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1. Featured News

GEOS-Chem 14.0.0 release is delayed due to bug found in 13.4

We recently discovered a GEOS-Chem Classic coding error introduced in GEOS-Chem 13.4.0. This will delay the release of GEOS-Chem 14.0.0 so that the bug fix can be benchmarked.

The cause of this error---located in the pressure fixer module pjc_pfix_mod.F90---was that several variables were set to zero prior to assignment, inadvertently introducing changes to the model. This was part of an effort to remove numerical differences that were caused by parallelization and precision issues.

The impact of the pressure fixer changes are visible in the 13.4.0 benchmark plots but went under the radar due to other changes introduced in that version. It is most noticeable as an increase in tropospheric ozone over the poles in GC-Classic between 13.3.0 and 13.4.0 that is not present in GCHP. See plots here and here for the 13.4.0 1-month benchmark comparisons that show this.

We have implemented a fix for this issue (geoschem/geos-chem PR #1387), and are currently re-running the GEOS-Chem 14.0.0 benchmark simulations.

If you have been using GEOS-Chem versions 13.4.0 through 14.0.0-rc.2, we ask that you update to the official GEOS-Chem 14.0.0 release when it is ready. Alternatively, you may pull this fix into your 13.4.0 through 14.0.0-rc.2 code using:

```
cd GCClassic/src/GEOS-Chem
git checkout -b bugfix/revert-pressure-fixer
git pull origin 13.4.0+revert-pressure-fixer
```

We sincerely apologize for the inconvenience.

Features that will be introduced in GEOS-Chem 14.0.0

GEOS-Chem 14.0.0 is a major version release that will break backwards compatibility with the version 13 release series. For a complete list of all version updates, including bug fixes and links to more information per update, please see the GEOS-Chem 14.0.0 version table on the GEOS-Chem wiki.

Important new features that will be introduced in GEOS-Chem 14.0.0 include:
● GCHP simulations now yield identical results whether they are run as a single stage or are broken up in time, and GEOS-Chem Classic simulations now yield fewer differences if run in multiple segments. *(Lizzie Lundgren, Harvard)*

● The `input.geos` configuration file (text format) is replaced with `geoschem_config.yml` (YAML format), as described in the previous newsletter. *(Bob Yantosca, Harvard)*

● Instances of the concentration array `State_Chm%Species(I,J,L,N)` are changed to `State_Chm%Species(N)%Conc(I,J,L)`, as described in the previous newsletter. *(Lizzie Lundgren, Harvard)*

● The fullchem and Hg chemistry mechanisms are now rebuilt with KPP 2.5.0, a more recent version of *The Kinetic PreProcessor*. *(Haipeng Lin, Harvard; Rolf Sander, MPIC, Mainz; Bob Yantosca, Harvard)*

● Offline emissions are updated for soil NOx and biogenic VOCs *(Honggian Weng, PKU)*

● HEMCO is updated to version 3.5.0. *(GEOS-Chem Support Team)*

● Nested-grid boundary conditions now may be archived in the first simulation timestep. *(Eloïse Marais, U. College London)*

● Updates are included for coupling GEOS-Chem 14.0 with external models, including NASA GEOS ESM, CESM, and WRF (aka WRF-GC). *(Haipeng Lin, Harvard; Lizzie Lundgren, Harvard; Thibaud Fritz, MIT)*

● There is now an automated GEOS-Chem user registration system through run directory creation. *(Lucas Estrada, Harvard)*

● Bug fixes include:
  ○ Revert the GEOS-Chem Classic global pressure fixer to version 13.3. *(Lizzie Lundgren, Harvard)*
  ○ Fix compilation errors with the custom chemistry mechanism option *(Bob Yantosca, Harvard)*
  ○ Fix methanol dry deposition over oceans *(Lizzie Lundgren, Harvard; Kelvin Bates, Harvard)*
  ○ Resolution of outstanding issues with the Hg simulation via KPP *(Ari Feinberg, MIT; Viral Shah, GMAO)*

