GEOS-Chem Steering Committee Meeting Minutes
2022-09-21

Present: Becky Alexander, Liam Bindle, Kevin Bowman, Jenny Fisher, Tzung-May Fu, Jeff Geddes, Barron Henderson, Chris Holmes, Hannah Horowitz, Jourdan He, Lu Hu, Daniel Jacob, Lyatt Jaeglé, Dylan Jones, Christoph Keller, Hong Liao, Lizzie Lundgren, Eloïse Marais, Randall Martin, Dylan Millet, Lee Murray, Jeff Pierce. Will Porter, Andrew Schuh, Melissa Sulprizio, Amos Tai, Katie Travis, Pam Wales, Yuxuan Wang, Bob Yantosca, Fangqun Yu, Yanxu Zhang

Absent: Seb Eastham, Mat Evans, Daven Henze, Prasad Kasibhatla, Jintai Lin, Jingqiu Mao, Clara Orbe, Jun Wang, Lin Zhang

IGC10 recap

It was an honor to host everyone at WashU for IGC10. We received very positive feedback from attendees.We hope to see you at IGC11 at WashU in 2024!

Some feedback to keep in mind for IGC11:

- Record meeting talks/clinics and keep them online for a finite time (e.g. ~1 month)
- Make sure that early career scientists have enough opportunities to ask questions.
- Break up 2-hour time blocks into shorter segments
- Offer more vegan/vegetarian food options, etc.

Working Group expansion

Based on discussion at IGC10, the following working groups have been reorganized:

- The Chemistry-Ecosystems-Climate WG is now the **Chemistry-Climate WG**.
    - Co-chairs: Hong Liao and Lee Murray

- The Emissions-Deposition WG is now the **Emissions WG**.
    - Co-chairs: Lyatt Jaeglé, Jintai Lin, and Eloïse Marais

- A new **Surface-Atmosphere Exchange** working group has been formed.
    - Co-chairs: Jeff Geddes, Chris Holmes, Dylan Millet, and Amos Tai.

The following topics now fall under the umbrella of the Surface-Atmosphere Exchange WG:

- Dry deposition
- Ecosystems
- Land and ocean processes
- Biogenic VOC emissions

- Sources and sinks that have an algorithmic dependence on land or ocean (e.g. biogenic VOC's,which depend on leaf area indices)

New GCSC members

Please join us in welcoming the newest GEOS-Chem Steering Committee members:

- Hannah Horowitz (UIUC), Hg and POPs WG co-chair
- Katie Travis (NASA/LaRC), Transport WG co-chair
- Lyatt Jaegle (UW), Emissions WG co-chair

New GCST members

Jourdan He and Saptarshi Sinha joined the GEOS-Chem Support Team this summer. They will be working in Randall Martin's group at WashU.

14.0.0 release update

The GEOS-Chem 14.0.0 10-year benchmark results were recently sent to the GCSC. Thanks to everyone who looked at them. We saw small changes between 14.0.0 and 13.4.0 as expected.

While investigating differences between the GEOS-Chem Classic and GCHP 1-year benchmarks for 14.0.0, Lizzie Lundgren and Bob Yantosca discovered that there was a bug in 13.4.0 that had escaped detection. In 13.4.0, many updates were introduced to resolve parallelization issues and numerical issues. A bug in the GEOS-Chem Classic pressure fixer module was inadvertently introduced along with these structural updates. Several chemistry updates (in particular, deactivating sea salt debromination in order to improve ozone concentrations) were also introduced into 13.4.0, and these masked the impact of the pressure fixer bug. This bug affected ozone, particularly at high latitudes.

The pressure-fixer bug is limited to GEOS-Chem Classic, as GCHP uses a different transport scheme. The bug also does not affect GEOS-Chem Classic nested-model simulations (although if you have been using version 13.4.0 or 13.4.1 to generate nested boundary conditions, then those boundary conditions will contain the signature of the bug).

The GCST has identified a path forward to resolve this issue:

1. Updates that were originally slated for 14.0.1 will be included into the 14.0.0 development branch, and evaluated with internal benchmarks.

2. When all of these updates have been validated, the GCST will revert to using the GEOS-Chem Classic pressure fixer from version 13.3.0, which does not have the bug.

