GEOS-Chem Newsletter—Summer 2015 Edition
10 Aug 2015

The GEOS-Chem Support Team
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IGC7 wrapup

The 7th International GEOS-Chem Meeting (IGC7) took place from May 4-7, 2015 at Harvard University. Please visit **igc7.geos-chem.org** to view the presentations and posters from the meeting.

GEOS-Chem v10-01 public release

GEOS-Chem v10-01 was publicly released on 17 Jun 2015. Key updates in this version include the HEMCO emissions component, the UCX strat-trop chemical mechanism, and the FAST-JX v7.0 photolysis mechanism.

We encourage all GEOS-Chem users who are still using older versions to migrate to GEOS-Chem v10- as soon as possible. For more information, please consult the following resources:

- GEOS-Chem Newsletter, SPECIAL EDITION: v10-01 public release
- GEOS-Chem v10-01 wiki page
- GEOS-Chem v10-01 benchmark history
- The GEOS-Chem v10-01 online manual
- The HEMCO User's Guide
- HEMCO Examples wiki page

GEOS-Chem v11-01 is now in development!

GEOS-Chem v11-01 is our current version in development. We changed the version number from v10 to v11 because the new FLEXCHEM chemical solver package will be introduced in this version. FLEXCHEM will render SMVGEAR obsolete, and SMVGEAR will be removed from v11-01. Therefore, v11-01 will be incompatible with prior versions.

Here is an update of what we have accomplished to date:

GEOS-Chem v11-01a

GEOS-Chem v11-01a includes Lizzie Lundgren's updates to account for moisture properly in various air mass quantities and unit conversions. Several related updates were also included. The 1-month benchmark for v11-01a was approved on 07 Jul 2015.

Feature	Type	Submitted by
Incorporate moisture into air quantities, tracer units, and tracer unit conversions	Science & Bug fix	Lizzie Lundgren (GCST) Meemong Lee (JPL)
Correct bug in below cloud average mixing ratio calculation in DO_MERRA_CONVECTION to improve mass balance	Bug fix	Lizzie Lundgren (GCST)
Added the capability to print out tracer masses every few hours, in order to check for mass conservation	Structural	Lizzie Lundgren (GCST)
Fix bug in RRTMG that prevents storage of O3 and CH4 RFs	Bug fix	David Ridley (MIT) Seb Eastham (MIT)
Prevent negative tracer concentrations at poles after advection	Bug fix	Lizzie Lundgren (GCST)

***Update 30 July 2015**:* A moisture signature is observed in CO2 concentrations during carbon simulations with zero emissions and constant 370 ppm initial conditions. The moisture signature is expected for wet mixing ratio (v/v total air) but not dry mixing ratio (v/v dry air). This issue is currently under investigation by the GEOS-Chem Support Team and the Carbon Cycle Working Group.

GEOS-Chem v11-01b

In GEOS-Chem v10-01b, we added several science updates and bug fixes that we had not been able to include into v10-01. The 1-month benchmark for v11-01b was approved on 04 Aug 2015. As of this writing, the 1-year benchmarks for v11-01b are still pending approval.

Feature	Type	Submitted by
Update DMS climatology to Lana	Science	Tom Breider (Harvard)
Impaction scavenging for hydrophobic BC	Science	Qiaoqiao Wang (Max Planck Inst.)
Homogeneous IN removal	Science	Qiaoqiao Wang (Max Planck Inst.)
Density of OA update	Science	Melanie Hammer (Dalhousie) Eloïse Marais (Harvard)
Improved dust size distribution scheme	Science	Li Zhang (Colorado U.) Daven Henze (Colorado U.)
Addition of BrC UV absorption to address impacts on OH • This feature is optional (default off)	Science	Melanie Hammer (Dalhousie)
Acid uptake on dust aerosols • This feature is optional (default off)	Science	T. Duncan Fairlie (NASA/LARC)
Now treat DST2-DST4 as coarse mode in wet scavenging	Bug fix	T. Duncan Fairlie (NASA/LARC)
Online emission of marine primary organic aerosol (POA) • This feature is optional (default off)	Science	Brett Gantt (NCSU) Matthew Johnson (NASA Ames)
Update of PMN + O3 reaction products in globchem.dat file	Bug fix	Dylan Millet (UMN)

Bug fix in RRTMG array sizes	Bug fix	Sebastian Eastham (MIT)
Bug fixes in rrtmg_rad_transfer_mod.F	Bug fix	Sebastian Eastham (MIT) David Ridley (MIT)
Bug fix for black carbon in ucx_mod.F	Bug fix	Sebastian Eastham (MIT)
Bug fix for archiving P(Ox)/L(Ox) from full-chemistry simulations via the ND20 diagnostic	Bug fix	GCST
Bug fix for linking files when compiling with PGI	Bug fix	GCST

GEOS-Chem v11-01c

The following updates are slated for GEOS-Chem v11-01c (timeline TBD).

