

# GEOS-Chem Steering Committee Meeting Minutes

## 2023-01-18

**Present:** Andrew Schuh, Becky Alexander, Barron Henderson, Bob Yantosca, Christoph Keller, Daniel Jacob, Dylan Jones, Eloïse Marais, Fangqun Yu, Hannah Horowitz, Jeff Pierce, Jeff Geddes, Jenny Fisher, Jingqiu Mao, Jintai Lin, Jourdan He, Katie Travis, Lee Murray, Lizzie Lundgren, Lu Hu, Lyatt Jaeglé, Melissa Sulprizio, Pam Wales, Prasad Kasibhatla, Randall Martin, Saptarshi Sinha, Sebastian Eastham, Will Porter

**Absent:** Amos Tai, Chris Holmes, Clara Orbe, Daven Henze, Dylan Millet, Hong Liao, Jun Wang, Kevin Bowman, Lin Zhang, Mat Evans, Tzung-May Fu, Yanxu Zhang, Yuxuan Wang

### General updates (Randall)

- See newsletter written by GCST
- Featured new item: New nested grid domains

### GEOS-Chem 14.1.0 benchmarks (Melissa, Randall)

Includes:

- Adaptive solver
- HTAP v3 (as option)
- Hg simulation updates for deposition, emissions
- Carbon simulation
- Satellite diagnostics as netCDF
- Update GMAO libraries in GCHP
- Fixed GCHP issues identified from 10-yr benchmark
  - Fraction of snow was all zeroes
  - HCFCs not defined properly
- GCHP operational run scripts – encourage users to send theirs via PR
- See GEOS-Chem 14.0.0 wiki page for full list

Sea salt alkalinity fix currently causes 1-month benchmark to crash

- Push off until 14.2

New capability: Autoreduction capability in KPP (Lin et al., JAMES, in press)

- Scheme to partition mechanism into fast and slow species based on prod/loss rates
- Reduce cost of integration by solving for slow species with separate calculation
- Implemented as an option (switch in config file)
  - Does well for tropospheric oxidants
  - Doesn't work as well for halogens, results in some issues in stratosphere
  - Useful for AQ applications and complex organic chemistry
- Offers significant speed up (30%)
- Can use it with nested simulations as well
- GMAO folks have tested it in GEOS and found it may not have as much of a speedup in an MPI environment, but they are looking into further improvements
- Useful for testing new mechanisms

- Not as much of a performance improvement as Lu Shen's mechanism reduction (reduction rates of up to 50%) but this is mechanism-agnostic so it's better suited for the standard model

## GCE2 (Eloise, Mat)

- Still in early stage of planning - booking venue
- Will be in London
- 2.5 days (Aug 14-16, 2023)
- No registration fee

## Plans for GEOS-Chem 14.2.0

Rationale for:

- Methane emissions from hydropower reservoirs (Daniel)
  - Delwiche et al. (2022)
  - Small source, generates hot spots
- ALK4 & R4N2 chemistry (Daniel)
  - Jared Brewer's work
  - Fixes bug - R4N2 was a common product of alkane, isoprene and monoterpene oxidation and produced organonitrate SOA - but we don't want ALK4 to produce organonitrate SOA
  - New tracer created
  - Decreases organic nitrate SOA globally by 14%
- Update reactions with JPL & IUPAC recommendations (Daniel)
  - Barron Henderson and Kelvin Bates working on this
  - Large change in IO + IO reaction causes big changes in iodine chemistry (still investigating). Should coordinate with Becky on Iy update.
- KORUSv5 inventory option (Daniel, Katie)
  - 2015 only
  - Not in CEDS
  - Useful for East Asia simulations - many projects currently using KORUS over SE Asia, MEIC over China
  - Implement as option and leave CEDS as the default
  - Received approval from KORUS developers for inclusion in GEOS-Chem
  - Q: Does it include VCP emissions as well? No, not ready
  - Consensus to add this as option
- Discussion of other regional inventories (all)
  - Should we also implement MEIC then?
    - MEIC is included in CEDS, but only for a few years
    - Some masking issues remain (if users overwrite KORUS over CEDS they may need to manually add MEIC back in)
  - MIX emissions coming out soon (2010-2017)
    - Includes MEIC, REAS, and other regional inventories
      - REAS is included in HTAPv3
    - GC doesn't currently include MIX - it was retired in favor of more recent CEDS emissions
    - Should we reimplement MIX as an option? If it provides additional years or higher resolution then it makes sense