3. 1-month and 1-year benchmarks for GEOS-Chem Classic and GCHP 14.0.0 will be re-run. If these pass scrutiny, then we can proceed to release GEOS-Chem and GCHP 14.0.0.

4. The 10-year benchmarks for 14.0.0 will also be rerun. The 10-year benchmarks take several weeks to run, so we will not let this hold up the 14.0.0 release.

5. The GCST has added a bug fix (**Git tag: 13.4.0+revert-pressure-fixer**) with the reverted pressure fixer so that people who are still using 13.4.0 or 13.4.1 can simply apply the bug fix. See the 2022 Newsletter, Issue 2 for instructions..

14.1.0 development and advocation of new features

There are several 14.1.0 development items that are currently in progress, as denoted on the model development priorities page.

We would like to begin a protocol that new features should be advocated for by a GCSC member in order to be prioritized for inclusion into the model. The floor was opened for discussion.

HTAPv3 emissions

Randall Martin advocated for the inclusion of HTAPv3 emissions into GEOS-Chem 14.1.0. This inventory has 0.1 degree emissions worldwide, at monthly time-resolution, from 2000-2018. The HTAPv3 emissions also include several regional emissions, and would be a way to provide a better inventory over North America than what we have at present. Implementation would only require updating the HEMCO configuration file to point to the HTAPv3 data files.

Points raised at discussion:

- It was agreed that CEDS will remain the default global inventory. But HTAPv3 could be a useful option, particularly for higher resolution simulations.
- Barron Henderson noted that not all countries provided data for all years, so some years of HTAPv3 data rely on extrapolations.
- HTAPv3 will use the same diurnal scaling factors as was done for HTAPv2.
- HTAPv3 contains lumped emissions, so some speciation will be necessary in order to translate emissions to the species carried by GEOS-Chem.
- The GCST will not perform an official benchmark simulation with HTAPv3 vs. CEDS, but perhaps this could be done with HEMCO standalone simulations. Working groups are encouraged to test with HTAPv3 data. Tests conducted by Dandan Zhang (WashU) and associated with the pull request document expected differences.
- We need to be especially clear with documentation during HTAPv3 implementation.

AMAP Hg emissions

Jenny Fisher advocated for including AMAP Hg emissions into GEOS-Chem 14.1.0, now that several bugs with the Hg simulation have been resolved. The AMAP data is a global standard and is needed for model intercomparison studies. Implementation would only require updating the HEMCO configuration file to point to the AMAP data. Sectoral data would also be valuable for the GEOS-Chem community.

Biomass burning updates

Dylan Millet advocated for adding several biomass burning updates into GEOS-Chem 14.1.0, including: (1) Updating VOC's to Andreae et al. (2019); (2) Adding biomass emissions for existing GEOS-Chem species that do not have biomass emissions, and (3) Adding 1 single lumped species (representing 3 compounds) for furans.

Coggon et al. (2019) have shown that furans are a big part of the reactivity of fires. Another furan oxidation species may also be necessary.

Geologic emissions

Dylan Millet (on behalf of Mat Evans) advocated for prioritizing geologic emissions of ethane and propane (cf. Evans & Rowlinson). This is not a huge source but it might explain an underestimate of emissions.

Updated soil NOx algorithm

Dylan Millet (on behalf of Jun Wang) advocated for including an updated soil NOx algorithm into GEOS-Chem 14.1.0 (based on Yi Wang et al. (2021)). The algorithm uses actual soil temperature (from MERRA-2) rather than an empirical estimate. It updates the temperature dependence of emissions at T > 20C to better fit observations over the USA. Global emissions increased by 22%.

Points raised at discussion

- **Chris Holmes** noted that there is inconsistency in the emission factors applied to different biomass burning inventories. This is a traceability challenge. We will need to make sure that emission factors are well documented and applied to all inventories if these changes are adopted.
- **Kevin Bowman** noted that soil temperature is a prognostic calculation. The new algorithm requires the MERRA-2 soil temperature field (TSOIL1), which we currently do not include in the met fields for GEOS-Chem. This will require having to download extra data for several years.

