# GEOS-Chem Newsletter
# Winter 2017 Edition + v11-01 Public Release

*GEOS-Chem Support Team*
*01 February 2017*

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## GEOS-Chem v11-01 public release

### Overview

We would like to thank all of you who submitted fixes for bugs and other technical issues during the v11-01 provisional release period. **We are happy to announce that GEOS-Chem v11-01 is officially released!**

GEOS-Chem v11-01 contains all of the features contained in the v11-01 provisional release, including:

- Addition of the FlexChem / KPP solver
- Complete removal of SMVGEAR and related legacy infrastructure
- Introduction of the GEOS-Chem species database
- Consistent physical properties for GEOS-Chem species
- Update to HEMCO v2.0
- Updated treatment of moisture in unit conversions and tracer concentrations
- Support for GNU Fortran Compiler and GNU Profiler
- netCDF I/O for GEOS-Chem restart files
- Updates to the specialty simulations (especially Hg)
- Fixes for bugs and technical issues in all areas of GEOS-Chem

User-submitted updates and fixes added during the provisional release period include:

| v11-01-Public-Release Feature | Type | Submitted by |
|---|---|---|
| Fixed incorrect timestamps in the GMI HCOOH stratospheric prod/loss file | Bug fix | Seb Eastham (Harvard) GCST |
| Turn on the traceback error output (i.e. set TRACEBACK=yes) by default | Structural | Seb Eastham (Harvard) GCST |
| Fixed a segmentation fault error in HEMCO v2.0 that was caused by an Intel Fortran compiler bug | Bug fix | Bob Yantosca (GCST) |
| GEOS-Chem error messages now advise the user to check the HEMCO log file | Structural | Bob Yantosca (GCST) |
| Fix for out-of-bounds error when using the brown carbon option | Bug fix | Melissa Sulprizio (GCST) |
| Bug fix: MAP_A2A now applies periodic boundary conditions only to global data sets during regridding | Bug fix | Seb Eastham (Harvard) GCST |
| Ocean grid boxes now use the timezone of the nearest land mass for computing emissions | Science | Seb Eastham (Harvard) |
| Bug fix for time interpolation in netCDF utility module_ncdf_mod.F90 | Bug fix | Christoph Keller (NASA/GSFC) Seb Eastham (Harvard) |
| Bug fix: Make sure nAdvect is initialized in EMISSCO2 | Bug fix | Bob Yantosca GCST |
| Fix units of O1D and O3P in ND43 diagnostic | Bug fix | Chris Holmes (Florida State) |
| Fix for compiling with CHEM=Custom | Bug fix | Prasad Kasibhatla (Duke) |

| v11-01-Public-Release Feature | Type | Submitted by |
|---|---|---|
| Print message to log file if OpenMP parallelization is turned off | Structural | Melissa Sulprizio (GCST) |
| Fix incorrect unit strings for ND65 diagnostic in diag3.F | Bug fix | Chris Holmes (Florida State)<br>Melissa Sulprizio (GCST) |
| Improve write speed of netCDF output files | Structural | Chris Holmes (Florida State) |
| GAMAP can now read GEOS-Chem restart files in netCDF format | Structural | Bob Yantosca (GCST) |
| Minor fix for ND68 entries in tracerinfo.dat | Bug fix | Melissa Sulprizio (GCST) |

For complete instructions on how to download and run GEOS-Chem v11-01 on your computer system, please see our GEOS-Chem Online User's Guide at **manual.geos-chem.org**.

## Validation

We have posted the results from the various benchmark simulations that were used to validate GEOS-Chem v11-01. For more information, please see:

- Comparing 1-year benchmark simulations for v10-01 and v11-01
- 1-year benchmark simulation for v11-01-public-release
- 1-month benchmark simulation for v11-01-public-release
- 7-day time test results (We encourage you to add your own results!)

## Selecting time steps for v11-01

Sajeev Phillip and Randall Martin recommend the following default GEOS-Chem timestep durations for future GC simulations when sufficient CPU resources are available:

> *Philip et al. (2016) examines the sensitivity of GEOS-Chem simulations to the duration of chemical and transport operators. Based on that study, we recommend chemical timesteps of* ***20 minutes*** *and transport timesteps of* ***10 minutes*** *for simulations when sufficient CPU resources are available. Fine horizontal resolution should take priority over fine temporal resolution. In some cases,* ***it may be beneficial to use coarser timesteps for initial simulations, and the recommended resolution (C20T10) for final simulations****. We encourage specification in publications of the duration of operators due to their effects on simulation accuracy.*

On 03 Feb 2016, the GEOS-Chem Steering Committee approved the optimal timestep settings recommended by Sajeev Philip and Randall Martin (listed above) for use with GEOS-Chem simulations.