- Jintai's group is using TROPOMI observations to produce summertime NO<sub>2</sub> emissions (in development, contact him if interested)
- Nitrate photolysis (Daniel)
  - Viral Shah has paper in press
  - Add as option
  - Harvard will do a validation with 14.2.0 to determine default recommendation
    - Nitrate phot on/off
    - SSA debromination on/off with Becky's alkalinity and Iy fixes
    - 1-year benchmarks will be completed for each and will be shared with interested parties
  - Seb recommends turning nitrate photolysis off in the stratosphere until better evaluated
  - This update doesn't impact nitrate concentration much
- Iy sink and SSA debromination (Becky)
  - Implications for ozone
  - Issue started in 13.4 when sulfate chemistry moved to KPP and SSA debromination was turned off by default
  - Becky added fixes for treatment of aerosol alkalinity, but it didn't fully solve the issue
  - Iy sink reactions were removed in 13.3 and turned into recycling reactions - Becky has reversed that
  - These two updates combined allow GC to run w/ SSA debromination on again
  - Ozone looks similar to previous versions of model (compared 13.0.0 and 13.4.0)
  - Consensus to add this along with nitrate photolysis evaluation
- Global continental chlorine (pCl and HCl) emissions (Becky)
  - Anthropogenic emissions of Cl are important for chemistry and thermodynamics
  - 1960-2014
  - Make sure to avoid double counting when turning on NEI (already includes Cl)
- Update surface methane boundary condition (Lee)
  - Straightforward update
  - IPCC is only meridional
  - GC is currently using product that Lee generated from NOAA flask data for 2016 extrapolated to 2020
  - This has now been updated through 2022
  - Will be updated annually going forward
  - Side note: Lee will also update constrained lightning through 2022 when those met fields are available at WashU
- CEDS at 0.1 degree resolution (Randall)
  - Standard version currently 0.5. Emma Knowland identified availability of the 0.1 degree dataset.
  - No significant changes expected because of coarse benchmark resolution
  - GMAO has these fields ready and working in GCHP/GEOS
- CEDS SO<sub>2</sub> Sat emissions option (Randall)
  - Emma Knowland identified this inventory.
  - Combines CEDS with OMI SO<sub>2</sub> to identify point sources
  - There is also an HTAP version of this product
  - Not clear if it's worth the effort - evaluate further before deciding

# Working Group updates and perspectives

## Aerosols (Becky, Jeff, Will, Fangqun)

- Items ready now:
  - TOMAS updates
    - Functionality in GCHP
    - Full integration with aqueous sulfate in KPP
    - Blowing snow sea-spray
  - DMS chemistry updates
  - Loretta: future dust and biomass burning emissions
    - Q about number of files and size of directory
  - Bug fixes on sea salt alkalinity and pH-dependent het. reactions on sea salt
  - Luo wet dep fixes (paper in prep, updated code ready within 3 months)
    - Will fix lag time in stratosphere
    - Will fix too-short lifetime for Pb210
- Planned work:
  - Bob Y. is cleaning up aerosol\_mod.F90, pulling out kinetic reactions from carbon\_mod.F90 and porting into KPP
    - Conversion of hydrophobic -> hydrophilic and conversion of SOA ported to KPP already
    - Need to determine how to bring in updated SOA from Jared Brewer
  - Brown carbon chemistry from Jingqiu Mao
    - Implemented in 12.7.2, but needs updating to current version and rate changes
  - Automated reduction in isoprene scheme from Dan Westervelt
- Discussion topics:
  - Directions for SOA scheme development
    - How to evaluate and tweak schemes going forward?
  - Future of thermodynamic models in GEOS-Chem
    - There seems to be a need to update from the current version of ISORROPIA, but need to discuss options
  - MAM 7 scheme in GEOS-Chem (Seb)
    - Still 12 months out
    - This will work in the stratosphere and troposphere
    - Will need advice from aerosols WG

