

GEOS-Chem Newsletter – SPECIAL EDITION, v10-01 PUBLIC RELEASE
17 Jun 2015

The GEOS-Chem Support Team
geos-chem-support@as.harvard.edu

GEOS-Chem v10-01 is now officially released!

Dear GEOS-Chem users,

We are happy to announce the public release of [GEOS-Chem v10-01](#) as of today, Wednesday, 17 Jun 2015! GEOS-Chem v10-01 contains many new important structural and scientific updates, [as described on the GEOS-Chem wiki](#).

Highlights of new features in v10-01:

- You can now choose from [4 chemistry mechanisms for NO_x-O_x-aerosol chemistry](#):

Mechanism	Description
NO_x-O_x-HC-Aer-Br aka “tropchem” formerly “fullchem”	This is our standard 66-tracer chemistry mechanism, which is applied from the surface to the tropopause. In addition to NO _x -O _x -hydrocarbon chemistry, this mechanism includes several aerosol and bromine species.
SOA	This chemistry mechanism adds secondary organic aerosol species to the NO_x-O_x-HC-Aer-Br mechanism. You have the option to use SOA formation from semi-volatile POA species.
UCX	This mechanism adds several stratospherically-important species (Br, Cl, and halogen species) to the NO_x-O_x-HC-Aer-Br mechanism. The UCX mechanism is applied from the surface to the stratopause.
Benchmark (default mechanism)	<p>This mechanism combines the UCX and SOA mechanisms. We now use the Benchmark mechanism for all GEOS-Chem benchmark simulations in v10-01 and higher versions.</p> <p>When you run GEOS-Chem “out-of-the-box”, the Benchmark mechanism will be selected unless you specify otherwise, as described here.</p>

- You can use the [HEMCO emissions component](#) to customize the emissions configuration for your GEOS-Chem simulations. [Many new emissions inventories and data sets](#) (in [COARDS-compliant netCDF format](#)) can be used with HEMCO.
- You can now compute online radiation diagnostics with the [RRTMG radiative transfer model from AER](#).
- You can take advantage of the following developments for **nested-grid simulations**:
 - [Updates for the 0.25 x 0.3125 nested-grid simulations](#)
 - [Two-way nesting between nested-grid and global-grid simulations](#)
- You can use the [GEOS-Chem CO2 simulation](#) with updated emissions and CO2 flux data.
- We also added code for [compiling GEOS-Chem with the PRECISION=4 option](#). This will declare many of GEOS-Chem's large data arrays as REAL*4 instead of REAL*8, which will save memory. This will greatly facilitate running GEOS-Chem in HPC environments. **This option has not been fully benchmarked & validated yet. It is still considered experimental. You can use this option for testing, but you should not use it in your production runs. We hope to have this ready for the next version, [v11-01](#).**

The v10-01 period of public comment ended on June 15, 2015

The PROVISIONAL RELEASE of GEOS-Chem v10-01 occurred on 01 May 2015. The **period of public comment for GEOS-Chem v10-01 lasted from May 1, 2015 to June 15, 2015**. During this time, we asked GEOS-Chem users to start using GEOS-Chem v10-01 and to report to us any:

1. Last-minute bugs
2. Technical issues with the GEOS-Chem code or data
3. Typos or omissions in the wiki or web documentation
4. Other issues (i.e. problems downloading or installing the code and/or required libraries)

so that we could begin to implement fixes. We received many such reports, and were able to resolve all of the issues that GEOS-Chem users reported to us. [You can see a complete list of all the issues we fixed during the public comment period on the wiki.](#)

Many of the issues that were reported to us involved typos in the input files used by HEMCO and GEOS-Chem. Other fixes removed errors in source code or data files.

We validated the v10-01 public release code with benchmarks and unit tests

Benchmark	Description
v10-01-public-release-Run0	This 1-month benchmark was done with the UCX chemical mechanism. It validates the updates that we added to GEOS-Chem during the public comment period. It is compared against the prior benchmark GEOS-Chem v10-01i.
v10-01-public-release-Run1	This 1-month benchmark was done with the new Benchmark chemical mechanism (which combines the UCX mechanism with the SOA mechanism).
v10-01-RnPbBe	This 1-year benchmark was done with the GEOS-Chem Rn-Pb-Be simulation.
Unit test	Description
v10-01-provisional-release	The complete set of unit tests (i.e. short simulations designed to reveal various common errors) that we ran prior to the v10-01 provisional release on May 1, 2015.
v10-01-public release	The complete set of unit tests that we ran prior to the v10-01 public release on June 17, 2015.

