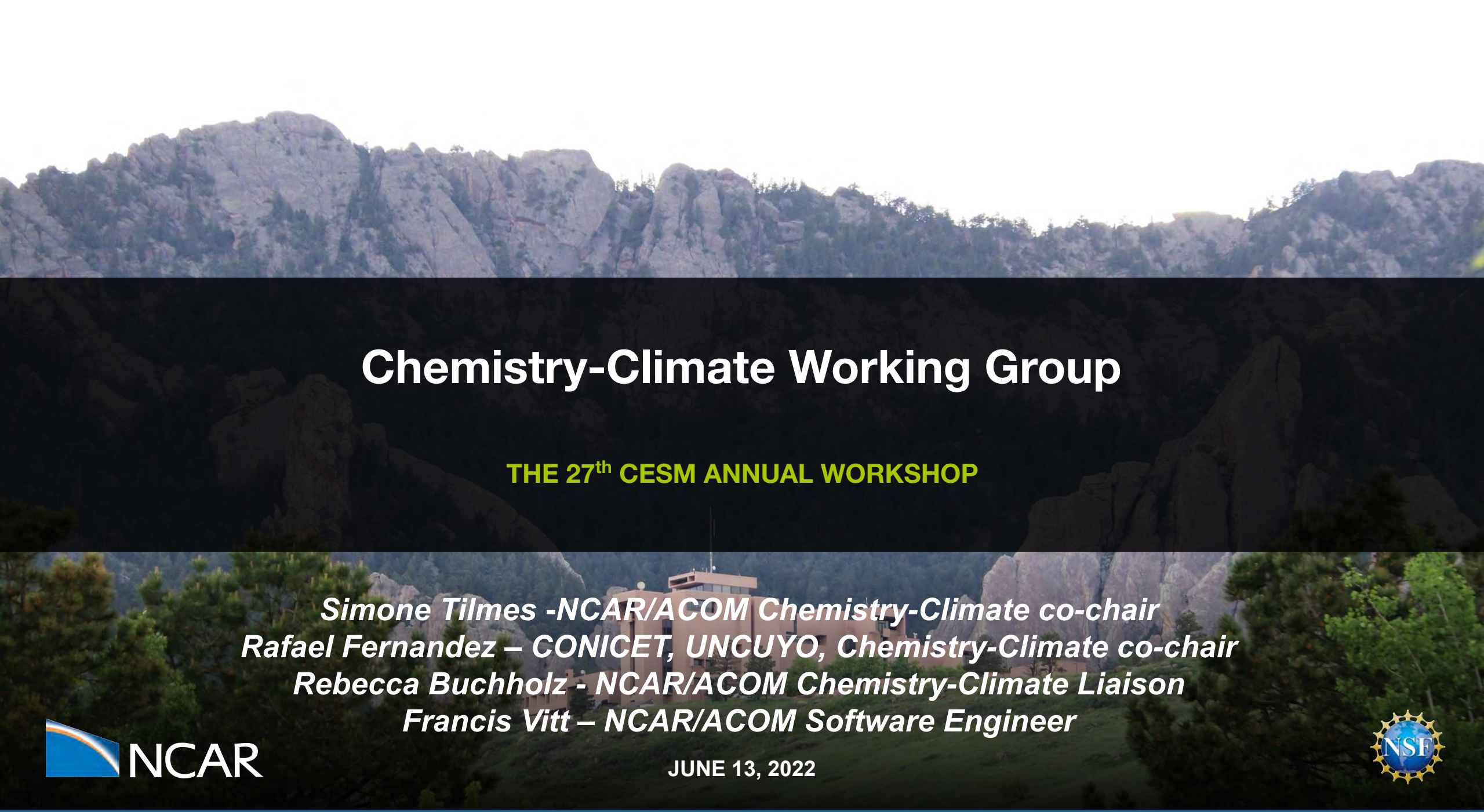


Chemistry-Climate Working Group

THE 27th CESM ANNUAL WORKSHOP

Simone Tilmes -NCAR/ACOM Chemistry-Climate co-chair
Rafael Fernandez – CONICET, UNCUYO, Chemistry-Climate co-chair
Rebecca Buchholz - NCAR/ACOM Chemistry-Climate Liaison
Francis Vitt – NCAR/ACOM Software Engineer

JUNE 13, 2022

This material is based upon work supported by the National Center for Atmospheric Research, which is a major facility sponsored by the National Science Foundation under Cooperative Agreement No. 1852977.

Achievements during the Last Year

MUSICA-v0 Regional Refinement using the Spectral Element Dycore

- MICM, MusicBox, MUSICA-v0 Tutorial, Fall 2021 - Spring 2022 -> talk by Louisa Emmons
- Investigation of regional and local air quality over specific refined regions -> Wednesday talks
- Producing a chemical forecast model for the ACCLIP Aircraft campaign (August 2022)

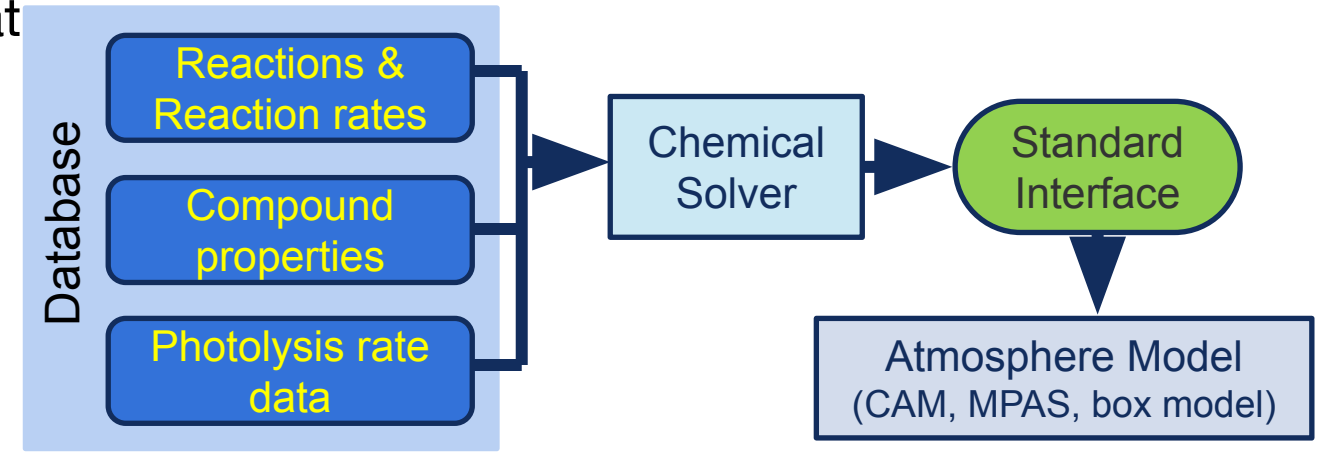
Model-Independent Chemistry Module (MICM)

