Spring 2020 Newsletter

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Featured News

The upcoming GEOS-Chem 13.0.0 release

Several important structural updates will be added in version 13.0.0

GEOS-Chem 13.0.0 features several important structural updates. Updates impacting both GEOS-Chem Classic and GCHP include retiring carbon-based units for VOC species, more efficient allocation of diagnostic arrays for a reduced memory footprint, retiring GNU Make and replacing it with a CMake build system, and starting to separate out emissions and dry deposition from non-local PBL mixing. Notably, both GEOS-Chem Classic and GCHP will be run from new wrapper repositories containing GEOS-Chem and HEMCO as separate git submodules. These updates are needed to facilitate the interfacing of GEOS-Chem into several external models, such as the NASA/GEOS-GCM, CESM, WRF, and NOAA models. All GEOS-Chem updates in 13.0.0 are purely structural and will not impact output beyond numerical noise.

The table below summarizes all structural updates slated for version 13.0.0. Further below are details of updates specific to GEOS-Chem Classic and GCHP respectively.

Feature or fix in version 13.0.0	Authors
Retire carbon-based units for VOCs	Melissa Sulprizio, GCST
Retire the GNU Make build system in both GEOS-Chem Classic and GCHP and replace with CMake	Liam Bindle, GCST
Retire the GEOS-Chem Unit Tester repository and move GEOS-Chem run directory creation to the GEOS-Chem source code repository	Melissa Sulprizio, GCST
Use GEOS-Chem and HEMCO as separate git submodules inside a new GEOS-Chem Classic wrapper repository	Lizzie Lundgren, GCST
Updates to HEMCO for compatibility with CESM	Haipeng Lin, Harvard
Reduction of memory for HISTORY diagnostics with a species dimension	Bob Yantosca, GCST
Removal of HEMCO code from within the non-local PBL mixing modules	Bob Yantosca, GCST
GCHP update: Retire the existing GCHP repository and replace with a new wrapper repository that uses ESMF as an external library and integrates GEOS-Chem and NASA/GMAO GEOS-ESM git repositories as git submodules	Lizzie Lundgren, GCST

GCHP update: Separate HEMCO from GEOS-Chem to use as an ESMF gridded component in GCHP	Lizzie Lundgren, GCST
Enable a stretched grid capability in GCHP to run global simulations at regional high resolution	Liam Bindle, GCST
Updates for compatibility with MAPL 2.1.	Lizzie Lundgren and Liam Bindle, GCST

GEOS-Chem Classic 13.0.0

Starting in 13.0.0, GEOS-Chem will be embedded within a new GEOS-Chem Classic wrapper repository called GEOS-Chem-Classic. HEMCO will be its own repository and will be included as a git submodule within the wrapper alongside GEOS-Chem.

The GEOS-Chem Unit Tester Github repository will officially be retired in this version. Run directory files and a run directory creation script will be included within the “run” subdirectory of the GEOS-Chem repository, following what is already done for GCHP.

GCHP 13.0.0

GCHP version 13.0.0 will feature a new GCHP repository, called GCHPctm, which will serve as a wrapper around GEOS-Chem, HEMCO, and GMAO libraries. These libraries will be used as Git submodules. The existing GCHP repository used within GEOS-Chem will be retired, and the structure of GCHP will be essentially inverted to make the functional structure of the model more clear. ESMF will no longer be included in the GCHP download and it will be separately downloaded and built for use as an external library. The removal of ESMF and the switch to a new build system (CMake) will significantly reduce GCHP compile time.

GCHP 13.0.0 will feature the latest release of the GMAO MAPL library which will fix the remaining long-standing GCHP issues, namely the persistent memory leak limiting run duration and the minimum input resolution required for when running at high grid resolutions. The upgrade will also provide several new functionalities including a stretched grid capability (work-in-progress by Liam Bindle of Wash U.), 1D diagnostic output, the capability of reading input data on the cubed-sphere, and improved error handling.

GCHP Stretched-grid Capability

GCHP 13.0.0 will feature a new capability to define a high-resolution cubed-sphere face over an area of interest (such as North America, Europe, or Asia), while reducing the resolution of the remaining grid faces. One of the great benefits of using a stretched-grid simulation over a nested-grid simulation is that you will no longer need to generate transport boundary conditions from a separate global simulation. The stretched-grid simulation implicitly handles the two-way nesting (transport of species into and out of the high-resolution grid face). This work is currently being validated by GCST member Liam Bindle.