Because we added several changes into GEOS-Chem v10-01 during the period of public comment, we ran the following benchmarks and unit tests listed above. We are confident that GEOS-Chem is performing as expected.

Instructions for installing the v10-01 public release code and data

The GEOS-Chem Online User's Guide (manual.geos-chem.org) contains instructions on how you can download and install GEOS-Chem v10-01 on your system. Please visit these links for further information:

- [Chapter 2: Installation](#)
- [Chapter 3: Compilation](#)
- [Chapter 4: Data Directories](#)
- [Chapter 5: Run Directories](#)

Also see these pages on the [GEOS-Chem wiki](#) for important installation instructions:

- [Installing libraries for GEOS-Chem](#)
- [Downloading GEOS-Chem source code and data](#)
- [Setting up the ExtData directory](#)

- [HEMCO data directories](#)
- [Debugging with the GEOS-Chem Unit Tester](#)
- [Creating GEOS-Chem run directories](#)

Because GEOS-Chem v10-01 contains many new features w/r/t the prior version [v9-02](#), we have completely overhauled the [GEOS-Chem manual](#) and several related wiki pages, including the [HEMCO User's Guide](#) and [HEMCO examples](#) pages. Please be sure to consult these resources before using GEOS-Chem v10-01.

Before compiling and running GEOS-Chem, we recommend that you first [generate a run directory from the GEOS-Chem unit tester](#) for the type of simulation that you want to perform. This will ensure that you have all of the correct input files, and restart files, and Makefiles for the given simulation.

We have updated some data files since the v10-01 provisional release

Since the v10-01 provisional release on 01 May 2015, we have added the following data sets for use with GEOS-Chem, via HEMCO.

- The [GFED4 biomass burning emissions](#) that shipped with the v10-01 provisional release on 01 May 2015 were preliminary data. The **official GFED4 biomass burning data** were released later in May 2015 and are now used in the GEOS-Chem v10-01 public release. You should download these new data files from the HEMCO data directory `$ROOT/GFED4/v2015-06/`.
- The [FINNv1 biomass burning emissions](#) are now available as a research option. We fixed [a couple of minor issues regarding FINNv1](#) during the public comment period.
- The **QFED2 biomass burning emissions** are also available as a research option.
- We fixed an issue with the unit string in the **UVALBEDO** data files used for the FAST-JX photolysis mechanism. You can download these data files from the HEMCO data directory `$ROOT/UVALBEDO/v2015-03/`.

The best way to download these data is with our `hemco_data_download` package. Please see [our Downloading the HEMCO data directories wiki entry](#) for more information on how you can install this package.

NOTE: Since the v10-01 provisional release, we have modified the default behavior of the `hemco_data_download` installer. The first time you use `hemco_data_download`, it will download all of the data that you specify in the configuration file. But the next time you use `hemco_data_download`, it won't start downloading everything from scratch again, but will only get the newer data files (as judged by the file timestamps). This will save you time on future data download operations.

Things you should be aware of when using GEOS-Chem v10-01

GEOS-Chem v10-01 includes many new features (such as [HEMCO](#) and [new chemistry mechanism options](#)), as well as many structural updates in order to facilitate running in high-performance computing environments. Therefore, several GEOS-Chem “behaviors” have changed since not only the prior version (v9-02) but also since the v10-01 provisional release.

