Newsletter 2022, Issue 1

24 Feb 2022

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1. Featured News

Registration is now open for IGC10 (June 7-10, 2022)

We cordially invite you to attend **IGC10** (The 10th International GEOS-Chem Meeting), which will be held **at Washington University in St. Louis from June 7-10, 2022**. The meeting style will be primarily in-person, while offering some hybrid capability for those unable to travel.

The scope of IGC10 encompasses all topics of research in atmospheric composition. All research scientists, students, and stakeholders worldwide are welcome to attend and contribute presentations. For GEOS-Chem users, the meeting will provide a platform for sharing information about the model and learning about new model developments. Working Group breakouts will focus on specific aspects of the model.

Several GEOS-Chem Clinics will be offered on June 6, 2022 (the day prior to IGC10 kick-off). The clinics will benefit both novice and experienced users who wish to become more familiar with the workflow of running GEOS-Chem simulations. Holding all of the clinics on the same day will allow sufficient time for demonstrations and Q&A sessions.

Registration will remain open through March 31, 2022. To register, please visit the official IGC10 website: **https://igc10-2022.wustl.edu**. Information about lodging will be posted at the IGC10 web site in the coming weeks.

Nested grid simulation issue in 12.9.0 through 13.0.2

An update to the HEMCO time cycle flags in GEOS-Chem 12.9.0 caused the boundary conditions in nested grid simulations to only update once at the beginning of the simulation. In GEOS-Chem 13.1.0, this issue was resolved by changing the time cycle flag in HEMCO_Config.rc from “EF” to “EFY” to ensure the boundary conditions are updated continuously. See Github issue #700 for more details. ***If you are using a nested grid simulation with any of these GEOS-Chem versions, you should update to GEOS-Chem 13.1.0 or later.***

Integrated Methane Inversion capability

The **Integrated Methane Inversion (IMI)** is a user-friendly, cloud-based facility for estimating regional methane emissions by analytical inversion of satellite observations from the TROPOspheric Monitoring Instrument (TROPOMI). It enables researchers and stakeholders to infer methane emissions at up to 0.25° × 0.3125° resolution from TROPOMI satellite data resident on the Amazon Web Services (AWS) cloud, without requiring expert knowledge of inverse methods or cumbersome data download.

The IMI uses the GEOS-Chem 3-D chemical transport model, also resident on AWS, as the forward model for the inversion.

Key resources for getting started (including links to the source code repository and documentation page) can be found on the IMI website. If you are interested in beta-testing the IMI, please contact **Daniel Varon** (danielvaron@g.harvard.edu).

Reference: Varon, D.J., D.J. Jacob, M. Sulprizio, L.A. Estrada, W.B. Downs, L. Shen, S.E. Hancock, H. Nesser, Z. Qu, E. Penn, Z. Chen, X. Lu, A. Lorente, A. Tewari, and C.A. Randles, *Integrated Methane Inversion (IMI 1.0): A user-friendly, cloud-based facility for inferring high-resolution methane emissions from TROPOMI satellite observations*, submitted to Geophys. Model Dev., 2022.

Updated mercury simulation (as a KPP mechanism)

GEOS-Chem 13.4.0 will contain an updated mechanism for $Hg^0/Hg^I/Hg^{II}$ atmospheric cycling, based on the work of Shah et al [2021]. Unlike prior versions of the mercury simulation, the Shah et al [2021] mechanism is implemented via the Kinetic PreProcessor (KPP), which makes the mechanism easier to maintain and update.

This mercury simulation in GEOS-Chem 13.4.0 is currently being validated by the GEOS-Chem Hg and POPs working group. Until this validation is completed, we ask interested GEOS-Chem users to continue using the standard mercury simulation. Fixes for bugs or other issues discovered during validation will be added to GEOS-Chem patch versions (such as 13.4.1, 13.4.2, etc.).

Reference: Shah, V., D.J. Jacob, C.P. Thackray, X. Wang, E.M. Sunderland, T.S. Dibble, A. Saiz-Lopez, I. Cernusak, V. Kello, P.J. Castro, R. Wu, and C. Wang, *Improved mechanistic model of the atmospheric redox chemistry of mercury*, Environ. Sci. Technol., 55, 14445-14456, 2021.