● Minor issues in run directory configuration files have been resolved:
  ○ CO2 simulations will now use the most recent CEDS emissions data. *(Bob Yantosca, Harvard)*
  ○ A typo in `HEMCO_Config.rc` for GCHP fullchem simulations is now fixed. *(Killian Murphy, York)*
  ○ Minor issues when creating run directories for GCAP2 meteorology are fixed *(Lee Murray, Rochester)*

● Several updates specifically for GCHP include:
  ○ Updated GMAO libraries, including from MAPL 2.6.3 to 2.18.3. *(Liam Bindle, WashU; Lizzie Lundgren, Harvard)*
○ Add the option to use cubed-sphere mass fluxes at c720 resolution. (Liam Bindle, WashU)
○ Add a fix for the scale factor error in the GCHP vertical mass flux diagnostic. (Liam Bindle, WashU)

**Updated documentation for GEOS-Chem and related software**

**Manuals for GEOS-Chem and related software are now at ReadTheDocs**

We now use ReadTheDocs to publish user manuals for GEOS-Chem and related software. ReadTheDocs is a flexible documentation system that allows you to view not only the current manual, but manuals for previous versions as well. You may also convert the documentation to one of several formats (PDF, HTML, e-Book) for off-line reading.

In anticipation of the GEOS-Chem 14.0.0 release, we have given the GEOS-Chem documentation a major overhaul! Important updates include:


- The GCHP user manual ([gchp.readthedocs.io](https://gchp.readthedocs.io)) has been updated with information for GCHP 14.0.0 and contains several expanded sections.

- The HEMCO manual has been migrated from the wiki to [hemco.readthedocs.io](https://hemco.readthedocs.io).

- Several GEOS-Chem Guides have been migrated from the wiki to the Supplemental Guides and Help & Reference sections of [geos-chem.readthedocs.io](https://geos-chem.readthedocs.io), [gchp.readthedocs.io](https://gchp.readthedocs.io), and [hemco.readthedocs.io](https://hemco.readthedocs.io). These include:
  ○ Work with netCDF files
  ○ Prepare COARDS-compliant netCDF files
  ○ Load requested libraries
  ○ Build libraries with Spack
  ○ Debug GEOS-Chem and HEMCO errors
  ○ View GEOS-Chem species properties
  ○ Update chemical mechanisms with KPP (formerly at kpp.readthedocs.io)
  ○ View related documentation
  ○ Contributing guidelines
  ○ Support guidelines

The old wiki pages now contain links to the updated content at ReadTheDocs.
All other GEOS-Chem-related information (except the ReadTheDocs documentation described above) will remain at the GEOS-Chem web site and GEOS-Chem wiki. GEOS-Chem support issues will remain on Github.

Information about software maintained by GEOS-Chem users

We have recently compiled a list of software tools maintained by GEOS-Chem users. These include tools for data assimilation, pre-processing input files, post-processing GEOS-Chem output, etc.

The GCST takes no responsibility for these tools (other than maintaining this list). If you should encounter problems with the tools and/or documentation, please contact the listed maintainer(s) directly.

If you would like to add your software package to the list, please contact the GEOS-Chem Support Team at geos-chem-support@g.harvard.edu. This list is now linked from the front page of the GEOS-Chem wiki and from the “Software Tools” menu of the GEOS-Chem web site.

GEOS-Chem user registration

Lucas Estrada (Harvard) has implemented an automated GEOS-Chem user registration system into GEOS-Chem 14.0.0. The first time you create a run directory with GEOS-Chem or GCHP on a new system, you will be asked to provide your name, email, institution, and how you plan to use GEOS-Chem. This information will be kept on a secure cloud-based database (only accessible by the GCST) and will help us to keep an accurate record of GEOS-Chem users worldwide.