GCPy 1.0.0 to be released concurrently with GEOS-Chem 13.0.0

We have added many new features to GCPy since the last newsletter. Much of this effort has been focused on improving our capability to produce plots and tables for validating the GEOS-Chem 1-month and 1-year benchmark simulations. In particular:

- Benchmark plots and tables can now be created in parallel, significantly reducing the overall time required to generate output from benchmark simulations.
- Single-level plots can now be generated at any resolution for any area of the globe. Zonal mean plots can also now be produced for the 72 level full vertical grid or the 47-level reduced vertical grid. In the future, we hope to also include a new algorithm that can vertically regrid between arbitrary grids.
- New routines have been introduced to compute budget tables for both the full-chemistry and TransportTracers benchmarks.

While much progress has been made, there are still many development tasks left to complete, namely:

- Refactoring the GCPy code so that it is separated into modules in a more logical manner than at present.
- Updating the GCPy documentation in the code itself, as well as rewriting the GCPy manual pages online.
- Adding example scripts for the benefit of users.

All of this development work will culminate with a **GCPy 1.0.0** release that will be issued concurrently with the GEOS-Chem 13.0.0 release. GCPy 1.0.0 will be the official public release of GCPy. Until then, all versions of GCPy should be considered unofficial development versions

One of the great benefits of using open-source Python code such as GCPy is that it can be easily ported between computer systems and to the AWS cloud..

Meeting updates

Remote GCE1 Meeting: September 2020 (tentative)

As you are aware, the GEOS-Chem Europe Meeting (GCE1) was originally scheduled to be held from June 22-24 at Leeds, UK, but was postponed due to concerns about COVID-19.

The organizers of GCE1 (Mathew Evans, York U; Eloise Marais, U. Leicester; and Paul Palmer U. Edinburgh) still hope to be able to host a remote GCE1 meeting, using Zoom or similar teleconferencing. They have proposed that remote GCE1 take place on **September 1-2, 2020**, but this is preliminary and the schedule may still change.

We will keep you apprised of further developments. When we have more information, we will update the GCE1 meeting website (**gce1.geos-chem.org**).

The GCA2 Meeting has been cancelled

The Second GEOS-Chem Asia Meeting (GCA2), scheduled to happen later this year, has now been cancelled. We hope to be able to hold this meeting in 2022.

The 10th International GEOS-Chem Meeting (IGC10)

Add more text about IGC10 after the telecon when we have details

GEOS-Chem Version Updates

The GEOS-Chem 12 versions listed below were released since our last newsletter (Feb 2020):

12.7.1

Release date: 19 Feb 2020; **DOI:** zenodo.3676008

This version includes the following features and bug fixes:

Feature or fix in version 12.7.1	Authors
Prevent excessive scavenging in the stratosphere in the Luo et al 2019 wet deposition scheme • NOTE: Luo et al 2019 wetdep is a research option, which is turned off by default	Gan Luo, Albany; Transport Working Group Bob Yantosca, GCST
Bug fixes for the TOMAS microphysics simulation	Dana McGuffin, CMU; Bob Yantosca, GCST
Bug fix for ND51/ND51b satellite timeseries w/ nested-grid simulations	Bob Yantosca, GCST
Bug fix in computation of AOD from isoprene SOA diagnostic	Jun Meng & Bob Yantosca, GCST
Bug fixes for ObsPack diagnostic re: instantaneous sampling	Charley Fite, FSU Bob Yantosca, GCST
Fix for segmentation fault when dry deposition is turned off	Lizzie Lundgren, GCST

Fix WRF-GC SetGridFromCtrEdges interface	Haipeng Lin, Harvard
Fix bug where GCHP 12.7.0 standard run failed if emissions are turned off	Lizzie Lundgren, GCST
Update MEGAN file used in GCHP 12.7.0 that caused run failure if using gfortran	Lizzie Lundgren, GCST
Add MODEL_GCHP (and MODEL_CLASSIC) as CPP options in GEOS-Chem	Lizzie Lundgren, GCST
Now make sure the HEMCO standalone gets the proper met field name and grid resolution	Jun Meng and Bob Yantosca, GCST
Prevent overwriting restart variables H2O2AfterChem and SO2AfterChem if present	Lizzie Lundgren, GCST
GCHP fix: Fix incorrect vertical flipping of MAPL 3D imports impacting mesospheric chemistry	Lizzie Lundgren, GCST; Seb Eastham, MIT
GCHP fix: Fix incorrect mapping between internal state H2O2AfterChem and the equivalent State_Chm field	Lizzie Lundgren, GCST
GCHP fix: Fix two timestep delay in update time for LAI upon day change	Lizzie Lundgren, GCST

For more information about the updates in GEOS-Chem 12.7.1 please click here.