Feature	Type	Submitted by
Updates to PAH code	Science	Carey Friedman (MIT)
Harmonizing Henry's Law coefficients across wet and dry deposition (SO2 treated as effective Henry's Law)	Science	GCST
Bug fix for sea salt alkalinity in sulfate_mod.F	Bug fix	Johan Schmidt
Correct problem in OTD-LIS local redistribution files for GEOS-5	Bug fix	Christoph Keller (Harvard) Lu Hu (Harvard)
Bug fixes for the ND21 diagnostic	Bug fix	Sebastian Eastham (MIT)
Bug fix for custom nested grid in tpcore_bc_mod.F	Bug fix	Shannon Koplitz (Harvard)
GEOS-Chem Timers: Adding the capability to determine how long transport, chemistry, emissions, and other operations take to execute (see below)	Structural	Matt Yannetti (GCST)

GEOS-Chem v11-01d

The following updates are slated for GEOS-Chem v11-01d (timeline TBD).

Feature	Type	Submitted by
CO2 direct effect on isoprene emissions	Science	Amos Tai (CUHK)
Criegee intermediates	Science	Dylan Millet (U. Minnesota) Eloïse Marais (Harvard)
PAN updates	Science	Emily Fischer (CSU)
Update biomass burning emissions to GFED4.1, includes: • Daily and diurnal factors	Science	Prasad Kasibhatla (Duke) Christoph Keller (Harvard)
Metal catalyzed oxidation of SO2 (as a switch)	Science	Becky Alexander (UW)
Monthly mean surface methane distributions	Science	Lee Murray (NASA GISS/LDEO)

Updates still "in the pipeline" for GEOS-Chem v11-01

The following features are slated to be brought into GEOS-Chem v11-01, timeline TBD.

Feature	Type	Submitted by
Implementation of FLEXCHEM chemical solver (see below)	Science	Mike Long (GCST) John Linford (ParaTools Inc) GCST
Developing a common data structure for species properties (see below)	Structural	GCST
Adding support for MERRA2 meteorology (see below)	Structural	GCST
NetCDF output: Flexible diagnostic package and tracer restart file	Science	GCST
Uniformity of units	Science	Lizzie Lundgren (GCST)
Fix to direct/diffuse radiation	Science & Bug fix	Katie Travis
Fix for NO3 + ISOP product	Science	Katie Travis
Update MODIS LAI fields through 2015	Science	Barron Henderson (UF)
Updated organic deposition	Science	Katie Travis (Harvard) Jenny Fisher (U. Wollongong)
Hg code updates (emissions, chemistry, ocean, land)	Science	Hg and POPs WG
EPA-derived BC/OA emissions over US (1990-2012)	Science	David Ridley (MIT)
Update density of BC to 1.8 and add absorption enhancement factor in input.geos	Science	Xuan Wang (MIT)
Updates to isoprene chemistry, includes: • Fast photolysis of carbonyl nitrates • Aerosol uptake of organic nitrates	Science	Jenny Fisher (U. Wollongong) Eloïse Marais (Harvard) Kelvin Bates (Caltech) Katie Travis (Harvard)
Nighttime isoprene chemistry updates	Science	Rebecca Schwantes (Caltech)
Remove dependence of species drydep on HNO3 drydep	Science	Katie Travis (Harvard) Jenny Fisher (U. Wollongong)
A snow NOx source from deep snowpack	Science	Maria Zatko (UW) Becky Alexander (UW)
Land cover module in GEOS-Chem	Science	Jeffrey Geddes (MIT) Michael Long (GCST)
Merge standard simulation with specialty simulations for OVOC, acids, aromatics, dicarbonyls, terpenes	Science	Dylan Millet (UMN) Xin Chen (UMN)
Automate redistribution of NOx in HEMCO	Science	Lee Murray (NASA GISS/LDEO)

Injection height for fire emissions	Science	Emily Fischer (CSU)
Improved lightning emission scheme	Science	Lee Murray (NASA GISS/LDEO)

Other fundamental software development efforts

GEOS-Chem timers

Matt Yannetti is creating a Fortran-based timing package for GEOS-Chem. You will be able to use these timers to determine how long individual operations (e.g. chemistry, transport, emissions, deposition, etc.) take to execute. We will also activate the timers in all GEOS-Chem benchmarking simulations, so that a record of execution times can be kept along with other benchmark output. This will help us to locate performance bottlenecks. We expect this new capability to be added into GEOS-Chem v11-01c.

