

# GEOS-Chem Newsletter

## Spring 2016 Edition

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*GEOS-Chem Support Team*

*16 May 2016*

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### GEOS-Chem v11-01 Development Overview

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GEOS-Chem v11-01 development continues to proceed rapidly! GEOS-Chem [v11-01f](#) was approved in April 2016, and [v11-01g](#) is under development as of this writing.

The clean and flexible reimplementations of the Kinetic PreProcessor package (aka KPP)—known as **FlexChem** – is nearing full integration into GEOS-Chem. Most of the remaining FlexChem development work will focus on replacing legacy infrastructure—which prevents GEOS-Chem from operating efficiently in high-performance computing (HPC) environments—with newer, more efficient algorithms.

We have also created a **GCHP development kit**, which you can use to install and run our MPI-enabled version of GEOS-Chem on your system. This is considered an “alpha” product (meaning it is ready for testing but not fully debugged).

More information on the Development Kit is included below.

## GEOS-Chem v11-01f

GEOS-Chem [v11-01f](#) was approved on 16 Apr 2016. This version contains important structural updates that needed to be made prior to the addition of the FlexChem in [v11-01g](#).

V11-01f also contains several user-submitted [bug fixes](#) for chemistry and emissions (most of which were discussed in the [GEOS-Chem Newsletter, Winter 2016 edition](#)). Also included in this version are the initial round of modifications for saving GEOS-Chem restart files using the [netCDF file format](#). Lastly, v11-01f introduces full compatibility with the [MERRA-2](#) met fields for all full-chemistry and specialty simulations.

Feature	Type	Submitted by
<a href="#">Bug fixes for hydrophobic aerosol properties</a>	Bug fix	Seb Eastham (Harvard)
<a href="#">Use an updated EMEP mask file to prevent zero emissions at 30 N</a>	Bug fix	Eloise Marais (Harvard)
<a href="#">Correct too-high emissions of Hg2 over China and EU</a>	Bug fix	Amanda Giang (MIT)
<a href="#">Fix typo in HEMCO extension module hcox_gc_RnPbBe_mod.F90</a>	Bug fix	Mat Evans (U. York)
<a href="#">Fix syntax error in globchem.dat for the MOBA + OH --&gt; MOBAOO reaction rate</a>	Bug fix	Will Porter (MIT)
<a href="#">Fix bug in reaction ISNOOA + NO2 --&gt; PMN in globchem.dat</a>	Bug fix	Mike Long (Harvard)
<a href="#">Fix an emissions error in the SOA-SVPOA simulation</a>	Bug fix	Prasad Kasibhatla (Duke) Melissa Sulprizio (GCST)
<a href="#">Add a script (NcdfUtil/perl/isCoards) to determine if a netCDF file is COARDS-compliant</a>	Structural	Bob Yantosca (GCST)
<a href="#">Consistent physical parameter values throughout GEOS-Chem</a>	Structural	Lizzie Lundgren (GCST)
<a href="#">Add optimal timestep settings to the standard GEOS-Chem run directories (via the GEOS-Chem Unit Tester)</a>	Structural	Sajeev Philip (Dalhousie) Randall Martin (Dalhousie)
<a href="#">Drive full-chemistry simulations with MERRA-2 met fields</a> <ul style="list-style-type: none"><li>• Compute various scale factors (dust, lightning, etc.)</li></ul>	Structural	Melissa Sulprizio (GCST) Lee Murray (NASA GISS/LDEO)
<a href="#">NetCDF Output Phase 1:</a> <ul style="list-style-type: none"><li>• Input and output restart file in netCDF format for all simulations except mercury</li></ul>	Structural	Lizzie Lundgren (GCST)
<a href="#">Add further fixes for compiling GEOS-Chem with PGI Fortran</a>	Structural	Bob Yantosca (GCST)
<a href="#">Correct bug introduced in v11-01e where emissions were disabled in the stratosphere for specialty simulations</a>	Bug fix	Lizzie Lundgren (GCST)

## GEOS-Chem v11-01g

This version will contain the FlexChem chemical solver package, plus several additional structural modifications ([including a new faster way to look up species indices from their names](#)).