****IMPORTANT**** In GEOS-Chem v11-01, this timestep configuration (C20T10) is included by default in the input files that ship with the GEOS-Chem Unit Tester. Running GEOS-Chem with the recommended time steps from S. Philip et al (2016) has been shown to increase run times with respect to v10-01 by approximately a factor of 2. To speed up GEOS-Chem simulations, users may choose to:

(1) RUN WITH COARSER TIMESTEPS FOR FASTER TURNAROUND AND LOWER ACCURACY.

Using these transport timesteps (as was done prior to v11-01) should speed up your simulation by a factor of 2:

| Resolution | Chemistry & Emissions Timesteps | Transport & Convection Timesteps |
|---|---|---|
| 4° x 5° | 60 minutes | 30 minutes |
| 2° x 2.5° | 30 minutes | 15 minutes |

(2) SELECT ONE OF THE MECHANISMS IN WHICH DETALED STRATOSPHERIC CHEMISTRY IS OMITTED.

- These are: Tropchem, SOA, SOA-SVPOA.

## GEOS-Chem v11-02 Development Overview

Because many of the updates that went into GEOS-Chem v11-01 required widespread structural changes to the code (e.g. FlexChem, species database, etc.), several important science updates had to be postponed to v11-02. Here is our current plan for adding these updates into v11-02. These may be subject to change depending on circumstances.

*NOTE: v11-02a, v11-02b, etc. denote our proposed 1-month benchmark simulations, which are designed to evaluate GEOS-Chem's performance at intermediate stages of development.*

## GEOS-Chem v11-02a

The following updates are planned for v11-02a. These are mostly chemistry updates plus a few minor structural updates and bug fixes.

| v11-02a Feature | Type | Submitted by |
|---|---|---|
| Updating chemistry rate constants based on *JPL Publication 15-10* | Science | Barron Henderson (U. Florida)<br>Mat Evans (U. York)<br>Oxidants and Chemistry WG |
| Fixes to correct ALK4 lumping issue | Science | Barron Henderson (US EPA) |
| PAN updates | Science | Emily Fischer (CSU) |
| Monthly mean NEI2011 emissions | Science | GCST |
| Implement ISORROPIA v2.0 as a Fortran module (eliminating `COMMON` blocks) | Structural | Seb Eastham (Harvard)<br>GCST |
| Update to HEMCO v2.0.004 | Structural | Christoph Keller (GMAO) |
| Fix error in production of SO4S and NITs in SEASALT_CHEM routine | Bug fix | Prasad Kasibhatla (Duke) |
| Fix bug in CHEM_NIT routine | Bug fix | Prasad Kasibhatla (Duke) |

## GEOS-Chem v11-02b

GEOS-Chem v11-02b will contain updates to the halogen chemistry and SOA mechanism.

| v11-02b Feature | Type | Submitted by |
|---|---|---|
| Halogen chemistry updates | Science | Tomás Sherwen (York)<br>Johan Schmidt (Harvard)<br>Oxidants and Chemistry WG |
| Enhance default GEOS-Chem simple SOA | Science | Aerosols Working Group |

## GEOS-Chem v11-02c

GEOS-Chem v11-02c will contain an updated isoprene chemistry. It will be benchmarked with both 1-month and 1-year simulations.

| v11-02c Feature | Type | Submitted by |
|---|---|---|
| Updates to isoprene chemistry, includes:<br>• Fast photolysis of carbonyl nitrates<br>• Aerosol uptake of organic nitrates | Science | Jenny Fisher (U. Wollongong)<br>Eloïse Marais (Harvard)<br>Kelvin Bates (Caltech)<br>Katie Travis (Harvard) |

## GEOS-Chem v11-02d

GEOS-Chem v11-02d will contain several aerosol updates, as well as an update for the UCX mechanism:

| v11-02d Feature | Type | Submitted by |
|---|---|---|
| Update density of BC to 1.8 and add absorption enhancement factor in input.geos | Science | Xuan Wang (MIT) |
| Add aqueous isoprene uptake to SOA scheme | Science | Eloise Marais (Harvard) |
| Monthly mean surface methane distributions | Science | Lee Murray (NASA GISS/LDEO) |
| Radon flux diagnostic | Benchmark | GCST |
| UCX stratospheric water boundary condition update | Science | Chris Holmes (UC Irvine)<br>Seb Eastham (Harvard) |