Implementation of FLEXCHEM into v11-01

Our new FLEXCHEM chemical solver package is now ready for implementation into GEOS-Chem! Mike Long will begin the process of integrating FLEXCHEM on top of the v11-01b base code. It will be introduced into the standard model as soon as it is ready. It will be benchmarked separately from other GEOS-Chem updates.

FLEXCHEM is a more flexible implementation of the KPP chemistry solver. We expect to be able to use the KPP-Accelerated (KPPA) solver from John Linford (ParaTools, Inc.). KPPA is a newer, faster version of the previous KPP chemical solver software. Preliminary tests show significant speedup (50-70%) over the existing SMVGEAR chemical solver software.

The implementation of KPPA into GEOS-Chem has been named FLEXCHEM, for “flexible chemistry”. The advantage of using FLEXCHEM over the existing SMVGEAR/KPP code is that you will be able to make changes to the chemistry mechanism by just changing an input file and recompiling GEOS-Chem. This will make it very simple to bring new chemistry mechanisms into GEOS-Chem.

Creating a common data structure for storing physical properties of species

The GEOS-Chem Support Team is creating a common data structure that will store all of the various physical properties for GEOS-Chem species. Currently, these properties are defined (and sometimes redefined) in several locations in the code.

For example, the effective Henry's law value *Heff* is calculated differently in the wet deposition module than in the dry deposition module. The GEOS-Chem wet deposition module assumes a pH value of 4.5 for rainwater, and thus uses a set of Henry’s law constants that are appropriate for this pH. On the other hand, the GEOS-Chem dry deposition module assumes a pH of 7 for water, and therefore uses a different set of Henry’s law constants. Keeping two independent sets of Henry’s law constants can lead to confusion.

In the v10-01 public release, Christoph Keller implemented a new GEOS-Chem module that can compute *Heff* for each species as a function of pH and the species-specific Henry's law constants K0, CR, and pKA. These Henry's law constants can be obtained from the literature (cf. Sander, Atmos. Chem. Phys. 15, 4399-4381, 2015, or similar references). We would like to use Christoph's new module to compute *Heff* in a consistent way everywhere in GEOS-Chem.

We would also like to store these Henry's law constants together with other relevant physical parameters such as molecular weight, density, aerosol radius, reactivity factor for drydep (F0), etc. for each species. Keeping all of these physical properties in a single data structure will streamline the code and help to reduce confusion.

We have already started on this effort, and expect that it can be included into the standard GEOS-Chem code shortly. The adoption of different physical constants with respect to the previous code will likely cause small numerical differences in the output. Therefore, we will benchmark this new feature separately from other new GEOS-Chem code updates.

Adding support for MERRA2 meteorology into GEOS-Chem

NASA/GMAO is currently preparing to release the MERRA2 met field product. MERRA2 will be a long-term reanalysis data product (similar to the prior MERRA product) generated with the GEOS-Data Assimilation System version 5.12.4. The native resolution of MERRA2 data will be 0.5° lat x 0.625° lon x 72 vertical layers. The 72-layer vertical grid used by MERRA2 is identical to that used by the GEOS-5, MERRA, and GMAO "forward processing" (i.e. what we call GEOS-FP) met data products.

The MERRA2 file structure is very similar to that used by the GEOS-FP data product. Because of this similarity, it was straightforward to extend our existing GEOS-FP data processing software to download and regrid MERRA2 data. Bob Yantosca has validated the MERRA2 regridding software with some sample data obtained directly from GMAO.

MERRA2 is slated to "go live" in the near future. MERRA2 "raw" data files will eventually be available for download through the NASA GES-DISC data distribution service. In the meantime, we have prepared some MERRA2-related pages on the GEOS-Chem wiki.

- MERRA2
- List of MERRA2 met fields used as input to GEOS-Chem
- MERRA2 implementation details (under construction!)

The list of MERRA2 met fields for GEOS-Chem that we have compiled is by no means exhaustive. We are planning to get most of the same fields that are also present in our GEOS-FP data archive. If you or your research group has a need of a MERRA2 met field that is not present, then please contact the GEOS-Chem Support Team.

We believe that the initial code modifications for MERRA2 will be ready in time for v11-01c or v11-0d. It will of course take longer to completely validate MERRA2 in GEOS-Chem. This validation will

require a couple of years of regridded MERRA2 data, so that we can run our GEOS-Chem usual benchmark simulations.