2. List of recent GEOS-Chem publications

Here is a list of the most recent GEOS-Chem publications. We strongly recommend that you browse through this list to keep up with what is happening in the GEOS-Chem world that may be relevant to your research.

For the complete list (with links to each article), please visit our GEOS-Chem Publications Page on Google Scholar. This page is generously maintained by GEOS-Chem user Gongda Lu (gongda.lu@ucl.ac.uk). If you find that any of your GEOS-Chem co-authored papers are missing from the Scholar page, please email Gongda with the title of the publication.


● Statistical and machine learning methods for evaluating trends in air quality under changing meteorological conditions, M Qiu, C Zigler, NE Selin, Atmospheric Chemistry and Physics, 22 (16), 10551-10566, 1, 2022.


● Integrated Methane Inversion (IMI 1.0): A user-friendly, cloud-based facility for inferring high-resolution methane emissions from TROPOMI satellite observations, DJ Varon, DJ Jacob, M Sulprizio, LA Estrada, WB Downs, L Shen, et al., Geoscientific Model Development, 15 (14), 5787-5805, 2022.


● Contributions of Various Sources to the Higher-Concentration Center of CO within the ASM Anticyclone Based on GEOS-Chem Simulations, Y Yang, Q Li, H Wang, Z Bai, D Li, W Wang, J Bian, Remote Sensing, 14 (14), 3322, 2022.


● A New Chemistry-Climate Model GRIMs-CCM: Model Evaluation of Interactive Chemistry-Meteorology Simulations, S Lee, RJ Park, SY Hong, MS Koo, JI Jeong, SW Yeh, SW Son, Asia-Pacific Journal of Atmospheric Sciences, 1-20, 2022.


● **Burden of diseases in fifty-three urban agglomerations of India due to particulate matter (PM$_{2.5}$) exposure**, P Shende, A Qureshi, *Environmental Engineering Research* 27 (3), 2022.


● **The 2019 methane budget and uncertainties at 1° resolution and each country through Bayesian integration Of GOSAT total column methane data and a priori inventory estimates**, JR Worden, DH Cusworth, Z Qu, Y Yin, Z Zhang, AA Bloom, S Ma, et al., *Atmospheric Chemistry and Physics*, 22 (10), 6811-6841, 2022.

● **The toxicity emissions and spatialized health risks of heavy metals in PM2.5 from biomass fuels burning**, J Wu, S Kong, Y Yan, Y Cheng, Q Yan, D Liu, S Wang, X Zhang, S Qi, *Atmospheric Environment*, 119178, 2022.


● **4D-Var Inversion of European NH$_3$ Emissions Using CrIS NH$_3$ Measurements and GEOS-Chem Adjoint With Bi-Directional and Uni-Directional Flux Schemes**, H Cao, DK Henze, L Zhu, MW


- Benefits of refined NH3 emission controls on PM2.5 mitigation in Central China, Z Zhang, Y Yan, S Kong, Q Deng, S Qin, L Yao, T Zhao, S Qi, *Science of The Total Environment*, 814, 151957, 2022.


3. GEOS-Chem Version Releases

Since our last newsletter, the following GEOS-Chem versions have been released:

GEOS-Chem 13.4.1

Release Date: 19 May 2022

GEOS-Chem 13.4.1 contains the following updates:

- Bug fixes in masking the anthropogenic CH₄ emissions over US, Canada, and Mexico for the CH₄ simulation only (Melissa Sulprizio, Harvard)

Please see the following pages for details on these updates, including benchmarks:

- 13.4.1 wiki page
- 13.4.1 Github milestone for geoschem/geos-chem

GEOS-Chem 13.4.0

Release Date: 02 May 2022

GEOS-Chem 13.4.0 contains the following updates:

- Disable sea salt debromination by default (Mike Long, GMAO; Viral Shah, GMAO)
- Migrated sulfate chemistry to KPP (Mike Long, Harvard; Viral Shah, GMA; Bob Yantosca, Harvard)
- Increased surface resistance for O₃ dry deposition on ice/snow (Ryan Pound, York; Shuting Zhai, UW)
- Benchmarks now use degassing-only volcano climatology (Christoph Keller, GMAO; Daniel Jacob, Harvard)
- Updated Rn$^{222}$ emissions from Zhang et al. (2021) (Bo Zhang, NIA; Hongyu Liu, NIA)
- Updates for automated run-directory creation (Liam Bindle, WashU; Melissa Sulprizio, Harvard)
- Updated Hg simulation via KPP following Shah et al. (2021) (Viral Shah, GMAO; Colin Thackray, Harvard; Bob Yantosca, Harvard; Ari Feinberg, MIT)
- Bug fixes for HCl uptake on seasalt and Henry's law computation in hetchem (Viral Shah, GMAO)
- HEMCO has been updated to version 3.4.0 (GEOS-Chem Support Team)
- Update AEIC aircraft emission to AEIC2019 (Seb Eastham, MIT; Thibaud Fritz, MIT)

Please see the following pages for details on these updates:

- 13.4.0 wiki page
- 13.4.0 Github milestone for geoschem/geos-chem
- 3.4.0 Github milestone for geoschem/HEMCO

Please note that we have identified a bug introduced in GEOS-Chem 13.4.0 that will be corrected in 14.0.0. If you are using GEOS-Chem versions 13.4.0 or 13.4.1 we ask that you update to the official GEOS-Chem 14.0.0 release when it is ready.

4. Model development priorities

**GEOS-Chem 14.1.0**

The following important updates (requested by the GEOS-Chem user community and prioritized by the GEOS-Chem Steering Committee) are slated to be introduced in GEOS-Chem 14.1.0:

**Emissions updates**

- Climatologies for open fire (Melissa Sulprizio, Harvard)
- Climatology for lightning NOx (Lee Murray, Rochester)
- AMAP Hg emissions following Steenhuizen et al (2022) (Helené Angot, MIT; Ari Feinberg, MIT; Noelle Selin, MIT)
- Bug fix for GFAS emissions in GCHP (Lizzie Lundgren, Harvard)
- Add HTAPv3 as an optional global emissions inventory (Dandan Zhang, WashU)

**Chemistry updates**

- TOMAS microphysics in GCHP (Betty Croft, WashU; Jourdan He, WashU)
• New carbon cycle (CH4-CO2-OCS) simulation via KPP (Beata Bukosa, NIWA; Kevin Bowman, JPL; Mike Long, GMAO)

• Updated chemical mechanism solver code with KPP 3.0.0 as documented in Lin et al. (2022) (Mike Long, GMAO; Haipeng Lin, Harvard; Bob Yantosca, Harvard); Lu Shen, PKU; Rolf Sander, MPIC Mainz)

• Adaptive solver option following Lin et al. (2022) (Haipeng Lin (Harvard))

• Furans chemistry following Carter et al. (2022) (Colette Heald, MIT; Jessica Haskins, MIT; Therese Carter, MIT)

• Nitrate photolysis from Shah et al. (2022) (optional) (Viral Shah, GMAO)

• Update Hg0 dry deposition from Feinberg et al. (2022) (Ari Feinberg, MIT; Noelle Selin, MIT; Thandolwethu Dlamini, MIT; Martin Jiskra, UBasel; Viral Shah, GMAO)

• Fix for ETO -> HO2 + 2CH2O reaction rate (Kelvin Bates, Harvard)

• Fix for HOBr + SO2 and HOCl + SO2 reactions (Xuan Wang, CUHK)

• Add MO2 + NO3 reaction (Kelvin Bates, Harvard)

Diagnostic updates

• New diagnostic for production of RO2 (Melissa Sulprizio, Harvard)

• New diagnostic for species concentration in molec/cm3 (Haipeng Lin, Harvard)