We will completely remove the obsolete SMVGEAR chemical solver and related infrastructure from [v11-01g](#). Because some existing diagnostic output depends on SMVGEAR arrays and variables, we will need to restore the equivalent functionality into GEOS-Chem. This work is ongoing.

We will validate v11-01g with both 1-month and 1-year benchmark simulations for the [various pre-built chemical mechanisms](#) (i.e. benchmark, tropchem, UCX, SOA, SOA-SVPOA).

Feature	Type	Submitted by	Status
<a href="#">FlexChem</a> <ul style="list-style-type: none"><li>Replacing SMVGEAR with a flexible implementation of KPP</li><li>Removing legacy SMVGEAR code and input files</li></ul>	Science	Mike Long and <a href="#">GCST</a>	Implemented into a development version of GEOS-Chem.  FlexChem has been parallelized and yields good results for all pre-built mechanisms w/r/t the prior code.  Removal of legacy infrastructure is ongoing.
<a href="#">NetCDF Output Phase 2:</a> <ul style="list-style-type: none"><li>Use NetCDF restart files for Hg simulation</li></ul>	Structural	Lizzie Lundgren ( <a href="#">GCST</a> )	Pending benchmark approval
<a href="#">Fix parallelization issues that prevented Hg simulations using GEOS-5 met fields from passing unit tests</a>	Bug fix	Bob Yantosca ( <a href="#">GCST</a> )	Pending benchmark approval
<a href="#">Update 4x5 soil Hg files and Hg simulation photoreduction and soil emission coefficients</a>	Science	Jenny Fisher (Wollongong)	Pending benchmark approval
<a href="#">Restore the tagged CO specialty simulation</a> <ul style="list-style-type: none"><li>Use HEMCO for CO tagged tracer emissions</li><li>Restore tagged CO unit tests</li></ul>	Structural	<a href="#">GCST</a>	Pending benchmark approval
<a href="#">Updates for High Performance GEOS-Chem (GCHP) Dev release</a> , includes: <ul style="list-style-type: none"><li><a href="#">Prevent segmentation fault in HEMCO that can happen with Intel Fortran Compiler v12 or newer</a></li></ul>	Structural & Bug fix	Seb Eastham (Harvard) <a href="#">GCST</a>	In development

<a href="#">Do not nullify local pointers in the same line where they are declared</a>	Structural	<a href="#">GCST</a>	Completed 29 Apr 2015
<a href="#">Improved species indexing, Phase 1:</a> <ul style="list-style-type: none"> <li>Phase 1: Removal of Hg, Rn, and POPs indexing variables from <code>tracerid_mod.F</code></li> <li>Phase 2: Implementation of a fast algorithm for species name lookup</li> </ul>	Structural	<a href="#">GCST</a>	Phase 1: Completed 02 May 2015  Phase 2: to be done concurrently with <a href="#">FlexChem</a> implementation

## Remaining updates for GEOS-Chem v11-01

During the integration of [FlexChem](#) into GEOS-Chem, we suspended all further science updates. We will introduce many of these into GEOS-Chem v11-01h and later versions.

Feature	Type	Submitted by	Status
<a href="#">Fix to remove moisture signature in dry mixing ratio</a>	Bug fix	Meemong Lee Kevin Bowman Richard Weidner (all JPL)	Delivered to GCST
<a href="#">Set ACTA and HCOOH to active</a>	Bug fix	Katie Travis (Harvard)	Delivered to GCST
<a href="#">Correct bug in units of EDGAR v4.2 SO2 emissions</a>	Bug fix	Jaegun Jung (Ramboll)	Delivered to GCST
<a href="#">Update HEMCO from version 1.1.016 to latest version available</a>	Structural	Christoph Keller and <a href="#">GCST</a>	In progress
<a href="#">Add option for QFED &amp; FINN emissions in the Hg simulations</a>	Science	Jenny Fisher (Wollongong)	Delivered to GCST. NOTE: Requires the latest HEMCO updates
<a href="#">Use TOMS ozone for all years when running simulations with GEOS-5</a>	Science	Jenny Fisher (Wollongong)	Delivered to GCST
<a href="#">NetCDF Output Phase 3a: Output diagnostics in NetCDF format</a>	Structural	<a href="#">GCST</a>	In progress
<a href="#">NetCDF Output Phase 3b: Updates to eliminate differences between single and multi-segmented GEOS-Chem runs</a>	Bug fix	Christoph Keller and <a href="#">GCST</a>	In progress
<a href="#">PAN updates</a>	Science	Emily Fischer (CSU)	Delivered to GCST, partially implemented into development code
<a href="#">Monthly mean surface methane distributions</a>	Science	Lee Murray (NASA GISS/LDEO)	Awaiting code from developer