MUSICA

Database of chemical mechanisms and dat needed for solving chemistry

Allows easily changing the chemical mechanism

Will allow use of the same chemistry in different atmosphere models



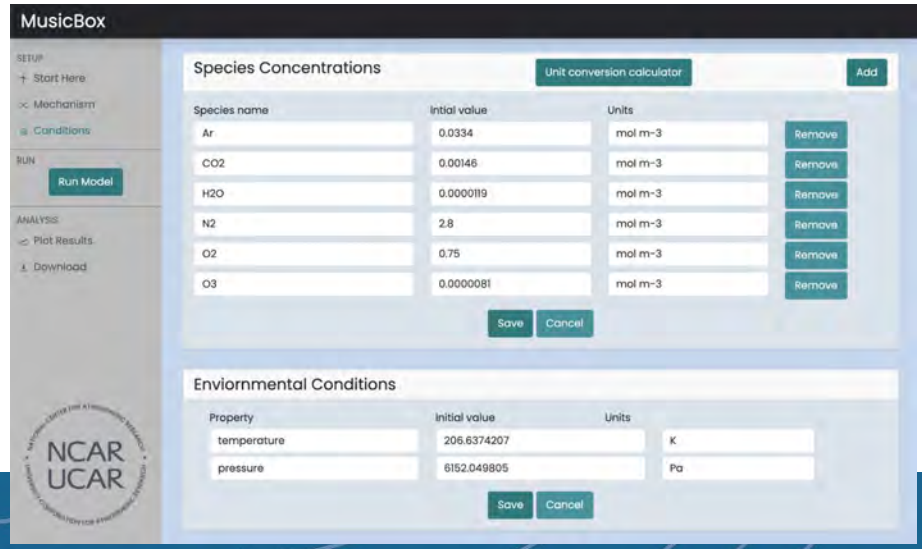
MusicBox: MICM in a box model: https://github.com/NCAR/music-box

Available with command-line control or browser interface

Allows for easy:

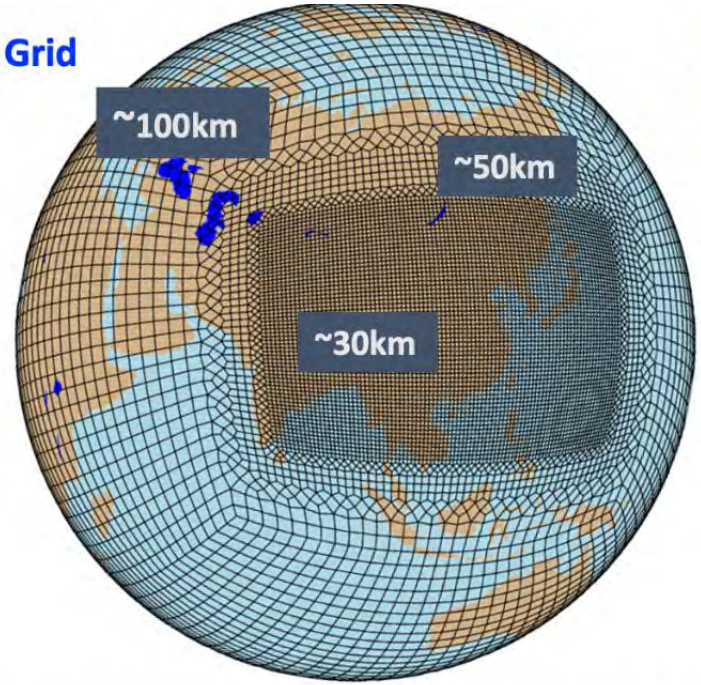
- Modification of chemical mechanism
- Specification of initial and time-varying environment

Browser interface plots results, allows comparison of 2 mechanisms



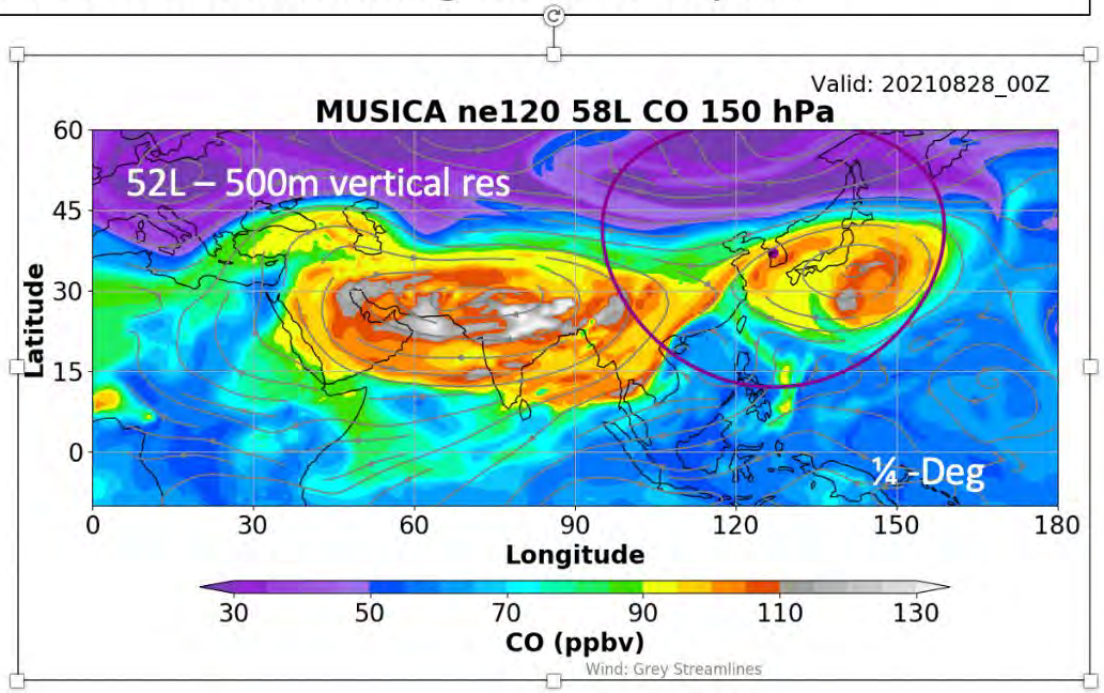
Regional Refinement for Asian Summer Monsoon in support of the NSF/NASA ACCLIP Field Mission