12.7.2

Release date: 09 Mar 2020; **DOI:** 10.5281/zenodo.3701669

This version contains bug fixes for GEOS-Chem “Classic” and GCHP:

Feature or fix in version 12.7.2	Authors
Restrict wet scavenging to troposphere in Luo et al 2019 wetdep scheme • NOTE: Luo et al 2019 wetdep is a research option, which is turned off by default	Gan Luo, Albany Transport Working Group Bob Yantosca, GCST
Bug fix for reading 3-hourly boundary condition files after hour 21	Melissa Sulprizio, GCST
Remove unused routines in regridding module regrid_a2a_mod.F90 -- this facilitates HEMCO restructuring.	Haipeng Lin, Harvard

GCHP fix: Fix pointer retrieval error in SET_CH4 introduced in 12.7.0 when running at c180+. This also corrects a long-standing and previously unidentified issue when running with reduced timesteps.	Lizzie Lundgren, GCST
GCHP fix: Use new Ordonez files to avoid error in MAPL when running at c360.	Lizzie Lundgren, GCST

For more information about the updates in GEOS-Chem 12.7.2, please click here.

12.8.0

Release date: 03 Feb 2020; **DOI:** 10.5281/zenodo.3634864

This version contains many new scientific updates:

Feature or fix in version 12.8.0	Authors
Isoprene chemistry	Kelvin Bates, Harvard
Wet deposition parameterization	Kelvin Bates, Harvard; Sarah Safieddine, MIT
Ozone deposition to the ocean	Ryan Pound & Mat Evans, York
Use online DustDead, MEGAN, SeaSalt, and SoilNOx emissions for benchmark simulations • NOTE: Standard simulations still use high-resolution offline emissions by default	Melissa Sulprizio, GCST
Shift CMIP6 time from middle to start of month to allow start in January	Lizzie Lundgren, GCST
GFED 4.1s beta emissions for 2017-2019	Maggie Marvin, Edinburgh
Replace `State_Chm%nAero` with `State_Chm%nAeroSpc` and `State_Chm%nAeroType`	Seb Eastham, MIT Bob Yantosca, GCST
Convert all files in GeosCore, GeosUtil, and Headers to .F90	Melissa Sulprizio, GCST
Change GEOS-Chem timers from a CPP switch to an option in input.geos	Melissa Sulprizio, GCST

Bug fix: Remove potential for surface CH4 retrieval error in SET_CH4 due to reliance on HEMCO emissions year	Christoph Keller, GMAO
GCHP bug fix: Fix leap year handling issue in GCHP multi-run script	Lizzie Lundgren, GCST
GCHP fix: Correct SH surface ozone bias	Seb Eastham, MIT LIzzie Lundgren, GCST

For more information about the updates in GEOS-Chem 12.8.0, please click here.

12.8.1

Release date: 03 Feb 2020; **DOI:** 10.5281/zenodo.3634864

****** THIS IS THE CURRENT STABLE VERSION OF GEOS-Chem ******

This version contains the following features and fixes:

Feature or fix in version 12.8.1	Authors
Disable FlexGrid checks to allow for running with any horizontal or vertical grid -- this facilitates WRF-GC development	Melissa Sulprizio, GCST
Update the dry-run download data script to make files group-writeable	Bob Yantosca, GCST
Add more timers for gas-phase chemistry	Melissa Sulprizio, GCST
Reduce the amount of memory that GEOS-Chem dry-runs require	Bob Yantosca, GCST
Add bounds-checking and floating point exceptions to CMake "Debug" target	Melissa Sulprizio, GCST
Fix incorrect indexing for AOD diagnostics	Melissa Sulprizio, GCST
Fix for instantaneous timeseries diagnostics to avoid overwriting hour zero	Bob Yantosca, GCST
Allow for missing species in boundary conditions	Melissa Sulprizio, GCST
Fix to allow diagnostics with frequency="End" to properly straddle year-end boundaries	Bob Yantosca, GCST
Fixes for WRF-GC and CESM-GC	Haipeng Lin, Harvard