<a href="#">Ocean ammonia emission inventory</a>	Science	Fabien Paulot (NOAA/GFDL)	Data files delivered to GCST; Needs to be implemented via HEMCO
<a href="#">Update density of BC to 1.8 and add absorption enhancement factor in input.geos</a>	Science	Xuan Wang (MIT)	Delivered to GCST

## In the Pipeline

The following features are slated for inclusion after the GEOS-Chem v11-01 public release.

Feature	Type	Submitted by	Status
Species Database Phase 3: <ul style="list-style-type: none"> <li>Harmonizing Henry's Law coefficients across wet and dry deposition</li> </ul>	Science	<a href="#">GCST</a>	TBD after FlexChem
<a href="#">Uniformity of units</a>	Science	Lizzie Lundgren ( <a href="#">GCST</a> )	Phase 2 (unit uniformity throughout chemistry) to be implemented after Flexchem  Phase 3 (unit uniformity in some specialty simulations) will be implemented in pieces with input from 3rd party developers.  Phase 4 (removal of area and area-dependent State_Met variables) will be ongoing.
<a href="#">Metal catalyzed oxidation of SO2</a> (as a switch)	Science	Becky Alexander (UW)	TBD
<a href="#">Temporary fix to remove SO2 scavenging in convective updrafts</a>	Science	Duncan Fairlie (NASA/LARC)	TBD
<a href="#">Update SO2 scavenging in convective updrafts for consistency</a>	Science	Duncan Fairlie (NASA/LARC)	TBD after FlexChem
Fix to direct/diffuse radiation	Science & Bug fix	Katie Travis	TBD after FlexChem
<a href="#">Fix for NO3 + ISOP product</a>	Science	Katie Travis	TBD after FlexChem
Update MODIS LAI fields through 2015	Science	Barron Henderson (UF)	TBD
Updated organic deposition	Science	Katie Travis	TBD after FlexChem

		(Harvard) Jenny Fisher (U. Wollongong)	
Hg code updates (emissions, chemistry, ocean, land)	Science	<a href="#">Hg and POPs WG</a>	Bug fixes for several issues were made in v11-01c and v11-01e. Team Hg is currently running a new Hg benchmark (Feb 2015)
EPA-derived BC/OA emissions over US (1990-2012)	Science	David Ridley (MIT)	TBD after FlexChem
Updates to isoprene chemistry, includes: <ul style="list-style-type: none"> <li>Fast photolysis of carbonyl nitrates</li> <li>Aerosol uptake of organic nitrates</li> </ul>	Science	Jenny Fisher (U. Wollongong) Eloïse Marais (Harvard) Kelvin Bates (Caltech) Katie Travis (Harvard)	TBD after FlexChem
Nighttime isoprene chemistry updates	Science	Rebecca Schwantes (Caltech)	TBD after FlexChem
Remove dependence of species drydep on HNO3 drydep	Science	Katie Travis (Harvard) Jenny Fisher (U. Wollongong)	TBD after FlexChem
A snow NOx source from deep snowpack	Science	Maria Zatko (Ramboll) Becky Alexander (UW)	TBD after FlexChem
Land cover module in GEOS-Chem	Science	Jeffrey Geddes (MIT) Michael Long (Harvard)	TBD after FlexChem
Merge standard simulation with specialty simulations for OVOC, acids, aromatics, dicarbonyls, terpenes	Science	Dylan Millet (UMN) Xin Chen (UMN)	TBD after FlexChem
Automate redistribution of NOx in HEMCO	Science	Lee Murray (NASA GISS/LDEO)	TBD after FlexChem
Injection height for fire emissions	Science	Emily Fischer (CSU)	TBD after FlexChem
Improved lightning emission scheme	Science	Lee Murray (NASA GISS/LDEO)	TBD after FlexChem
Updated halogen chemistry	Science	Tomás Sherwen (York) Johan Schmidt (Harvard)	TBD after FlexChem