Flexible precision will be declared an official option when FLEXCHEM is added

Flexible precision is a language feature that was introduced in Fortran-90. It allows you to define GEOS-Chem's floating-point variables with 4 bytes (aka REAL*4) or with 8 bytes (aka REAL*8) when you compile the code. We invite you to read our *Flexible precision in GEOS-Chem* wiki page to learn more about the specifics involved.

The ability to switch between 4-byte and 8-byte precision in GEOS-Chem will have tremendous benefits. By using 4-byte precision, we will be able to reduce GEOS-Chem's memory footprint dramatically. This will facilitate running GEOS-Chem at very fine resolution in high-performance computing environments. It will also reduce the amount of memory required to run the current nested-grid simulations.

GEOS-Chem Support Team member Matt Yannetti made the necessary modifications to bring flexible precision into GEOS-Chem v10-01. But due to leftover legacy code (in particular, the SMVGEAR chemical solver), we were not able to take full advantage of flexible precision as of yet. Once FLEXCHEM is integrated into GEOS-Chem v11-01 (and the legacy SMVGEAR modules are removed), we expect to declare flexible precision as an "official" GEOS-Chem option. Stay tuned…

Correcting inaccuracies in the computation of air mass and related quantities

The current method of converting tracer units from vol/vol to kg in GEOS-Chem uses the air mass in a grid box and the molecular weight of dry air, implicitly assuming dry air mass. This algorithm assumes that the surface pressure (which we obtain from the GEOS met data archive) is based on dry air content. But more recent versions of the GEOS met data products—which are used to drive GEOS-Chem—now account for water vapor in the computation of surface pressure, thus rendering this assumption invalid.

GEOS-Chem Support Team member Lizzie Lundgren is working to correct this situation and similar instances of dry air assumptions in GEOS-Chem. She has implemented the following solutions:

1. Grid box dry air partial pressure-edge and pressure-center arrays are now computed in GEOS-Chem and are used for air number density unit conversions and gas partial pressure calculations in chemistry. Input moist air pressure continues to be used for all other pressure applications.
2. Both moist and dry air mass is now computed and dry air mass is used in the initial conversion from vol/vol to kg.
3. Vol/vol dry air is now converted to kg/kg total air for convection and advection.
4. Box height is now computed using the hypsometric equation with water vapor taken into account.
5. Both moist and dry air densities are now computed using the partial pressures of dry air and water vapor in the ideal gas law.
6. The computations of relative humidity (only necessary if using GEOS-4 or GCAP meteorology in GEOS-Chem) and water vapor volume mixing ratio were previously calculated by approximating the specific humidity (mass water / mass total air) as mass water per dry air.

> Both computations have been updated to take into account the more precise definition of specific humidity.

These updates were incorporated into GEOS-Chem v11-01a (approved on 07 Jul 2015). Please also see our wiki page entitled Air Quantity Updates for v11-01a.

The inclusion of moisture appears to have introduced a moisture signature in vol/vol dry air that would instead be characteristic of vol/vol total air. The GEOS-5 AGCM includes a scaling of the mixing ratio to ensure the dry air concentration is not affected by moisture and changes in moisture and GEOS-Chem may need to an analogous implementation. This issue is currently under investigation by the GEOS-Chem Support Team and the Carbon Cycle Working Group.

In the pipeline: Making units consistent throughout GEOS-Chem

GEOS-Chem has traditionally carried tracers in units of kg, and then has converted them to v/v mixing ratio and molec/cm3 in other areas of the code as needed. But these unit conversions rely upon the surface area of each grid cell. GEOS-Chem currently computes surface areas assuming a Cartesian grid. On the other hand, the latest generation of Earth System Models—including NASA's GEOS-5 GCM—often use cubed-sphere grids. This renders the assumption of a Cartesian grid invalid.

We are planning to recode GEOS-Chem such that tracer and species concentrations are carried in mass mixing ratio units, such as [kg gas/kg air]. This will:

- Remove the burden of having to know what the surface area of each grid box is,
- Remove several commonly-repeated multiplications and divisions, thus increasing computational efficiency,
- Facilitate coupling GEOS-Chem with the GEOS-5 GCM and other Earth System Models

Lizzie Lundgren is currently leading the effort to make the units consistent throughout GEOS-Chem. She writes:

> This work will complement our work to correctly incorporate air moisture into GEOS-Chem. We intend to use [kg/kg dry air] throughout GEOS-Chem except in transport where units will be in kg/kg total air.