Managing input data with the bashdatacatalog

The **bashdatacatalog** is a command-line utility that will help users download and manage input data for GC-Classic and GCHP. This command-line tool can perform operations such as:

- listing the input files for a specific version of GEOS-Chem (X.Y version specific)
- customization to include data collections for optional emissions and specialty simulations
- filtering by date range (e.g., files needed for 2015-2019, or for 2018-03-01 onwards)
- local input data management for:
    a. listing missing files (i.e., needed but absent),
    b. listing files that are corrupt (local files with an incorrect checksum), and

    c. listing files that are unnecessary for a given date range
- creating file lists for passing to other tools:
    a. downloading input data with cURL, wget, or Globus,
    b. transfering data with rsync (locally or via SSH),
    c. executing commands on every file (e.g., for file sizes, changing permissions, etc.)
    d. your own reference

The bashdatacatalog was developed to help GEOS-Chem users download and manage input data, but it is a general purpose data catalog. Users might find the bashdatacatalog useful for keeping track of internal data collections (e.g., observations or custom emissions inventories), transferring large datasets over SSH, or for distributing their own data products. Those interested are welcome to contact GEOS-Chem Support Team member **Liam Bindle** (liam.bindle@wustl.edu) for instructions on setting up data collections.

The bashdatacatalog has an automatic installer and the only dependency is bash, which all major Linux distros have by default (macOS has bash too). The initial version of the **bashdatacatalog, v0.1.0, will be released on February 28th, 2022**. Here is the link to the Instructions for GEOS-Chem Users.

2. List of recent GEOS-Chem publications

Here is a list of the most recent GEOS-Chem publications. For the complete list (with links to each article), please visit our GEOS-Chem Publications Page on Google Scholar.

The Google Scholar page is generously maintained by GEOS-Chem user **Gongda Lu** (gxl642@student.bham.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.

- U.D. Baruah, S.M. Robeson, A. Saikia, N. Mili, K. Sung, P. Chand, *Spatio-temporal characterization of tropospheric ozone and its precursor pollutants NO2 and HCHO over South Asia*, Science of The Total Environment, 809, 151135, 2022.

- H. Tan, L. Zhang, X. Lu, Y. Zhao, B. Yao, R.J. Parker, H. Boesch, *An integrated analysis of contemporary methane emissions and concentration trends over China using in situ and satellite observations and model simulations*, Atmospheric Chemistry and Physics, 22 (2), 1229-1249, 2022.

- H. Zhang, J. Wang, L.C. García, M. Zhou, C. Ge, T. Plessel, J. Szykman, R.C. Levy, B. Murphy, T.L. Spero, *Improving Surface PM2.5 Forecasts in the United States Using an Ensemble of Chemical Transport Model Outputs: 2. Bias Correction With Satellite Data for Rural Areas*, Journal of Geophysical Research: Atmospheres, 127 (1), e2021JD035563, 2022.