		<a href="#">Oxidants and Chemistry WG</a>	
<a href="#">Sedimentation of stratospheric aerosols</a>	Science	Sebastian Eastham (Harvard, formerly MIT)	TBD after FlexChem
<a href="#">Quick fix for low Pb tropospheric lifetime against deposition in GEOS-FP and MERRA-2</a>	Science	Bo Zhang, Hongyu Liu (NIA / NASA Langley)	Under further study by Transport Working Group

## Details for Bug Fixes

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### Fix to restore stratospheric emissions in specialty simulations

Emissions in the stratosphere were disabled in a HEMCO June 2015 update to prevent build-up of stratospheric concentrations due to aircraft emissions (mainly VOCs). This [HEMCO update](#) was merged into GEOS-Chem [v11-01e](#).

While this modification was intended for the [full-chemistry simulations](#), it also inadvertently shut off all emissions above the tropopause in [GEOS-Chem's specialty simulations](#). In particular, the original [v11-01f 1-year Rn-Pb-Be benchmark simulation](#) displayed lower-than-expected stratospheric Be7 fluxes to the troposphere and imbalanced Be7 trop+strat sources and sinks. Christoph Keller recommended maintaining disabled emissions in the stratosphere for at least the full-chemistry simulation.

To correct this, we now only restrict emissions in the stratosphere if performing a full-chemistry simulation and if the [UCX mechanism](#) is turned off. Emissions in the stratosphere are enabled for all specialty simulations. This fix was added to [v11-01f](#) (approved 16 Apr 2016).

### Parallelization bug fix for GEOS-5 Hg simulations

Bob Yantosca ([GCST](#)) found and fixed two parallelization errors that had been causing the GEOS-5 Hg simulations to fail unit tests. Lizzie Lundgren described this error on the wiki:

*There are [inconsistent differences in the diagnostics and ocean restart files](#) when running unit tests on GEOS-5 4x5 and 2x2.5 mercury simulations in [v11-01c](#). When running a test of ten GEOS-5 4x5 Hg unit tests, the trac\_avg file failed with differences seven times and the ocean restart file failed with differences eight times. We have isolated the issue to a single call to depo\_mercury\_mod.F routine ADD\_HG2\_SNOWPACK that occurs in convection\_mod.F routine NFCLDMX. Commenting out the call and conducting ten GEOS-5 4x5 Hg unit tests results in all*

tests passing. The issue appears to be an optimization problem but is currently unresolved.

For specific details about how this problem was fixed, please see [this post on our Mercury wiki page](#).

## Bug fix for incorrect pointer initializations

Bob Yantosca ([GCST](#)) discovered that local pointer variables were being initialized incorrectly in several GEOS-Chem routines. In some instances, this caused GEOS-Chem simulations to exit with a [particular type of error](#) from parallelized DO loops.

In [v11-01g](#), we have now updated the pointer initializations to avoid encountering such errors. For complete information about this fix, please see [this post on our GEOS-Chem v11-01 wiki page](#).

We also believe that this fix will solve [a previously-reported segmentation fault error](#) that sometimes occurs in HEMCO when using [Intel Fortran Compiler](#) version 12 or higher.

## Details for Structural Updates

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### Migration from binary punch file format to netCDF file format

The [HEMCO emissions component](#) contains the capability to save diagnostic output (time-averaged or instantaneous) as well as end-of-run restart information to netCDF files. In v10-01, this feature is used only for emissions-related data. The [GEOS-Chem Support Team](#) is currently leveraging HEMCO's I/O capabilities **to replace all binary punch I/O with netCDF within GEOS-Chem v11-01**. This work has started in [v11-01f](#) and will continue into future internal versions.

Migrating to netCDF format will bring the following benefits:

- Using HEMCO's diagnostic archival capability will ensure that all quantities will be archived consistently throughout GEOS-Chem.
- Using netCDF I/O will facilitate further GEOS-Chem High Performance (aka [GCHP](#)) development, because binary files cannot be written efficiently in high-performance computing (HPC) environments.
- Using netCDF I/O will give GEOS-Chem users more options for visualizing GEOS-Chem output. Many free and open-source software packages (e.g. [Python tools](#)) are compatible with netCDF format. Users will no longer have to rely on expensive proprietary software for visualization (e.g. IDL).