Add fix for POPs emissions diagnostics	Melissa Sulprizio, GCST
Avoid memory corruption bug in HEMCO when certain debug flags are on	Seb Eastham, MIT
Fix bug causing seg fault when ConcAboveSfc diagnostic collection is on	Lizzie Lundgren, GCST
Fix bug causing crash if not starting on the first day and time of the month	Lizzie Lundgren, GCST
GCHP fix: Now use correct GCHP config file entry for surf_iodide source file in 12.8.0	Lizzie Lundgren, GCST
GCHP fix: Avoid unexpected behavior if dynamic timestep is changed to non-default values	Lizzie Lundgren, GCST
GCHP fix: Fix timestamps in offline biogenic VOCs data to avoid crashing in late Dec/early Jan	Lizzie Lundgren, GCST
GCHP fix: Add internal state met variables to benchmark and transport tracers simulations -- needed for benchmarking	Lizzie Lundgren, GCST
GCHP fix: Enable all budget diagnostics output in GCHP transport tracer simulation by default -- needed for benchmarking	Lizzie Lundgren, GCST

For more information about the updates in GEOS-Chem 12.8.1, please click here.

12.8.2

Release date: TBD; **DOI:** TBD

This version contains the following features and fixes:

Feature or fix in version 12.8.2	Authors
Bug fix: Update version numbers to 12.8.2	Bob Yantosca, GCST
Updates to facilitate WRF-GC development	Haipeng Lin, Harvard

For more information about the updates in GEOS-Chem 12.8.1, please click here.

GEOS-Chem 12.9.0

This version will feature a major revision of tropospheric halogen chemistry based on Wang et al (2019), and including further updates to bromine chemistry (Zhu et al, 2019), cloud entrainment (Holmes et al 2019), and cloud acidity (Shah et al, 2020).

This version will also contain the following features and fixes:

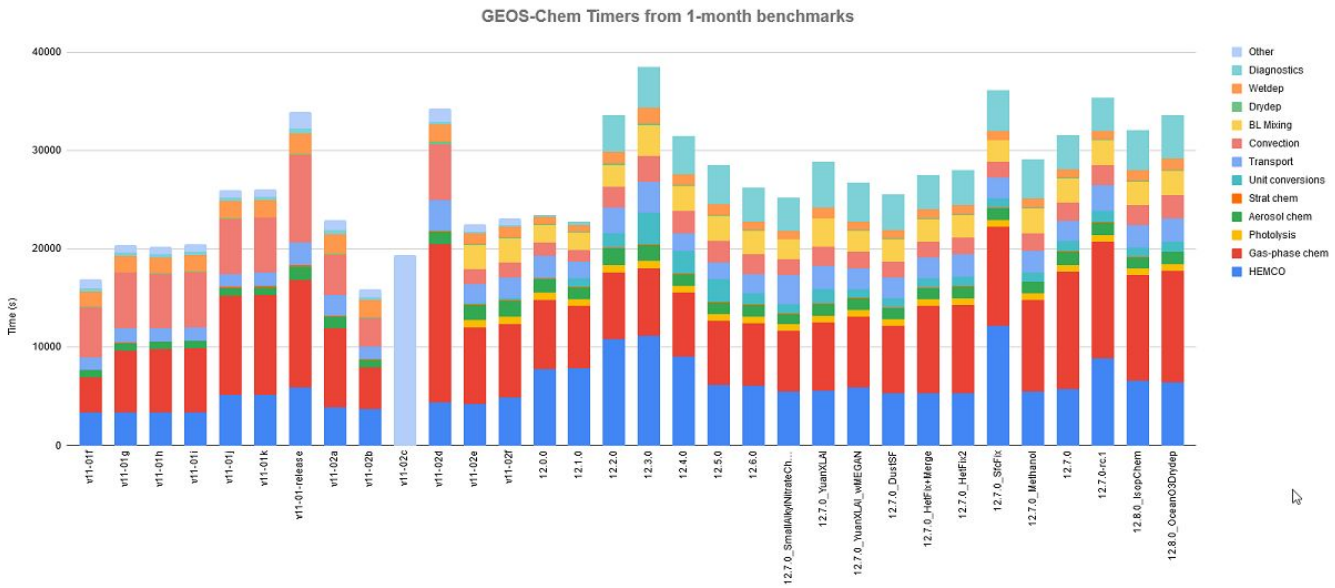
Feature or fix in version 12.9.0	Authors
Updated halogen chemistry	Xuan Wang, Harvard
Improved cloud water pH	Viral Shah, Harvard Jonathan Moch, Harvard
Update lightning data through Dec 2019	Lee Murray, Rochester
Convert GEOS-Chem species database to YAML format	Bob Yantosca, GCST Melissa Sulprizio, GCST
Properly apply masks and scale factors to non-emissions data obtained from HEMCO	Lizzie Lundgren, GCST

For more information about the updates in GEOS-Chem 12.9.0, please click here.