We expect to introduce this change into GEOS-Chem v11-01, following the integration of FLEXCHEM.

Migrating diagnostics from binary output to netCDF output

For many years, GEOS-Chem has saved diagnostic output to binary punch file format—that is, unformatted Fortran binary output with standardized data fields. But binary files cannot be read efficiently in distributed high-performance computing environments. Therefore, we have begun to recode GEOS-Chem so that diagnostic outputs can be saved to COARDS-compliant netCDF files.

Christoph Keller has modified HEMCO so that we can use HEMCO's internal data structure to archive

diagnostic output for any GEOS-Chem quantity. We have opened a new branch of development into which we are placing these modifications. We envision that netCDF diagnostic output will be standardized in GEOS-Chem v11-01 (timeline TBD).

We will also work on code that will save restart file quantities to netCDF format, instead of the current binary punch format (timeline also TBD).

High-performance computing with GEOS-Chem

GEOS-Chem HP update

We have succeeded in compiling and running GEOS-Chem in a high-performance computing (HPC) environment. GEOS-Chem can now utilize the Earth System Modeling Framework (ESMF) with Message-Passing Interface (MPI) parallelization to run on distributed computing architectures. It also uses the MPI-enabled NASA/GMAO finite-volume dynamics core (FVdycore) as the transport operator.

We are currently doing some test runs with our standalone GEOS-Chem HP on the Odyssey supercomputer at Harvard. We have also created some wiki documentation to assist interested users in setting up GEOS-Chem HP on their systems.

If you would like to take the new GEOS-Chem HP out for a spin on your local supercomputer or cluster, then please contact Mike Long (mlong [at] seas [dot] Harvard [dot] edu) and Matt Yannetti (myanneti [at] seas [dot] Harvard [dot] edu).

Electronic media updates

GEOS-Chem email lists are migrating to Google Groups

The Harvard University IT group is retiring the Mailman list server engine in favor of Google Groups, which provides similar functionality. Because of this change, the official names of the GEOS-Chem email lists will now use the **g.harvard.edu** domain name instead of the **seas.harvard.edu** name, as shown in the table below.

Old mailing list address (will still work, for backwards compatibility)	New mailing list address
geos-chem@seas.harvard.edu	geos-chem@g.harvard.edu
geos-chem-adjoint@seas.harvard.edu	geos-chem-adjoint@g.harvard.edu
geos-chem-aerosols@seas.harvard.edu	geos-chem-aerosols@g.harvard.edu
geos-chem-carbon@seas.harvard.edu	geos-chem-carbon@g.harvard.edu
geos-chem-emissions@seas.harvard.edu	geos-chem-emissions@g.harvard.edu
geos-chem-hg-pop@seas.harvard.edu	geos-chem-hg-pop@g.harvard.edu
geos-chem-organics@seas.harvard.edu	geos-chem-organics@g.harvard.edu

geos-chem-hp@seas.harvard.edu	geos-chem-hp@g.harvard.edu
geos-chem-organics@seas.harvard.edu	geos-chem-organics@g.harvard.edu
geos-chem-oxidants@seas.harvard.edu	geos-chem-oxidants@g.harvard.edu
geos-chem-regional@seas.harvard.edu	geos-chem-regional@g.harvard.edu
geos-chem-transport@seas.harvard.edu	geos-chem-transport@g.harvard.edu

For purposes of maintaining backwards compatibility, mail that is sent to the old mailing list addresses (e.g. geos-chem@seas.harvard.edu) will still be delivered as before. But the commands for subscribing and unsubscribing from the lists will now be different. The GEOS-Chem Support Team will provide instructions on how to use the new email lists in the coming days.

New and updated wiki pages

We have added a few new GEOS-Chem wiki pages since the last newsletter. We have also updated content on several pages in order to remove obsolete information. Please see the following wiki pages for more information:

- Coupling GEOS-Chem with RRTMG
- GEOS-Chem model development priorities
- GEOS-Chem v11-01 and GEOS-Chem v11-01 benchmark history
- MERRA2 and List of MERRA2 met fields for GEOS-Chem
- Leaf area indices in GEOS-Chem (updates for GEOS-Chem v11-01)
- Mineral dust aerosols (updates for v11-01)
- PGI compiler
- Version history of GMAO met data products
- Wet deposition (updates for v11-01)

Thank you for your continued support of GEOS-Chem!

Sincerely,

Bob Yantosca
on behalf of the entire GEOS-Chem Support Team
(Melissa, Matt, Lizzie, Mike, Junwei, Yanko)
10 Aug 2015