• Satellite diagnostic in netCDF (and removing ND50, ND51 bpch diagnostics) (Eloïse Marais, U. College London)

Structural updates

• Identify and remove memory leaks and similar issues (Bob Yantosca, Harvard)

• Update TransportTracers simulation for consistency with the NASA GEOS ESM (Melissa Sulprizio, Harvard)

• Use pointers to MAPL internal state for species arrays in GCHP/GEOS (Lizzie Lundgren, Harvard)

We anticipate a GEOS-Chem 14.1.0 code freeze in mid-November. Any items on this list that are not implemented by this date will be slated for version 14.2.0.

Other updates slated for inclusion into GEOS-Chem

The GEOS-Chem Steering Committee regularly prioritizes science updates for inclusion into GEOS-Chem. Please view our Model Development Priorities wiki page to view a list of prioritized updates as of this writing. The current list reflects priorities that were assigned at the IGC10 meeting in June 2022.

We encourage you to bring new GEOS-Chem developments to the attention of the relevant Working Group Chair(s) for addition to the model development priorities list.
5. Steering Committee News

Presentations from IGC10 are now online

To view presentations and clinics from the recent IGC10 meeting (held at Washington University in St. Louis this past June), please visit igc10.geos-chem.org.

Working Group reorganization

The following updates to Working Groups were approved at the GEOS-Chem Steering Committee (GCSC) meeting (held at the IGC10 meeting in St. Louis).

- A standalone Emissions Working Group was created from the former Emissions and Deposition Working Group.
  - Co-chairs: Lyatt Jaeglé, Jintai Lin, and Eloïse Marais.
- A new Chemistry-Climate Working Group was created from the former Chemistry-Ecosystems-Climate Working Group.
  - Co-chairs: Hong Liao and Lee Murray.
- A new Surface-Atmosphere Exchange Working Group has been created. Deposition and Ecosystems now fall under the purview of this working group.
  - Co-chairs: Jeff Geddes, Chris Holmes, Dylan Millet, and Amos Tai.

As always, we encourage you to join the Working Group(s) that corresponds to your area(s) of research by signing up for the relevant Working Group email list(s).

New GEOS-Chem Steering Committee members

Please join us in welcoming the following new GCSC members!

- Hannah Horowitz (UIUC) will co-chair the Hg and POPs Working Group with Jenny Fisher and Yanxu Zhang.
- Lyatt Jaeglé (UW) will co-chair the Emissions Working Group with Jintai Lin and Eloïse Marais.
- Katie Travis (NASA/LaRC) will co-chair the Transport Working Group with Clara Orbe and Andrew Schuh.
Notes from the most recent Steering Committee meeting

The GEOS-Chem Steering Committee met on 21 September 2022. We invite you to read the meeting minutes as well as the following related presentations:

- Update from the Chemistry-Climate Working Group -- see the GCSC meeting minutes
- Update from the Surface-Atmosphere Exchange Working Group

6. Support Team News

Jourdan He and Saptarshi Sinha joined the GCST this summer. They will be working with Randall Martin’s group at Washington University in St. Louis. Please join us in welcoming Jourdan and Saptarshi to the team!

Lucas Estrada left full-time status on the GCST on September 1st---but he hasn’t gone far! Lucas is now a first-year graduate student in Daniel Jacob’s research group at Harvard University and will continue to contribute to GEOS-Chem Support Team activities on a consulting basis.

Liam Bindle will be leaving the GCST in October, as he has accepted a new position in Vancouver, Canada. Yanshun Li will be stepping back from his GCST duties (processing and archiving met fields to disk) in order to focus on his Ph.D. thesis at Washington University in St. Louis. We would like to thank Liam and Yanshun for their tremendous contributions to GEOS-Chem. Thank you for all of your hard work and best of luck in your new endeavors!

Thanks for your continued support of GEOS-Chem!

Happy modeling!

The GEOS-Chem Support Team:
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