## Stratosphere (Dylan J., Seb, Pam)

- Featured news:
  - Paper validating GEOS-Chem stratosphere in GEOS-FP (Knowland et al, 2022)
    - Uses GEOS-Chem coupled to GEOS
    - More accurately forecast ozone hole featured on GMAO website
- Items ready now:
  - Implement GMI update for NO<sub>x</sub> source from galactic cosmic rays
  - Urgent but unresolved item to extend UCX into the mesosphere
- Benchmarking:
  - Water vapor looks better in 14.0.0 10-year benchmark
  - No new major issues
  - Ongoing issues

- ClO and HCl biased low
    - N<sub>2</sub>O is biased high in lower strat, low in upper strat (issue w/ resolution, mixing in UTLS)
  - Propose expansion of stratospheric benchmarking using existing data from GEOS-CF comparison
    - Tracer-tracer comparisons (e.g. NO<sub>y</sub> vs NO)
    - Bring in SF<sub>6</sub> observations
    - ACE-FTS Cl<sub>y</sub>, NO<sub>y</sub>
    - Stratospheric CO
- Looking ahead:
  - Many updates impact the stratosphere without explicitly being assigned as stratospheric WG items
  - WG will add persistent/known issues to Stratospheric WG wiki page
  - KPP autoreduce may not be appropriate for GEOS-Chem stratosphere
  - Mass fluxes vs winds evaluation on stratospheric impact is ongoing
  - Plan to submit benchmarking updates as PR? WG is still thinking about this, will follow up with GCST

## Other WG updates

- Transport WG
  - Development of GCClassic – GCHP – GEOS-replay comparisons
    - Need transport tracers consistent between models, update coming soon to GC simulation
    - Emma will do GEOS IT 2019 replay simulation
    - Lizzie will run many simulations to evaluate
  - GF vs RAS differences relative to transport (role of GEOS-IT)
- Hg and POPs WG
  - Ari Feinberg (MIT) updated Hg<sub>0</sub> soil emissions parameterization (paper to be submitted Jan 2023)

## GMAO update (Christoph)

- TEMPO has been delayed from mid-March to mid-April
- QFED files are being pushed on a monthly basis to WashU (ready by mid-month)
- GEOS-IT
  - 1998-present, updated in NRT
  - Will put files needed for GCHP on NASA Pleiades
  - Includes cube-sphere archive of met fields
  - Already being pulled to WashU archive

## Living document listing existing simulations or specialty restart files (Prasad)

- Would it be useful to make some simulation results (tied to papers) available?
  - We should not take on the responsibility of archiving but can encourage users to archive their own work. A public spreadsheet with links to model output would facilitate.

- The location of these archives can be documented on the GEOS-Chem wiki
- Resources/requirements for archiving are dependent on publication and university
- Restart files for specialty simulations
  - Want to initialize simulations (e.g. CO<sub>2</sub>, CH<sub>4</sub>) with restart file for exact month and year and have these data constrained by observations if possible, but GCST currently only provides one sample restart file (e.g. Jan 2019) per simulation
  - This is different from full-chemistry simulations, which require a spinup to remove impact of initial conditions and where mechanism evolves rapidly

### Update on status of GEOS-Chem within CESM (Lizzie)

- GEOS-Chem and HEMCO in CESM, review is ongoing should be merged soon to get GC from direct CEDS download
- H. Lin doing comparison of GEOS-Chem and CAM-Chem

### Exploring the prospect of a GEOS-Chem Center proposal (Randall)

- Attract additional resources to support GCST, sustain growth of community
- Still in early stages
- Reaching out for interest and input