MODEL Grid



Scientific Objectives: Obtain a comprehensive suite of dynamical, chemical, and microphysical measurements in the ASM anticyclone to address: 1) transport pathways to the global UTLS; 2) chemical content; 3) aerosol size and composition for determining radiative impact

- Cube sphere grid; resolution around 1-Deg down to a fine resolution of 0.25 degree.
- Covers the ASM deep convection; anticyclone over the Tibetan Plateau and eastward eddy shedding over the western pacific region.
- Allows for better representation of regional processes and chemistry of surface emissions. This model had detail tropospheric and stratospheric chemistry.



talks by Ren Smith and Doug Kinnison, Jun Zhang

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Chemistry Developments / Evaluation

- New chemistry including HONO etc: Investigation of the effects of COVID on air quality
- MELODIES /MONET: Model EvaLuation using Observations, DIagnostics and Experiments Software

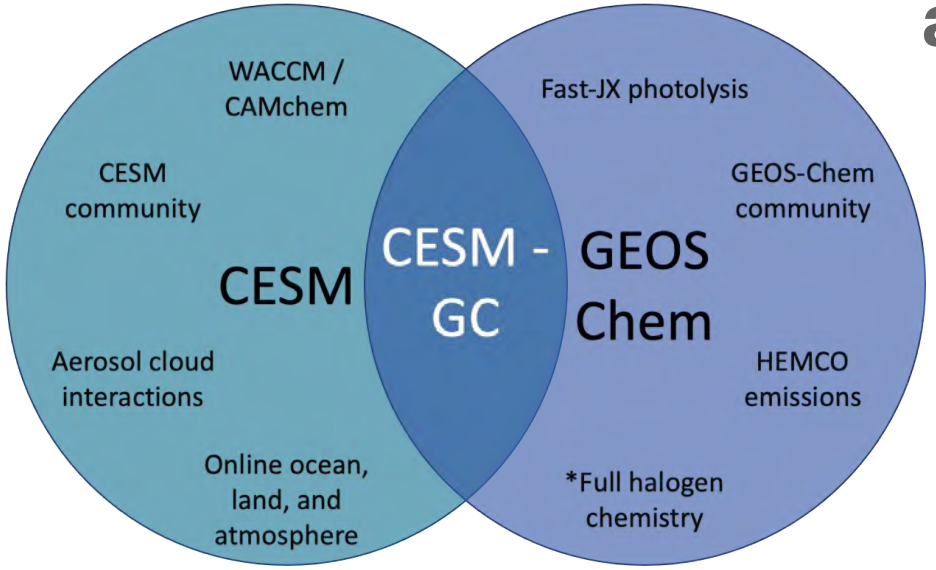
Aerosol Developments

- Aerosol scavenging in convective clouds (Yunpeng Shan, Xiaohong Liu)
- Online ocean DMS emissions (OASISS parameterization by Siyuan Wang)
- MAM5 - Stratospheric sulfate coarse mode, CESM1-MAM4 mode widths (Ziming Ke, Xiaohong)

New coupling of GEOS-chem into CESM2 (Harvard)

- CESM-GC
- HEMCO -> talk by Sebastian Eastham (Harvard)

GEOS-Chem merge into CESM2.1.1 (CESM-GC) and HEMCO CESM



Goal: Merge benefits from two very different Chemistry Modeling frameworks

- Identify differences in model results
- Identify differences in parameterizations and reasons for differences
- Merge User Communities
- Improve model capabilities and applications

HEMCO *(Keller et al., 2014)* was developed as an on-line emissions component for GEOS-Chem

- Runs as arbitrary horizontal resolution component within CAM, runs on CAM vertical grid
- Rectilinear latitude-longitude grid used internally in HEMCO
- Input is regridded to the vertical every file update (usually daily/monthly), not model time step
- Future: Will support arbitrary “internal grid” when CDEPS support is added

[Lin, Haipeng, et al., https://doi.org/10.5194/gmd-14-5487-2021]