## Priorities for future development

The GEOS-Chem Steering Committee has prioritized the following features for inclusion into the next version of GEOS-Chem, which will be assigned version name v11-02. The features are grouped by type. The priorities list will be further updated at the IGC8 meeting this May.

| v11-02 Feature | Submitted by |
|---|---|
| **Emissions updates** | |
| EDGAR v4.3 emissions | Chi Li (Dalhousie) |
| EPA-derived BC/OA emissions over US (1990-2012) | David Ridley (MIT) |

| v11-02 Feature | Submitted by |
|---|---|
| Historical CAC emissions | Chi Li (Dalhousie) |
| Default US emissions to NEI after 2011 | Dalhousie group |
| Ammonia from Arctic birds | Dalhousie group |
| Ocean ammonia emission inventory | Fabien Paulot (NOAA/GFDL) |
| A snow NOx source from deep snowpack | Maria Zatko (UW)<br>Becky Alexander (UW) |
| Non-agricultural NH3 for use with MASAGE | Amos Tai (CUHK) |
| **Aerosol, deposition, and radiation updates** | |
| Fix to direct / diffuse radiation | Katie Travis (Harvard) |
| Species Database Phase 3:<br>• Harmonizing Henry's Law coefficients across wet and dry deposition | GCST |
| Updated organic deposition | Katie Travis (Harvard)<br>Jenny Fisher (U. Wollongong) |
| Remove dependence of species drydep on HNO3 drydep | Katie Travis (Harvard)<br>Jenny Fisher (U. Wollongong) |
| Update SO2 scavenging in convective updrafts for consistency | Duncan Fairlie (NASA/LARC) |
| Sedimentation of stratospheric aerosols | Sebastian Eastham (Harvard) |
| **Structural updates** | |
| Uniformity of units | GCST |
| NetCDF Output Phase 3a: Output diagnostics in NetCDF format | GCST |
| NetCDF Output Phase 3b: Updates to eliminate differences between single and multi-segmented GEOS-Chem runs | GCST<br>Christoph Keller |

| v11-02 Feature | Submitted by |
|---|---|
| **Specialty simulation updates** | |
| PCB simulation | Carey Friedman (MIT)<br>Helen Amos (Harvard) |
| Hg code updates (chemistry, ocean, land) | Hg and POPs Working Group |
| Surface ocean Hg boundary conditions from MITgcm | Hannah Horowitz (Harvard) |
| **Other miscellaneous updates** | |
| Additional modifications for FlexChem, including:<br>• Rebuild the pre-built chemistry mechanisms (Standard, Tropchem, UCX, SOA, SOA-SVPOA) with Kppa<br>• Add capability for custom chemistry mechanism by building KPP on-the-fly in GEOS-Chem | Mike Long (Harvard)<br>GCST |
| FlexGrid: Use HEMCO I/O and regridding capabilities to read and regrid met fields | Jiawei Zhuang (Harvard)<br>Jintai Lin (PKU) |
| Merge standard simulation with specialty simulations for OVOC, acids, aromatics, dicarbonyls, terpenes | Dylan Millet (UMN)<br>Xin Chen (UMN) |
| Nested CO2, CH4, Hg, TOMAS, adjoint, etc. | Nested Model Working Group |
| Update ISORROPIA from v2.0 to v2.2, in order to remove persistent noise in output | Seb Eastham (Harvard) |

# GEOS-Chem Steering Committee News

## IGC8 News

The 8th International GEOS-Chem Meeting will take place from May 1-4, 2017 at Harvard University. Registration is free and the deadline is **February 15, 2017**. For more information about IGC8, and to register online, please visit **igc8.geos-chem.org**.

# GEOS-Chem High Performance News

The GEOS-Chem HP development team is working on validating scientific output generated with GCHP against similar output generated with GEOS-Chem "Classic". They plan on presenting their results at IGC8.

In the meantime, we invite you to the GEOS-Chem HP wiki page for the latest information: **wiki.geos-chem.org/GEOS-Chem_HP**.

# Conclusion

We have completed GEOS-Chem v11-01 development! We invite you to use the GEOS-Chem v11-01 public release in your research. We believe that you will find it much easier to modify the chemistry and emissions mechanisms in GEOS-Chem v11-01 than in prior versions.

Several new updates to chemistry, emissions, and aerosols are currently planned for GEOS-Chem v11-02. Please stay tuned for further updates.

Thank you for your continued support of GEOS-Chem! Please do not hesitate to contact us if you have any further questions or concerns.

Sincerely,

Bob Yantosca
with the GEOS-Chem Support Team
(Melissa, Lizzie, Mike, Junwei, Yanko)