This work will be done in four phases. **Phase 1** added the following updates to [v11-01f](#) (approved 16 Apr 2016):

- Changed the default input and output GEOS-Chem tracer restart files from binary punch to netCDF format (except for the [mercury](#) simulation).
- Saved [chemical species](#) concentrations in the output netCDF restart file in units of [mol/mol] along with [advected tracer](#) concentrations (for full-chemistry simulations).
- Added compile-time options (BPCH\_RST\_IN=y, BPCH\_RST\_OUT=y) to enable reading from or writing to binary punch restart files.

**Phase 2** will bring the following changes into [v11-01g](#) (currently in development):

- Change default input and output GEOS-Chem tracer restart files from binary punch to netCDF format for the mercury simulation.
- Save ocean mercury restart data along with advected tracer concentrations to the output netCDF restart file (for mercury and tagged mercury specialty simulations).
- Remove the compile-time options to enable input and output binary punch restart files (BPCH\_RST\_IN=y, BPCH\_RST\_OUT=y). From this point on, only the netCDF restart files will be used.

**Phase 3** is currently slated for v11-01h, with **Phase 4** to follow. For more information about these phases of development, please see [this post on our GEOS-Chem Output Files wiki page](#).

## Improved species indexing and faster name search

GEOS-Chem versions prior to v11-01 carry **advected tracers** and **chemical species** in separate arrays. This is due to the structure of the original models from which GEOS-Chem was constructed.

**Advected tracers** in GEOS-Chem are those species which are subject to [transport](#), [cloud convection](#), [boundary layer mixing](#), and [wet deposition](#). (They may also [dry deposit](#).) Historically, advected tracers have been read from restart files in volume mixing ratio, then were converted to kg and further converted to molec/cm<sup>3</sup> before being passed into the chemistry modules. Prior to [GEOS-Chem v9-02](#), advected tracers were stored in the STT array (which has since been replaced with State\_Chm%Tracers).

Indices of advected tracers are currently stored in integer variables (beginning with the letters IDT) in the module tracerid\_mod.F. These IDT\* variables were initialized in a big DO loop in routine TRACERID ([see this wiki post](#) for more information) during the initialization phase.

**Chemical species** are those GEOS-Chem species that are listed as reactants or products in one of [GEOS-Chem's chemistry mechanisms](#) (e.g. benchmark, tropchem, UCX, SOA, or SOA-SVPOA). Chemical species, which traditionally have been read from a separate binary punch restart file, are stored in the SMVGEAR solver array CSPEC and have units of molec/cm<sup>3</sup>.

Many chemical species (such as NO, O<sub>3</sub>, CO, etc.) are also [advected tracers](#); that is, they are moved around by the winds and convective mass fluxes. On the other hand, several species (notably OH) are not advected tracers. This is because the lifetime of these species are so small that they never get transported outside of the confines of the grid box where they are created.

The SMVGEAR chemistry solver routines used a separate set of integer variables to store indices of species in the chemical mechanism. These variables (which began with ID) were defined in a separate DO loop in routine SETTRACE, also located in module GeosCore/tracerid\_mod.F ([see this wiki post](#) for more information).

Further complicating matters is the fact that [the mercury simulation modules rely on separate indexing variables](#) which are also stored in tracerid\_mod.F.

As the number of GEOS-Chem full-chemistry and specialty simulations increased, more tracer ID's (the IDT\* variables) and species ID's (the ID\* variables) had to be added to tracerid\_mod.F. This was not only a very messy approach, but it also complicated the setup of new chemistry mechanisms. The implementation of the Hg tagged tracer indices was also cumbersome and needed to be streamlined.

In [GEOS-Chem v11-01](#), we shall retire the SMVGEAR chemistry solver and replace it with FlexChem, a new, clean implementation of the KPP chemical solver. This is necessary in order to obtain the best performance when running GEOS-Chem in HPC environments. FlexChem will also allow GEOS-Chem users to change chemistry mechanisms on-the-fly, without having to hardwire many variables in many different locations throughout GEOS-Chem.

The new [GEOS-Chem species database](#)—added in intermediate version [v11-01e](#)—now provides a central location for storing the [physical properties of GEOS-Chem species](#), including names, indices, molecular weights, and Henry's law constants. It also contains logical flags that denote whether a given species is advected, dry deposited, or wet scavenged, as well the location of the species in the KPP chemical solver matrix.