- A. Zammit-Mangion, M. Bertolacci, J. Fisher, A. Stavert, M. Rigby, Y. Cao, N. Cressie, *WOMBAT v1. 0: a fully Bayesian global flux-inversion framework*, Geoscientific Model Development, 15 (1), 45-73, 2022.
- W. Peng, C. Le, W.C. Porter, D.R. Cocker III, *Variability in Aromatic Aerosol Yields under Very Low NOx Conditions at Different HO2/RO2 Regimes*, Environmental Science & Technology, 2022
- M.J. Cooper, R.V. Martin, M.S. Hammer, P.F. Levelt, P. Veefkind, L.N. Lamsal, N.A. Krotkov, J.R. Brook, C.A. McLinden, *Global fine-scale changes in ambient NO2 during COVID-19 lockdowns*, Nature, 601 (7893), 380-387, 2022.
- Q. Yan, S. Kong, Y. Yan, X. Liu, S. Zheng, S. Qin, F. Wu, Z. Niu, H. Zheng, et al., *Emission and spatialized health risks for trace elements from domestic coal burning in China*, Environment International, 158, 107001, 2022.
- X. Yu, D.B. Millet, D.K. Henze, *How well can inverse analyses of high-resolution satellite data resolve heterogeneous methane fluxes? Observing system simulation experiments with the GEOS-Chem adjoint model (v35)*, Geoscientific Model Development, 14 (12), 7775-7793, 2021.
- Y. Sun, H. Yin, X. Lu, J. Notholt, M. Palm, C. Liu, Y. Tian, B. Zheng, *The drivers and health risks of unexpected surface ozone enhancements over the Sichuan Basin, China, in 2020*, Atmospheric Chemistry and Physics, 21 (24), 18589-18608 2, 2021.
- K.H. Bates, D.J. Jacob, K. Li, P.D. Ivatt, M.J. Evans, Y. Yan, J. Lin, *Development and evaluation of a new compact mechanism for aromatic oxidation in atmospheric models*, Atmospheric Chemistry and Physics, 21 (24), 18351-18374, 3, 2021.
- X. Liu, A.P.K. Tai, Y. Chen, L. Zhang, G. Shaddick, X. Yan, H.M. Lam, *Dietary shifts can reduce premature deaths related to particulate matter pollution in China*, Nature Food, 1-8, 2021.
- S. Baray, D.J. Jacob, J.D. Maasakkers, J.X. Sheng, M.P. Sulprizio, D. Jones, A.A. Bloom, R. McLaren, *Estimating 2010–2015 anthropogenic and natural methane emissions in Canada using ECCC surface and GOSAT satellite observations*, Atmospheric Chemistry and Physics, 21 (23), 18101-18121, 10, 2021.
- M.O. Nawaz, D.K. Henze, C. Harkins, H. Cao, B. Nault, D. Jo, J. Jimenez, S. C. Anenberg, D. L. Goldberg, Z. Qu, *Impacts of sectoral, regional, species, and day-specific emissions on air pollution and public health in Washington, DC*, Elementa, 9 (1), 2021.
- E. Brattich, H. Liu, B. Zhang, M.Á. Hernández-Ceballos, J. Paatero, D. Sarvan, V. Djurdjevic, L. Tositti, J. Ajtić, *Observation and modeling of high-7Be concentration events at the surface in northern Europe associated with the instability of the Arctic polar vortex in early 2003*, Atmospheric Chemistry and Physics, 21 (23), 17927-17951, 2, 2021.
- N. Zeng, P. Han, Z. Liu, D. Liu, T. Oda, C. Martin, Z. Liu, B. Yao, W. Sun, P. Wang, *Global to local impacts on atmospheric CO2 from the COVID-19 lockdown, biosphere and weather variabilities*, Environmental Research Letters, 17, 2021.

- X. Jiao, R. Ni, L. Chen, J.A. Adeniran, H. Weng, J. Wang, Y. Chen, S. Ren, X. Liu, *Environmental Benefits of Ultra-Low Emission (ULE) Technology Applied in China*, Atmosphere, 12 (12), 1693, 2021.

- R. Tian, X. Ma, T. Sha, X. Pan, Z. Wang, *Exploring dust heterogeneous chemistry over China: Insights from field observation and GEOS-Chem simulation*, Science of The Total Environment, 798, 149307, 1, 2021.

- H. Yin, X. Lu, Y. Sun, K. Li, M.Gao, B. Zheng, C. Liu,*Unprecedented decline in summertime surface ozone over eastern China in 2020 comparably attributable to anthropogenic emission reductions and meteorology*, Environmental Research Letters, 2, 2021.

- S. Zhai, D.J. Jacob, J.F. Brewer, K. Li, J.M. Moch, J. Kim, S. Lee, H. Lim, H.C. Lee, et al., *Relating geostationary satellite measurements of aerosol optical depth (AOD) over East Asia to fine particulate matter (PM2.5): insights from the KORUS-AQ aircraft campaign and GEOS-Chem model simulations*, Atmospheric Chemistry and Physics, 21 (22), 16775-16791, 1, 2021.

- P.I. Palmer, L. Feng, M.F. Lunt, R.J. Parker, H. Bösch, X. Lan, A. Lorente, T. Borsdorff, *The added value of satellite observations of methane for understanding the contemporary methane budge*t, Philosophical Transactions of the Royal Society A, 379 (2210), 20210106, 2, 2021.

- A.Y.H. Wong and J.A. Geddes, *Examining the competing effects of contemporary land management vs. land cover changes on global air quality*, Atmospheric Chemistry and Physics, 21 (21), 16479-16497, 2021.

- Hammer, M. S., van Donkelaar, A., Martin, R. V., McDuffie, E. E., Lyapustin, A., Sayer, A. M., Hsu, N. C., Levy, R. C., Garay, M. J., Kalashnikova, O. V. and Kahn, R. A., *Effects of COVID-19 lockdowns on fine particulate matter concentrations*, Sci. Adv., 2021.