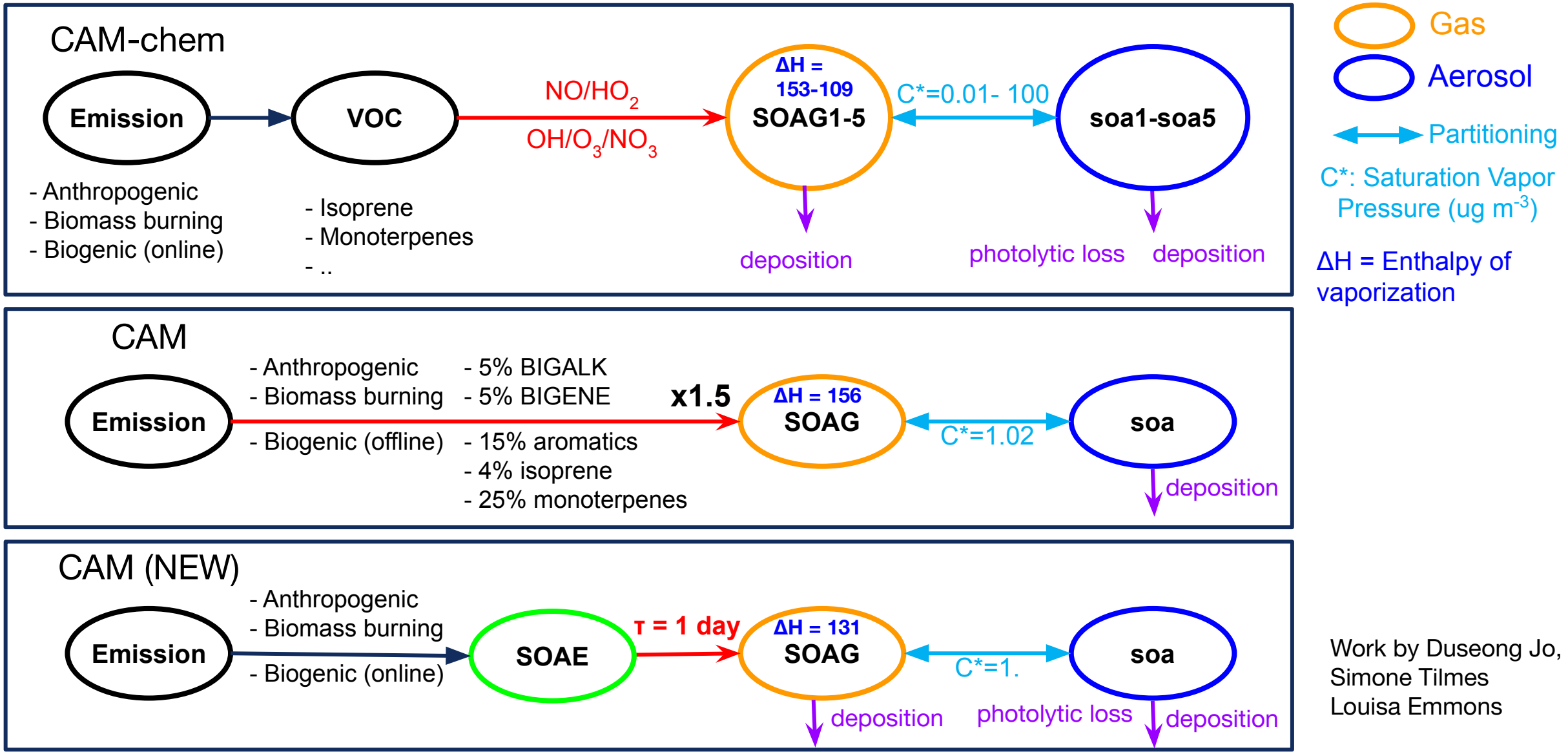
Thibaud M. Fritz, Sebastian Easthan, Louisa K. Emmons, Haipeng Lin, Elizabeth W. Lundgren, Steve Goldhaber, Steven R.H. Barrett, and Daniel J. Jacob

Ongoing Developments

Aerosol Developments

- Improving simple SOA chemistry for CAM -> talk by Duseong Jo (Wednesday)
- New dust emissions scheme in connection to MAM5 development (TAMU/Cornell)
- Implementing Marine Organic Aerosols to CESM2 (Zhao and Liu, TAMU/NCAR)
- Updated dry deposition of aerosols (TAMU/Cornell)

Improvement of simple SOA chemistry in CAM



Gas

Aerosol

Partitioning

C*: Saturation Vapor Pressure (ug m^{-3})