GEOS-Chem performance

This GEOS-Chem Support Team has been tracking model performance using the GEOS-Chem timers feature introduced in v11-01f. The wall time by model components for public and internal 1-month benchmark simulations are shown in the stacked bar chart below. Some differences in wall time may be attributed to performance issues on Harvard's cluster, but these have been avoided when possible by running on all 24 CPUs of a dedicated node.

The largest changes in wall time can be attributed to HEMCO and gas-phase chemistry. The switch from BPCH to netCDF diagnostics in 12.2.0 introduced a large increase in the diagnostic wall time; however, it's important to note that the benchmark simulations save out many more diagnostics than needed by the typical user. Changes in HEMCO wall time may generally be attributed to the introduction of newer emissions inventories and non-emissions datasets available at high spatial and temporal frequency. Changes in gas-phase chemistry can often be attributed to major changes in the chemistry mechanism (e.g. halogen chemistry). In GEOS-Chem 12.8.1, several new timers have been introduced in the gas-phase chemistry (i.e. FlexChem) component to further diagnose the changes to wall time in that component. See slides 30-44 of this presentation for a breakdown of updates that caused discernable jumps in the wall times.



GEOS-Chem development news

This section contains information about ongoing software engineering efforts:

HEMCO restructuring

Lizzie Lundgren (GCST) and **Haipeng Lin** (Harvard) are leading the effort to restructure the HEMCO emissions component so that it is separate from GEOS-Chem and can be more easily implemented into external ESMs. This work will be ongoing and will involve the following:

1. Move HEMCO out of the GEOS-Chem source code repository and into its own Github repository. HEMCO will then become a Git submodule in GEOS-Chem. This work is complete and will be included in GEOS-Chem 13.0.0.

2. Move model-specific code (i.e. I/O, regridding, and model-to-HEMCO interfaces) into separate layers that can be turned on or off depending on which external model is being connected to HEMCO.

3. Implement an optional HEMCO intermediate grid on which masks and scale factors may be applied to emissions before emissions are regridded to the coarser model resolution.

Improving chemistry code and unifying offline simulations via the Kinetic Pre-Processor (KPP) solver

We have obtained funding from the EPA/STAR program to transform GEOS-Chem's existing chemistry mechanisms. This will allow us to improve and streamline the various chemistry mechanisms that are used in GEOS-Chem.

This work will entail the following:

- Clean up and optimization of the heterogeneous chemistry functions used by KPP (**Bob Yantosca**, GCST)
- Porting aerosol chemistry to the KPP solver as much as possible (Bob Yantosca, GCST)
- Unifying offline simulations via KPP chemistry mechanisms. For example, the CO2, CO, and CH4 specialty simulations can be combined into a single KPP mechanism.

This work will proceed once GEOS-Chem 12.9.0 (which contains a new Halogen chemistry mechanism) is stable.

Communications and media

GEOS-Chem narrative and new developments have been updated for version 12.8.0

The GEOS-Chem narrative description and GEOS-Chem new developments web pages are updated to highlight the contributions of individual developers to **GEOS-Chem 12.8.0**, which was the last version in which new science updates were introduced..

For more information, please follow these links:

1. http://www.geos-chem.org/geos_new_developments.html
2. http://www.geos-chem.org/geos_chem_narrative.html

We shall continue to update the GEOS-Chem narrative and GEOS-Chem new developments pages for every feature release (i.e. 12.9.0, 13.0.0, ...).

Sign up to receive notifications from the GEOS-Chem Github repository!

We would like to invite you to sign up for notifications from (aka “watch”) our GEOS-Chem Github repository (https://github.com/geoschem/geos-chem). This will ensure that you’ll receive notifications for all GEOS-Chem version releases. We also encourage you to watch any other GEOS-Chem-related repositories on GitHub that you are interested in. GCST member Lizzie Lundgren has prepared a video tutorial that will walk you through the process.

Our Youtube channel has more than 100 subscribers!

Our GEOS-Chem Youtube Channel recently broke the 100 subscriber mark! Thanks to all of you who have subscribed!.

Because we now have more than 100 subscribers, we have obtained a custom URL. You can now use **youtube.com/c/geoschem** to reach the site. Our prior redirect **youtube.geos-chem.org** now points to this new URL (for backwards compatibility).

If you have not yet subscribed to the GEOS-Chem Youtube Channel, we ask that you please take a moment to do so. Navigate to the site, click on the subscribe button, and also click on the bell icon. You will receive notifications every time we post a new GEOS-Chem tutorial video.

Thanks for your continued support of GEOS-Chem!
Happy modeling!

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