As a result, the distinction between advected tracers and chemical species is now becoming a little more blurry. We can now speak of everything as a GEOS-Chem "species". Some species are advected, some are dry-deposited, and some are wet-deposited. Some species are contained in one of the KPP chemical mechanisms, and others are not. We therefore needed a new method for obtaining information about a species from its name.

We will bring the following improvements into GEOS-Chem [v11-01g](#), simultaneously with the FlexChem implementation:

1. We will now use a single array field to store all GEOS-Chem species concentrations. Instead of having to store tracer concentrations in `State_Chm%Tracers` and species concentrations in `State_Chm%Species`, we can store all concentrations in `State_Chm%Species`. We can then select a desired subset of species from `State_Chm%Species` and then pass them to the various chemistry, convection, transport, wet deposition, and dry deposition modules as needed.
2. We will also give GEOS-Chem a [faster algorithm to return the index of a species given its name](#). The new algorithm relies on integer searches instead of string comparisons, and is approximately 30-40 times faster. This will allow us to look up the index of any species stored in `State_Chm%Species` without having to add specific integer variables to `tracerid_mod.F`.
3. Lastly, we will move the index arrays used by the mercury simulations out of `tracerid_mod.F` and into the `State_Chm` derived-type object. This will finally allow us to retire `tracerid_mod.F` once and for all.

For more detailed information, please see [our new \*Species indexing in GEOS-Chem\* wiki page](#).

## Details for Notable Emissions Fixes

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### Restoration of the tagged CO simulation

Bob Yantosca ([GCST](#)) has added several modifications to the tagged CO simulation in order to allow HEMCO to compute emissions for the various tagged CO tracers. An updated `HEMCO_Config.template` file will now ship with the [GEOS-Chem Unit Tester](#).

The tagged CO simulation is set up to read QFED biomass emissions from disk by default. It is straightforward to split the total QFED emissions among the various tagged tracers by [applying regional masks](#) (as specified in the HEMCO configuration file).

At present, HEMCO cannot split GFED or FINN biomass emissions into regional tagged tracers, because these emissions are implemented as HEMCO extensions. Users who wish to run tagged CO simulations with GFED or FINN biomass emissions can (1) use the [HEMCO standalone interface](#) to save offline GFED or FINN biomass emissions to netCDF files and (2) update the HEMCO configuration file to read the offline emissions from the netCDF files and apply the relevant regional masks.

For more information, please see [this post on our \*Tagged CO simulation\* wiki page](#).

## Updated photoreduction constants and soil emissions for Hg simulations

Jenny Fisher updated the photoreduction constants and [soil emissions](#) for consistency with the recent mercury updates added to GEOS-Chem v11-01 (for 4x5 resolution and GEOS-FP/GEOS-5 met fields). For more information, see the [note for new users](#). This update will be added to [v11-01g](#).

## Details for Notable Chemistry Fixes

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### Optimal transport and timestep settings are now the GEOS-Chem defaults

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 these optimal timestep settings for use with GEOS-Chem simulations. Starting with [GEOS-Chem v11-01f](#), the `input.geos.template` files in the [GEOS-Chem Unit Tester](#) now use these optimal timestep settings. When you generate a GEOS-Chem run directory for v11-01f and higher versions, these optimal timesteps will automatically be added to the `input.geos` file as defaults. Users may choose to run with coarser timesteps for faster turnaround with lower accuracy.

## Ongoing GEOS-Chem Development Projects

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### FlexChem status report

We have achieved the following milestones in our integration of the FlexChem chemistry solver package into GEOS-Chem:

Milestone	Developer	Date
Added FlexChem into v11-01c. Enabled the “tropchem” mechanism.	Mike Long	14 Dec 2015
Restored the OH and HO2 diagnostics (ND43)	Melissa Sulprizio	18 Dec 2015
Removed CSPEC array and replaced with State_Chm%Species	Melissa Sulprizio	22 Dec 2015
Enabled a workaround for family tracers (ISOPN, MMN)	Mike Long	25 Jan 2016
Enabled FAST-JX photochemistry	Mike Long	25 Jan 2016
Enabled the “benchmark” chemistry mechanism	Melissa Sulprizio	29 Jan 2016
Fixed HBr and HOBr hetchem rates for the “tropchem” mechanism	Melissa Sulprizio	04 Feb 2016
Fixed unit conversions for heterogeneous chemistry	Mike Long	18 Feb 2016
Restored the broken J-value diagnostic (ND22)	Melissa Sulprizio	15 Mar 2016
Parallelized the main KPP driver loop; fixed other minor issues	Bob Yantosca	30 Mar 2016
Enabled the SOA and SOA-SVPOA mechanisms	Lizzie Lundgren	01 Apr 2016
Added more parallelization fixes	Bob Yantosca	18 Apr 2016
Merged FlexChem with v11-01f	Melissa Sulprizio	20 Apr 2016
Added KPP repository to Bitbucket ( <a href="https://bitbucket.org/gcst/kpp">https://bitbucket.org/gcst/kpp</a> )	Mike Long	19 April 2016
Created new gckpp* files from the updated KPP solver package	Melissa Sulprizio	22 Apr 2016
Enabled the UCX mechanism	Melissa Sulprizio	26 April 2016
Introduced a prod/loss diagnostic into the KPP solver package	Mike Long	29 Apr 2016
Fixed various other bugs and cleaned up some leftover things	Melissa Sulprizio	04 May 2016
Completed unit tests and 1-month benchmarks for the tropchem, benchmark, UCX, SOA, and SOA-SVPOA simulations	Melissa Sulprizio Lizzie Lundgren	05 May 2016

The following tasks either still need to be completed, or already have been completed but are not merged into the FlexChem development code:

Milestone	Developer	Status
Remove tracer indices of Rn, Pb, Be, Hg, and POPs simulations from tracerid_mod.F. (This paves the way for us to retire tracerid_mod.F.)	Bob Yantosca	Done 02 May 2016; not yet merged with FlexChem
<a href="#">Add a fast species name lookup algorithm</a>	Bob Yantosca	Done 04 May 2016; not yet merged with FlexChem
Store the unique list of GEOS-Chem species in the <a href="#">GEOS-Chem species database object</a> . (In other words, we combine the list of <a href="#">advected tracers</a> with the list of <a href="#">KPP chemical species</a> and remove duplicate entries).	Bob Yantosca	Done 09 May 2016; not yet merged w/ FlexChem
Store the indices of each species in the KPP chemical reaction matrix in the GEOS-Chem species database object.	Bob Yantosca	Done 09 May 2016; not yet merged with FlexChem
Store all species concentrations in State_Chm%Species (thus making State_Chm%Tracers redundant)	GCST	Imminent
Remove tracerid_mod.F from GEOS-Chem. Rely totally on the GEOS-Chem species database for looking up a species index from its name.	GCST	Imminent
Remove 1-D array indices (e.g. JLOOP, IJLOOP) from GEOS-Chem	Melissa Sulprizio	In progress
Update the GEOS-Chem Makefiles so that a fresh version of KPP will be built (using a custom chemical mechanism that you specify) each time GEOS-Chem is compiled.	TBD	TBD
Attach KPP prod/loss diagnostics to GEOS-Chem's netCDF diagnostic output capability.	TBD	TBD
Remove the remaining family tracers (ISOPN, MMN). Henceforth, FlexChem will only work with individual species.	TBD	TBD
Validate FlexChem with additional debugging, unit testing, and benchmarking	TBD	TBD
Update GEOS-Chem documentation and user manual for v11-01	TBD	TBD

We will be working on the remaining FlexChem integration tasks this summer.

## MERRA-2 Update

GEOS-Chem can now be driven by the NASA/GMAO [MERRA-2](#) meteorological reanalysis data product. MERRA-2 is a long-term reanalysis (30+ years of data) created with version 5.12.4 of the NASA GEOS-5 Data Assimilation System. Several [GEOS-Chem specialty](#)

[simulations](#) (including Radon, Mercury, POPs, Tagged O3, and CH4) can already use the MERRA-2 meteorology. Melissa Sulprizio ([GCST](#)) has added compatibility for MERRA-2 into the full-chemistry simulations (benchmark, tropchem, UCX, SOA-SVPOA, etc.) in [v11-01f](#). For more information, please see the results of the [1-month benchmark](#) and [1-year benchmark](#) for v11-01f using MERRA-2 meteorology.