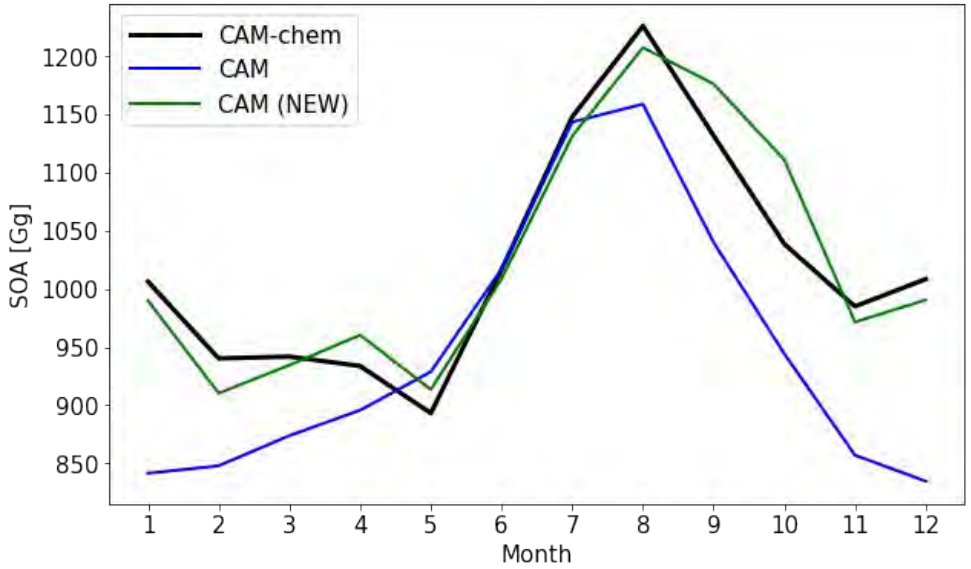
ΔH = Enthalpy of vaporization

Work by Duseong Jo,
Simone Tilmes
Louisa Emmons

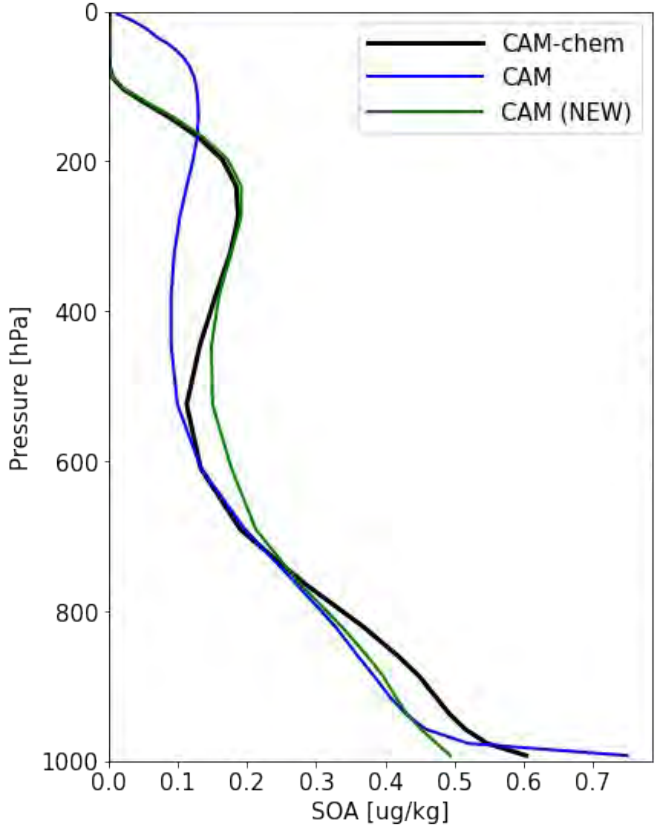
Improvement of simple SOA chemistry in CAM

1-year simulation with T, U and V nudged to MERRA2

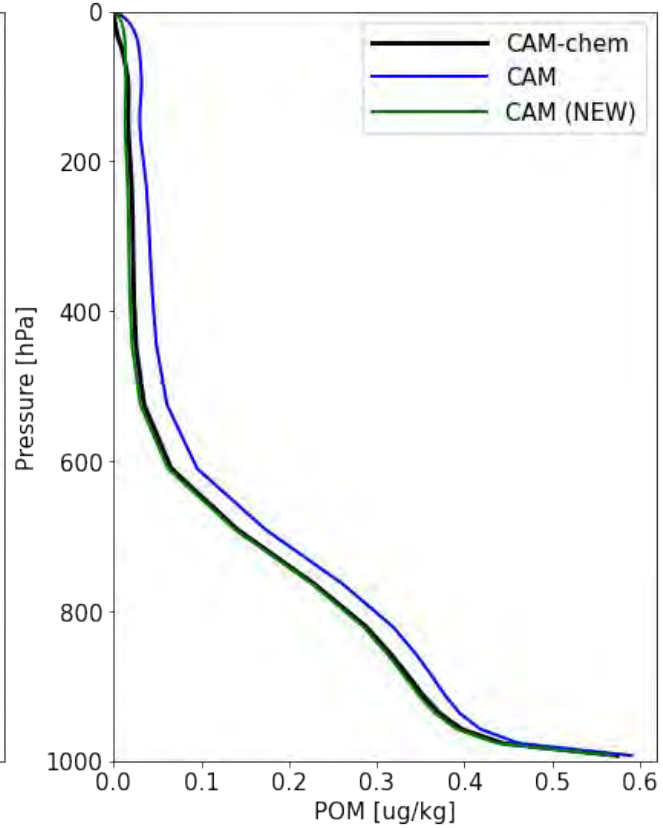
Secondary Organic Aerosol



Secondary Organic Aerosol



Primary Organic Aerosol



Radiative Forcing:

	CAMchem	CAM	CAM(NEW)
FSNT	**236.7**	238.2	**237.3**
FLNT	**238.7**	239.4	**239.3**
SWCF	**-50.5**	-49.1	**-49.8**
LWCF	**22.2**	21.6	**21.6**

- New SOA mechanism reduces the discrepancy between CAM-chem and CAM
- POM in CAM is also improved as a result of aerosol microphysics

Work by Duseong Jo,
Simone Tilmes
Louisa Emmons

Marine Organic Aerosol (MOA)

- **MOA is implemented into MAM4 of CESM2** Based on Zhao and Liu et al., 2021, ACP
  - New tracers: mom_a1 (accumulation mode), mom_a2 (Aitken mode), and mom_a4 (primary carbon mode)

• Emission method

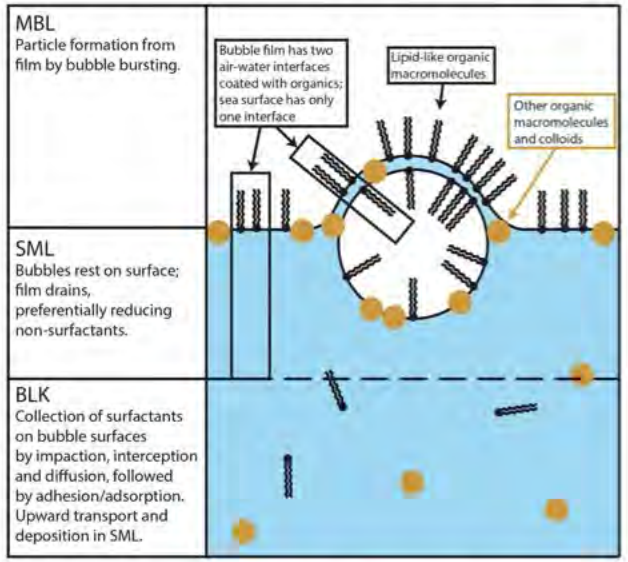
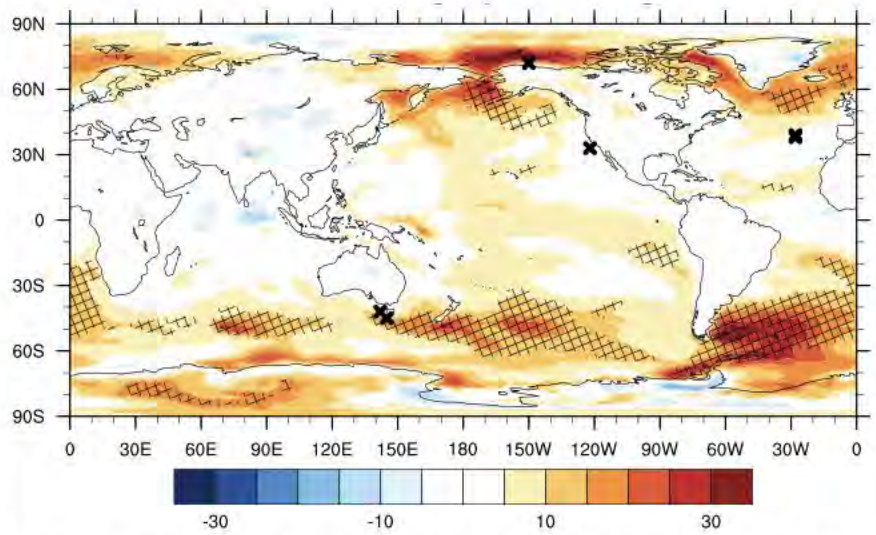