- McDuffie, E. E., Martin, R. V., Spadaro, J. V., Burnett, R., Smith, S. J., O'Rourke, P., Hammer, M. S., van Donkelaar, A., Bindle, L., Shah, V., Jaeglé, L., Luo, G., Yu, F, Adeniran, J. A., Lin, J. and Brauer, M., Source sector and fuel contributions to ambient PM2.5 and attributable mortality across multiple spatial scales., Nat. Commun. 2021.

- Meng, J., R. V. Martin, P. Ginoux, M. Hammer, M. P. Sulprizio, D. A. Ridley, and A. van Donkelaar (2021), *Grid-independent high-resolution dust emissions (v1.0) for chemical transport models: application to GEOS-Chem (12.5.0*), Geosci. Model Dev., 14(7), 4249-4260, 2021.

- van Donkelaar, A., M. S. Hammer, L. Bindle, M. Brauer, J. R. Brook, M. J. Garay, N. C. Hsu, O. V. Kalashnikova, R. A. Kahn, C. Lee, R. C. Levy, A. Lyapustin, A. M. Sayer, and R. V. Martin, *Monthly Global Estimates of Fine Particulate Matter and Their Uncertainty*, Environmental Science & Technology, 2021.

3. GEOS-Chem Version Releases

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

GEOS-Chem 13.3.3

Release Date: 02 Dec 2021

GEOS-Chem 13.3.3 contains the following updates:

- Upgrade to HEMCO version 3.2.2, which restores updating of manual diagnostics.
    - This had been inadvertently clobbered during a Git merge.
    - NOTE: This update affects CH4, Hg, and TOMAS simulations, as well as the MEGAN ISOP emissions, which use manual diagnostics internally.

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

- 13.3.3 wiki page
- 3.2.2 Github milestone for geoschem/HEMCO

GEOS-Chem 13.3.4

Release Date: 07 Dec 2021

***** THIS IS THE CURRENT STABLE GEOS-CHEM VERSION *****

GEOS-Chem 13.3.4 contains the following bug fixes:

- Bug fix: Now use proper restart file path for dry-run data download
- Bug fix: Now check GEOS-Chem Classic History diagnostic subset regions properly

Please see the following pages for details on these updates:

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

4. Model development priorities

GEOS-Chem 13.4.0

As of this writing, GEOS-Chem 13.4.0 is undergoing the benchmark review process. This version will include many important updates which had been requested by the GEOS-Chem user community, including:

- Migrating sulfate in-cloud and on-aerosol chemistry into the KPP fullchem mechanism
- Updated Hg chemistry implemented as a KPP mechanism (as noted above)
- Bug fixes in heterogeneous chemistry computations
- Updated surface resistance for O3 dry deposition on ice/snow
- Updated emissions for the CH4 and TransportTracers specialty simulations
- Unit conversion scale factor fixes for VOC species in the AEIC aircraft inventory
- Option to drive GEOS-Chem and GCHP with native meteorological data
- Ability to drive GCHP with mass fluxes on the cubed-sphere grid instead of winds
- GCHP advection now uses total pressure instead of dry pressure
- Updates to facilitate automatic run-directory generation
- Diagnostic updates for both GEOS-Chem Classic and GCHP
- Updates for compatibility of GEOS-Chem in GEOS

During the 13.4.0 benchmark review process, it was discovered that ozone concentrations in the southern hemisphere are much too low. We attribute this change to bromine chemistry; recent bug fixes have caused BrO to increase substantially. We will seek to rectify this situation by turning off sea salt debromination, which should reduce bromine species concentrations, and thus should restore ozone concentrations to normal levels. (We will leave sea salt debromination as an option that can be toggled by users if so desired for research purposes.)

A new round of benchmarking for GEOS-Chem 13.4.0 will be conducted and the results evaluated. This will push back the release timetable of both GEOS-Chem 13.4.0 by several weeks.

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.

We hope to be able to incorporate several of the remaining prioritized items into GEOS-Chem 14.0.0, which will be a major version release later this year. We will have more information about GEOS-Chem 14.0.0 in the months ahead.

The GEOS-Chem Steering Committee will meet at IGC10 (June 2022) to revise the list of model development priorities for the next two years going forward. There have been many exciting recent developments that need to be incorporated into GEOS-Chem and we look forward to adding these into subsequent model versions.