- **Jeff Geddes** noted that the existing temperature and flux relationship is based on many observations but the Wang et al Soil NOx scheme is based on data from a limited set of observations in a specific region. Is this a conceptual problem? How does this extrapolate to soil temperature in other parts of the world?
- **Jenny Fisher** noted that the Wang et al soil NOx is an online parameterization. Incorporating this will lead to an offset between offline & online emissions (unless the offline emissions are regenerated with the new algorithm).
- **Lee Murray & Kevin Bowman** noted that the surface air temperature is probably more robust than the surface soil temperature.
- **Daniel Jacob** noted that adding this new soil NOx scheme would be a big investment of time because of the need to regenerate the offline emission fields.

For these reasons, it was agreed to table this feature for the time being.

Nitrate photolysis

Daniel Jacob advocated for prioritizing Viral Shah's implementation of nitrate photolysis + sea salt debromination. With this new parameterization we can get a better representation of NOx and O3.

Because we do not want to break ozone, 4 different configurations (with and without nitrate photolysis, with and without sea salt debromination) will be informally benchmarked and reviewed by Mat Evans, Daniel Jacob, and Katie Travis. This will help to inform us as to what the best path forward is.

Points raised in discussion

- The nitrate photolysis includes a dependence on sea salt and nitrate.
- This update seems to affect the remote regions but not polluted regions. There is some concern that this might lead to excessive HOx production over the KORUS-AQ domain. This will indeed need to be examined.

Chemistry-Climate WG update

Lee Murray gave an update on the Chemistry-Climate WG, which focuses on reactive chemistry and its impact on climate (and vice versa). In particular

- The GCAP2 version of GEOS-Chem is now operational.
- WRF-GC is also operational
- Since IGC10, RRTMG has been updated by Seb Eastham
- There are SST future emission scenarios for CO2 & Methane
- ICECAP2 in 13.4.1 ready for inclusion in standard code. Met fields and data are served from the U. Rochester data portal.

- A new email list will be created (`geos-chem-chemistry-climate@g.harvard.edu`)

Surface-Atmosphere Exchange WG update

Jeff Geddes presented an introductory slide about the Surface-Atmosphere Exchange WG.

Points raised at discussion

- We need to make sure that all GEOS-Chem topics are covered by at least one WG.
- It would be useful to keep track of which WGs handle specialty simulations
- Is it possible to build a consistent system that accounts for land processes and that is propagated across to other areas?

GMAO Updates (Christoph Keller)

Christoph Keller informed us of a couple of issues with the MERRA-2 data

- There was an issue with the July-Aug 2022 pre-release MERRA-2 data
- Also, the June-Sep 2021 data was bad and has been replaced

The GCST will follow up to update the meteorological field data repository.

Google doc for GCPy developments

Dylan Jones mentioned that several of his students have re-invented the wheel when writing Python code to plot/analyze GEOS-Chem outputs. It would be great to have some kind of archive (a Google doc or similar) where people could find code that performs specific atmospheric computations. These routines (when mature) can eventually feed back into GCPy. Whichever method we choose should be easy for users to use and update.

Points raised at discussion

- We could have a wiki on the GCPy Github. But is this an activation energy barrier?
- Could people create HTML pages from their Jupyter notebooks for reference?
- We might need a multiple tier of documentation -- a Github for code that might be ready for GCPy, and a Google doc another with messy code for students, etc.
- There might be value in having similar lists for R or Matlab, etc.
- We could also consider a scripting sandbox: List the task to be accomplished next to the code snippet that does the task.
- This is a great idea and needs more discussion to find the best medium for sharing information about tools.

Updating benchmark observations

Lu Hu informed us that **Amy Christiansen** (Montana) is currently preparing an ozonesonde climatology up to the year 2019. Results will look quite different from the data set that we currently use for benchmark evaluation. There is 20 years of data available, but we will use the last 10 years of this data set for benchmark evaluations.

Offline aerosol simulation

Randall Martin has polled the Aerosols Working Group about the aerosol-only simulation. The responses indicated that the aerosol-only simulation is still being actively used, and the wiki has been updated accordingly. Oxidant fields for this simulation are taken from the most recent 10-year benchmark outputs.

Diagnosing GEOS-Chem transport errors

Daniel Jacob reported that **Emma Knowland** (GMAO) will run 1-year online simulation with the full tracer suite at c180 at GMAO. This data will be used as input to GEOS-Chem Classic and GCHP simulations (to be performed by **Lizzie Lundgren**) that will help diagnose potential transport errors and biases. A multi-year analysis can be performed in the future if the initial work is successful.