Figure 1. Conceptual schematic of bulk water (BLK), SML, and MBL aerosol enrichment processes.

A physically based framework for modeling the organic fractionation of sea spray aerosol from bubble film. [Burrows et al., 2014]

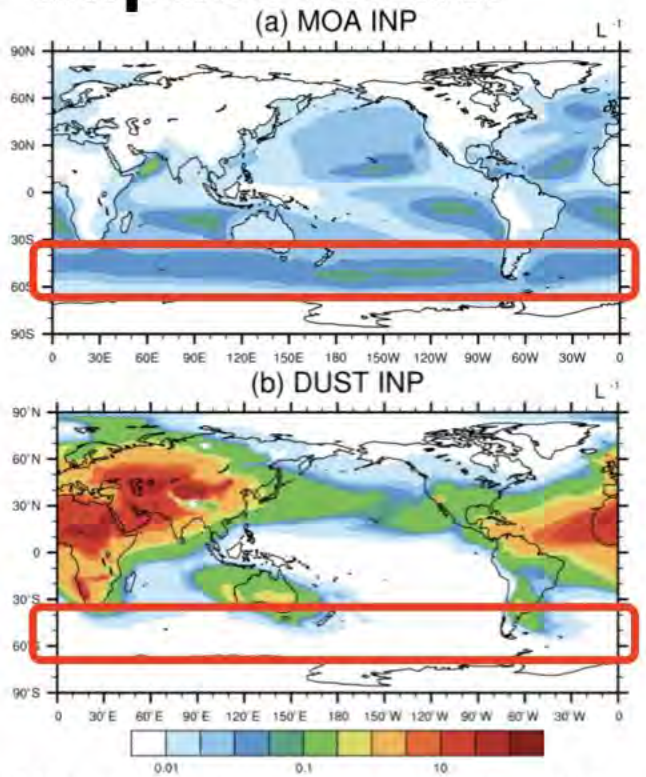
• Impact on CCN



CCN concentration is increased by 10-30% over Southern Ocean (SO) in winter

Implemented by: Xi Zhao, Xiaohong Liu (TAMU), Susannah Burrows (PNNL), Christina McCluskey (NCAR)