5. Ongoing Development

Infrastructure for automatic benchmarking

GCST members **Liam Bindle** and **Lucas Estrada** have created an infrastructure for running automated GEOS-Chem benchmarks on either the AWS EC2 cloud computing platform, or on the Wash U. Compute1 server. Benchmark output will be archived in an AWS S3 bucket, and a database of all submitted runs will be automatically updated. These improvements should substantially reduce the amount of manual work that the GEOS-Chem Support Team must do in order to run benchmark simulations and to generate the benchmark plots and tables.

Retiring input.geos in favor of a YAML format configuration file

Discussions between the GEOS-Chem Support Team and NASA GMAO have concluded that the name of the **input.geos** configuration file used in GEOS-Chem can be confusing since it implies configurations for inputs to the NASA GEOS ESM. The file instead contains primarily run-time switches and parameter values, not inputs, and is for GEOS-Chem, not GEOS. It is especially confusing within GEOS since all GEOS-Chem configuration files are stored in the same directory as other GEOS configuration files. For the sake of clarity, we propose retiring the input.geos file and replacing it with a configuration file in YAML format (which is the same format used for the GEOS-Chem Species database file).

Bob Yantosca has started on this update, which will be introduced into major version release 14.0.0. For more information, please see Github discussion geoschem/geos-chem #1111.

Unified mechanism for CO-CO2-CH4-OCS chemistry

One of the items on our to-do list is to combine the individual carbon-cycle specialty simulations into a unified chemistry mechanism, implemented via the Kinetic PreProcessor (KPP). This will build upon work previously done by **Beata Bukosa** (U. Wollongong and NIWA).

We hope to be able to have this ready soon, perhaps by the major version release of 14.0.0 (or if not, shortly thereafter). **Bob Yantosca** of the GCST will be performing this work.

Reference: B. Bukosa, J. Fisher, N. Deutscher, and D. Jones, *An improved carbon greenhouse gas simulation in GEOS-Chem version 12.1.1*, Geo. Model. Dev. Discuss., accepted, 2021.

Separating 4D species array into vector of 3D arrays

GCST member **Lizzie Lundgren** is working on a structural update to store species concentrations as one 3D array per species. The GEOS-Chem 14.0.0 major release will include this update with replacement of the existing 4D species concentration array with a vector of species objects containing the new 3D concentration arrays. Source code that previously looked like State_Chm%Species(I,J,L,N) will appear as State_Chm%Species(N)%Conc(I,J,L).

Users with their own development branches should take note of this change for the upcoming 14.0 release as they will need to make modifications in their code where they added or modified usages of State_Chm%Species. More information on this will be provided in the next newsletter accompanying the 14.0 release.

The motivation of this update is to reduce the memory requirement of GCHP and GEOS-Chem within GEOS when run at high resolution. Rather than store two copies of species concentrations, one in State_Chm and another in MAPL, we would like to store just one. Using 3D concentration arrays in State_Chm will allow using pointers rather than a copy to achieve this.

6. Steering Committee News

GEOS-Chem leadership news

Daniel Jacob is stepping down from the GEOS-Chem Model Scientist position, and former Co-Model Scientist **Randall Martin** is now Model Scientist. Daniel Jacob will remain in a supporting role as Co-Model Scientist.

Andrea Molod stepped down from the GEOS-Chem Steering Committee and has been replaced by **Clara Orbe** as Transport Working Group Co-Chair.

If you are potentially interested in serving on the GEOS-Chem Steering Committee, please see the GCSC functioning documentation to read about the required qualifications and expectations. If you are still interested we would love to hear from you, please contact Model Scientist Randall Martin (rvmartin@wustl.edu).

Notes from the most recent Steering Committee meeting

The GEOS-Chem Steering Committee met on **23 February 2022**. We invite you to read the meeting minutes as well as the following related presentations:

- Update from the Chemistry Working Group
- Update from the GCHP Working Group

- GCHP mass fluxes update presentation by Sebastian Eastham
- Bashdatacatalog and benchmarking on the AWS cloud presentation by Liam Bindle

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

The GEOS-Chem Support Team:
Bob, Melissa, Lizzie, Liam, Lucas, and Yanshun
geos-chem-support@g.harvard.edu