Junwei Xu ([GCST](#)) is now processing MERRA-2 met fields for the entire coverage period (1980–present). The MERRA-2 met fields will be available on the global 4°x5° and 2°x2.5° grids and on the nested Asia, Europe, and North America grids at 0.5°x0.625° resolution. The nested China/SE Asia grid for MERRA-2 is now referred to as the nested Asia grid since this domain has been expanded to include India and Japan (10°S–55°N, 60°E–150°E).

The following years of MERRA-2 data are now available for download at the Dalhousie server (rain.ucis.dal.ca): 2001-2007 and 2011-2015.

## GEOS-Chem High Performance update

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### You can now download the GCHP development kit!

We're excited to announce that the **GEOS-Chem High Performance Development Kit** ([GCHP Dev Kit](#)) is available!

GCHP is an MPI-capable version of the established GEOS-Chem model, and will eventually replace the standard, single-node code (henceforth known as "GEOS-Chem Classic"). This is the first field test of GCHP; if it goes well, we will use this as a template for a forthcoming public alpha release. Right now, GCHP has the following advantages over the GEOS-Chem Classic model:

- **Multi-node architecture:** As GCHP uses MPI rather than OpenMP for parallelization, it can be run on an arbitrary number of cores, and over an arbitrary number of machines.
- **Ultra-fine resolution global simulations:** Without the memory limits of a single-machine architecture, the only limit on GCHP is the resolution of your input data.
- **No more polar singularity:** GCHP uses the "cubed-sphere" geometry for all operations, leveraging the GFDL FV-cubed (FV3) transport core. This avoids the polar singularity inherent to regular lat-lon grids.
- **HEMCO used for all inputs:** Every initial and boundary condition is now read from NetCDF files through HEMCO. This means that all data, including met data, can be regridded on the fly.

- **Grid-independent compile process:** Grid resolution is set at run time, and no recompilation is required.

Currently, GCHP is still in alpha; it is **not yet ready for use in scientific analysis**. However, by downloading and setting up GCHP now, you will see the following advantages:

- **Future-proof your work:** By getting started with the development kit, you'll be ready to start simulations as soon as GCHP v1.0 is released. You can also make sure that the changes and advances you are working on with GEOS-Chem classic will be compatible with the next iteration of GEOS-Chem.
- **Narrow-focus support:** Once GCHP v1.0 becomes the standard version of GEOS-Chem, we anticipate a high volume of support requests. If you download and set up the GCHP development kit now, we can dedicate more resources to helping you get started.
- **Help bring launch day closer:** Even if all you do is install GCHP and run the first test case, you'll be helping to advance the code. We need to make sure that GCHP can be smoothly installed in as many environments as possible by as many users as possible, and that means we need to test it on as many different platforms and in as many different locations as we possibly can.

GCHP has some bugs that we know about, and almost certainly many others that we don't. To help us find and fix these, we've set up some tests which you can run after download. Instructions for downloading, compiling and running GCHP are available in the GCHP Development Kit Instructions, which can be found online on [our \*GEOS-Chem HP Dev Kit\* wiki page](#).

If you do download and install GCHP, please let us know! Even if everything went completely to plan, the more data points we have about people's experience with the install and test process, the better the experience will be by the "official" launch day. The point person for this release is Matt Yannetti - get in touch at [myannetti@seas.harvard.edu](mailto:myannetti@seas.harvard.edu).

## GCHP validation

Matt Yannetti has been creating plots comparing output from GCHP simulations to output obtained from GEOS-Chem "Classic". These will be available shortly.

## Conclusion

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We are currently working to merge several open lines of GEOS-Chem development together. Our highest priority is to add the new FlexChem chemistry solver into v11-01g. FlexChem will facilitate GEOS-Chem simulations at high-resolution, not only with our current nested model capability, but also with our high-performance GCHP model.



But before FlexChem can be completely integrated into GEOS-Chem, a significant amount of structural programming (updating diagnostics, adding the fast species indexing scheme, removing obsolete infrastructure) has to be done simultaneously. We will strive to complete this work this summer. We ask for your patience during this process.

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, Matt, Lizzie, Mike, Junwei, Yanko)