Here is a list of some items that you should be aware of when using GEOS-Chem v10-01:

- In GEOS-Chem v9-02 and prior versions, the [NOx-Ox-HC-Aer-Br chemistry mechanism](#) (formerly called “fullchem”, now called “tropchem”) was the default chemistry mechanism. This has been changed in v10-01. When you compile GEOS-Chem out-of-the-box, the new **Benchmark chemistry mechanism** will be selected unless you [manually specify another mechanism](#).
- Many modules that were present in prior GEOS-Chem versions have since been removed. Please see [our Removal of obsolete modules from GEOS Chem wiki page](#) for a complete list. If you are developing new features for GEOS-Chem based on the prior version v9-02, then be aware that the modules you modified in v9-02 may no longer exist in v10-01. Please feel free to consult the [GEOS-Chem Support Team](#) if you have questions.
- Dry deposition is now applied to all tracers in module `mixing_mod.F90`. Prior to this, dry deposition had been applied in several locations throughout the code, which was confusing and prone to error.
- Dry deposition fluxes (i.e. category DRYD-FLX) are now archived to the ND44 diagnostic in module `mixing_mod.F90`. **Furthermore, drydep fluxes are now archived with units of `molec/cm2/s` for all GEOS-Chem simulations.** In prior GEOS-Chem versions, some simulations (in particular [Rn-Pb-Be](#)) had archived drydep fluxes in units of `kg/s`. **Therefore, when analyzing output from GEOS-Chem v10-01, please make sure to modify your plotting or budget programs to expect drydep fluxes in units of `molec/cm2/s`.**
- When you [create GEOS-Chem run directories](#), each run directory will contain a HEMCO restart file. The dates in these HEMCO restart files are typically either 2006/07/01 or 2013/07/01. If you are trying to run a simulation for a different date, then you should tell HEMCO to not to read the restart file. In this case, HEMCO will use default values instead. To disable this option, set this switch at the top the HEMCO config file:

```
--> HEMCO_RESTART      :      false
```
- The GMAO operational data products (what we refer to as [GEOS-5](#) and [GEOS-FP](#)) actually change over time as new features and new science are added into the NASA GEOS-5 GCM. We have begun compiling a [version history of the GMAO data products](#) on the GEOS-Chem wiki which you can consult.

Tools that you can use to visualize GEOS-Chem output

You can use several tools for analyzing output archived from your GEOS-Chem simulations:

- [GAMAP](#) is our IDL-based visualization package for GEOS-Chem. We recently added a few minor updates and fixes to GAMAP, so you will want to make sure to download the latest changes. Please refer to our [GAMAP Online User's Guide](#) for more information.
- [pyGchem](#) is a free and open-source Python-based visualization package being developed by Benoit Bovy at the University of Liege, Belgium. PyGchem can read GEOS-Chem output and attach it to the SciPy stack, which contains many plotting and analysis functions. If you have experience in using the Python language, we encourage you to start using pyGchem for your GEOS-Chem analysis. Please send feedback about pyGchem to Benoit Bovy at: `bbovy [at] ulg.ac.be`.
- [Process Analysis Diagnostics](#): Barron Henderson has developed a free and open-source set of Python tools that will allow you to examine the change in each species due to each process and each reaction. If you work directly with chemical reaction networks, then this tool may be of great use to you. Please contact Barron for more information at: `barronh [at] ufl.edu`.

Other resources

For the most up-to-date information about GEOS-Chem, we invite you to visit the [GEOS-Chem wiki](#). In particular, please see the following pages:

- [GEOS-Chem v10-01](#)
- [GEOS-Chem v10-01 benchmark history](#)
- [Bugs and fixes](#)
- [Currently unresolved issues in GEOS-Chem](#)
- [HEMCO](#)
- [The HEMCO User's guide](#)
- [HEMCO examples](#)

If you are a new GEOS-Chem user, we also encourage you to view these wiki pages:

- [GEOS-Chem welcome letter for new users](#)
- [Frequently asked questions about GEOS-Chem](#)
- [Common GEOS-Chem error messages](#)

Coming attractions: GEOS-Chem v11-01

The next version of GEOS-Chem will be labeled [GEOS-Chem v11-01](#). Because v11-01 will contain the new FLEXCHEM solver—which will allow us to retire SMVGEAR—we are changing the version number from 10 to 11.

For a complete list of updates that are slated to go into GEOS-Chem v11-01, [follow this link](#).

--

Thanks for your continued support of GEOS-Chem. Happy Modeling!

Sincerely,

The GEOS-Chem Support Team

Bob Yantosca

Melissa Sulprizio

Matt Yannetti

Lizzie Lundgren

Mike Long

Junwei Xu

Yanko Davila

geos-chem-support [at] as.harvard.edu