• Impact on INP

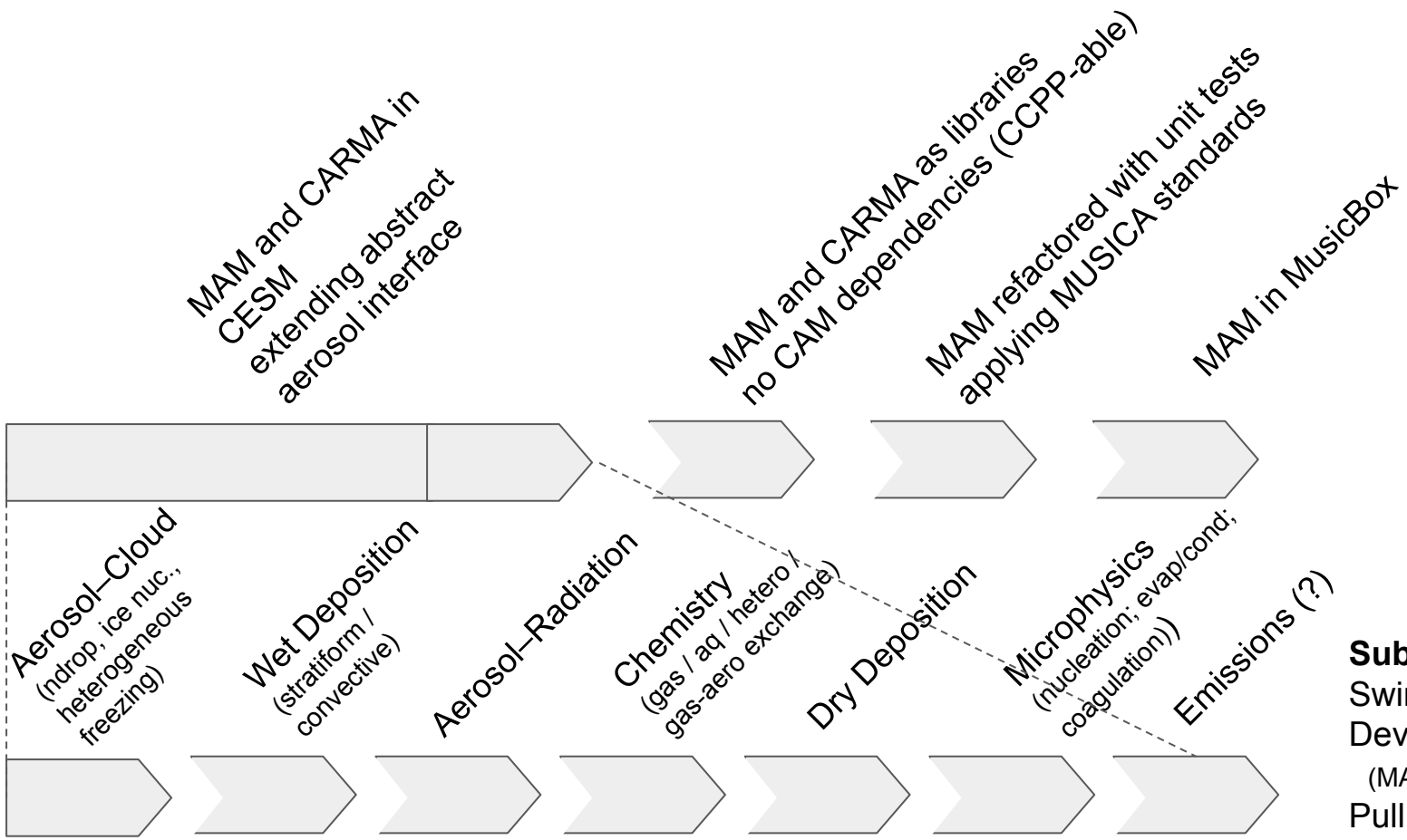


INP concentration is increased by one order of magnitude over SO

SIMA - Abstract Aerosol Interface

Goals of the design of the flexible aerosol interface in CAM:

- Identify and separate aerosol model specific calculation from host model (CAM)
- Keep interactions with aerosols in various place in the code independent of the aerosol model
- Allow easy way for adding new aerosols in one place in the code
- Move code to CCPP (no CAM dependencies)



Work by Matt Dawson, Francis Vitt, various others

Ongoing developments

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Implementation of the flexible aerosol interface

- MOSAIC, and other aerosol options (CESM sandbox)
- CARMA sectional aerosol model for troposphere and stratosphere (CESM sandbox)

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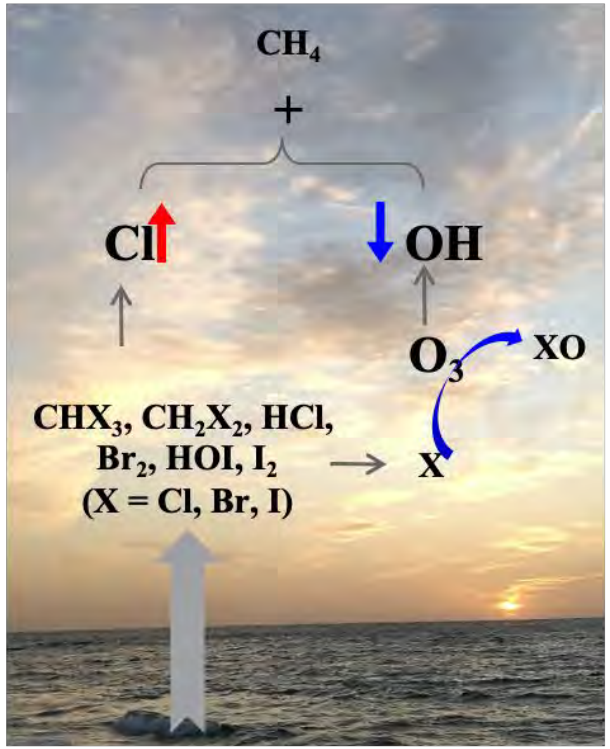
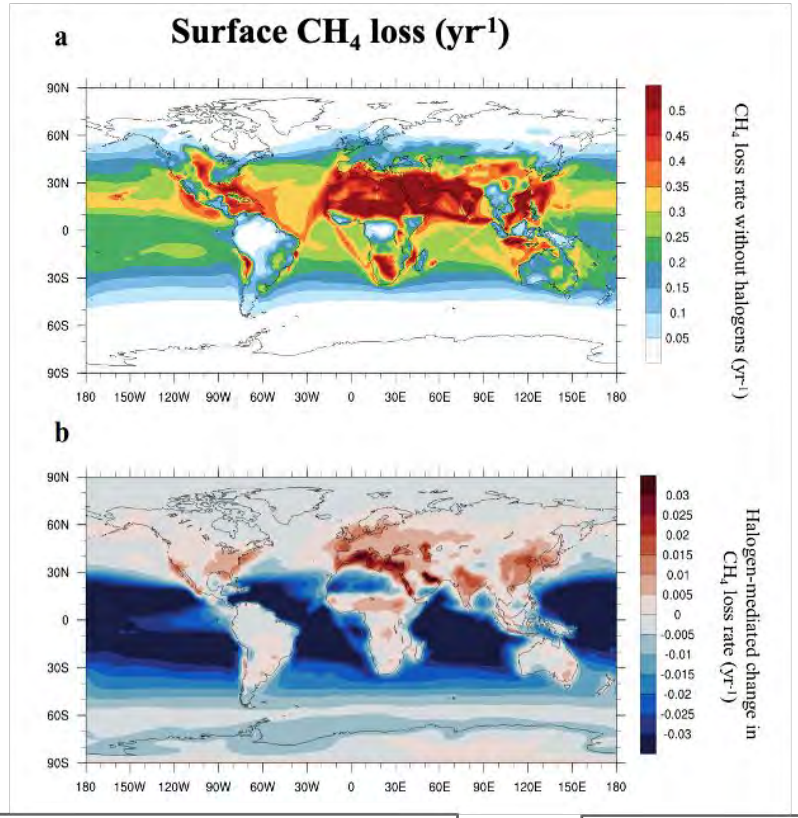
- Very short-lived (VSL) halogen implementation in CESM2 (Rafa Fernandez)
- Introduction of diurnal and vertical emissions: Investigation of the effects of fires
- TUV-x new photolysis scheme

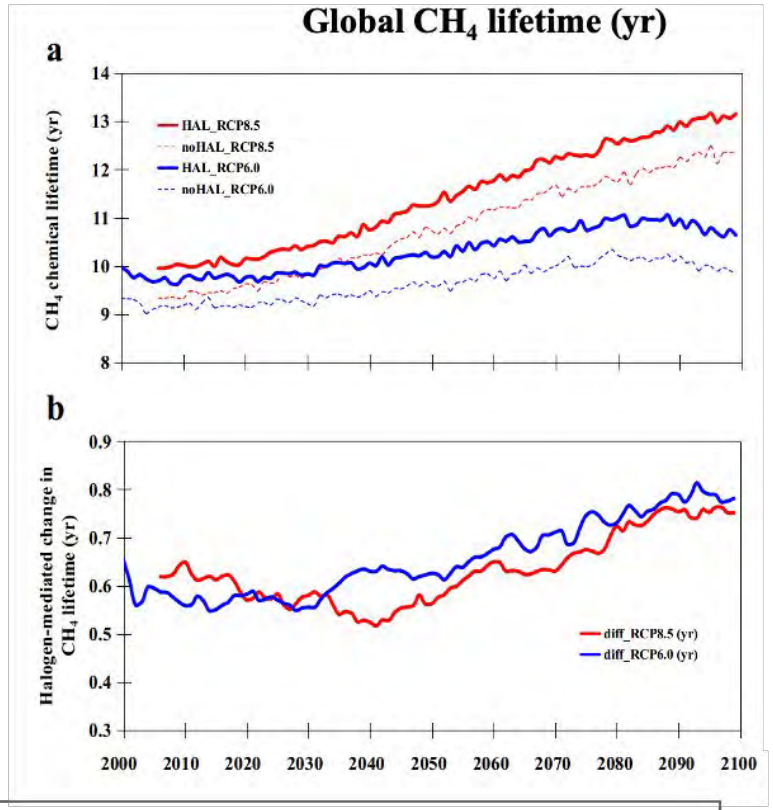
CAMchem VSL Halogens

- **Implementation of reactive chlorine sources & chemistry:**
  - **Evaluation of VSL Halogens Impact on CH_4 lifetime and burden**

Talk by Rafa Fernandez (Wed. 15th, 9:55)
Li et al., Nat. Comm., 2022







CH_4 loss is increased over the land at surface but mostly reduced over the vast opens ocean.

Global CH_4 lifetime is increased by halogens due to the indirect reduction in OH

Ongoing developments

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MUSICA-v0 /CAMchem

- Various different efforts and studies are ongoing, evaluation with WRF -> Wenfu Tang
- Running CAMchem with MPAS (Mary Barth)

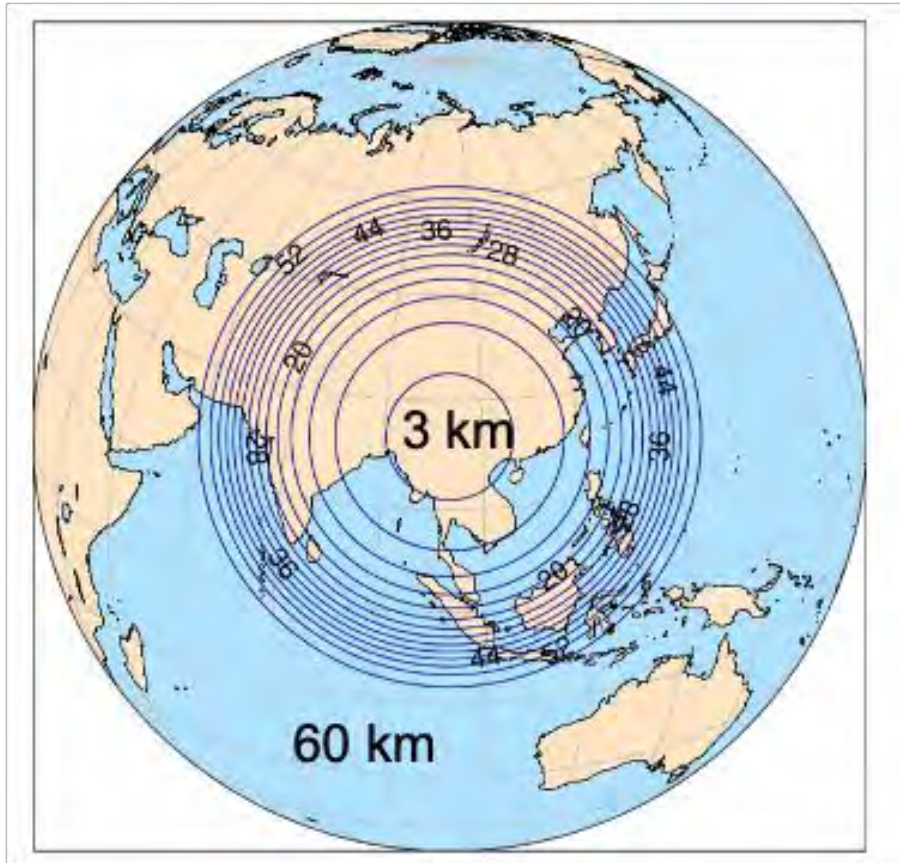
CAM-chem MPAS (SIMA)

Tests of CAM-MPAS-Chem over the Asian Summer Monsoon

Goal: Connects local-scale phenomena (convection) to hemispheric-scale phenomena using MPAS with Chemistry

Example: Asian Summer Monsoon in support of ACCLIP

- Initial tests with full chemistry is in progress:
  1.60 - 3 km grid mesh (0.84 million grid columns), 32 vertical layers, 168 trace gases & aerosols
- Test different numbers of compute nodes; check performance and memory
- Determine the number of constituents that need to be transported
- Run with more vertical layers (58 levels) (1-month simulation)
- Compare with WRF and Spectral Element Simulations



Work by Mary Barth and Francis Vitt

Joint Chemistry & Whole Atmosphere Session on Wednesday AM

Chemistry Working Group:
https://www.cesm.ucar.edu/working_groups/Chemistry/

CAM-chem wiki:
https://wiki.ucar.edu/display/camchem/Home

MUSICA:
https://www2.acom.ucar.edu/sections/multi-scale-chemistry-modeling-musica