

# GEOS-Chem Newsletter

## Summer 2016 Edition

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*GEOS-Chem Support Team*  
*19 August 2016*

### Table of Contents

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Table of Contents.....	1
GEOS-Chem Steering Committee news.....	2
Meeting minutes 19 August 2016.....	2
Guiding principles for updates to the GEOS-Chem model.....	2
GEOS-Chem v11-01 Development Overview.....	2
GEOS-Chem v11-01g.....	3
Remaining updates for v11-01.....	3
Structural Updates.....	5
Removal of the distinction between “tracers” and “species”.....	5
Removal of the State_Chm%Tracers array.....	6
Removal of the STT Pointers and Select Input_Opt Variables.....	7
Retirement of tracid_mod.F.....	7
Addition of the Ind_() function for species indexing.....	8
Migration of restart files from binary punch to netCDF file format.....	9
Chemistry Updates.....	9
FlexChem milestones.....	9
New production and loss diagnostics.....	11
Emissions updates.....	11
Correct bug in units of EDGAR v4.2 SO2 emissions.....	11
Prevent biofuel emissions from being double counted.....	12
Fix bug in CH4 emissions.....	12
Dynamics updates.....	12
Removal of moisture signature from tracer concentrations in dry mixing ratio.....	12
Other issues that will be resolved in v11-01.....	13

Fix to remove strange cycle in OH caused by TOMS overhead O3 errors.....	13
Update to GEOS-FP re-evaporation calculation.....	14
Fix for monthly stratospheric P/L rates in HEMCO.....	15
Fixed errors routine in DO_STRAT_CHEM.....	16
GEOS-Chem High Performance update.....	16
You can now download the GCHP development kit!.....	16
Future developments.....	18
Reading met fields via HEMCO and flexible grid definitions.....	18
Conclusion.....	18

## GEOS-Chem Steering Committee news

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### Meeting minutes 19 August 2016

The GEOS-Chem Steering Committee met by conference call on Friday 19 August 2016. We encourage you to [read the meeting minutes](#), which are posted online.

### Guiding principles for updates to the GEOS-Chem model

On 19 August 2016, the GEOS-Chem Steering Committee approved a document entitled [Guiding Principles for Updates to the GEOS-Chem Model](#), which is now posted online. This document gives some guidelines for developers and Working Group chairs on how best to prioritize and schedule new updates for inclusion into GEOS-Chem.

## GEOS-Chem v11-01 Development Overview

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GEOS-Chem v11-01 development is ongoing. We are validating the new [FlexChem](#) chemical solver in [v11-01g](#). FlexChem is currently producing output consistent with the prior [v11-01f](#).

In addition, we have nearly completed the process of removing SMVGEAR and its legacy infrastructure from GEOS-Chem. We expect that these updates will cause GEOS-Chem to perform much more efficiently than before.

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 v11-01g

GEOS-Chem v11-01g is still in development as of August 2016. This version will include the FlexChem solver, as well as some important new structural updates.

This version will require a 1-month benchmark simulation and a 1-year benchmark simulation.

Feature	Type	Submitted by	Status
<a href="#">FlexChem</a>	Science	Mike Long (Harvard) and <a href="#">GCST</a>	Validation of the existing code is ongoing.
<a href="#">NetCDF Output Phase 2: Use NetCDF restart files for Hg simulation</a>	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>	Structural	<a href="#">GCST</a>	Pending benchmark approval
<a href="#">Update High Performance GEOS-Chem (GCHP) Dev release</a>	Structural & Bug fix	Seb Eastham (Harvard) <a href="#">GCST</a>	In development
<a href="#">Parallelization bug fix: nullify local pointers outside declaration</a>	Structural	<a href="#">GCST</a>	Completed 29 Apr 2015
<a href="#">Improve species indexing</a>	Structural	<a href="#">GCST</a>	Completed 24 Jun 2016

## Remaining updates for v11-01

The updates listed in this table will be broken up into several distinct 1-month benchmark versions (v11-01h, v11-01i, etc.), denoted by alternating colors. Some updates will be introduced in v12.

Feature	Version	Type	Submitted by	Status
<a href="#">Fix to remove moisture signature in dry mixing ratio</a>	v11-01h	Bug fix	Meemong Lee (JPL) Kevin Bowman (JPL) Richard Weidner (JPL) Lizzie Lundgren (GCST)	Delivered to GCST

<a href="#">Fix bug in GEOS-FP re-evaporation calculation</a>	v11-0i	Bug fix	Virah Shah (UW) Bo Zhang (NIA) Hongyu Liu (NIA/NASA Langley)	Delivered to GCST (Jul 2016)
<a href="#">Add PM2.5 diagnostic</a>	v11-01i	Science	<a href="#">GCST</a>	TBD
<a href="#">Fix for TOMS/HEMCO to address strange cycle in OH output</a>	v11-01j	Bug fix	Barron Henderson (U. Florida)	Delivered to GCST (Jul 2016)
<a href="#">Correct bug in units of EDGAR v4.2 SO2 emissions</a>	v11-01j	Bug fix	Jaegun Jung (Ramboll Environ)	Delivered to GCST (Apr 2016)
<a href="#">Prevent biofuel emissions from being double counted in EDGAR v4.2</a>	v11-01j	Bug fix	<a href="#">GCST</a>	Delivered to GCST (May 2016)
<a href="#">Fix for monthly stratospheric P/L rates in HEMCO</a>	v11-01j	Bug fix	Christoph Keller (NASA GSFC)	Delivered to GCST (Jul 2016)
<a href="#">Fix bug in CH4 emissions</a>	v11-01j	Bug fix	Melissa Sulprizio (GCST)	In progress
<a href="#">Update HEMCO from version 1.1.016 to latest version available</a>	v11-01j	Structural	Christoph Keller (NASA GSFC)	In progress
<a href="#">Add option for QFED &amp; FINN emissions in the Hg simulations</a>	v11-01j	Science	Jenny Fisher (Wollongong)	Delivered to GCST (Apr 2016)  NOTE: Requires the latest HEMCO updates
<a href="#">Use TOMS ozone for all years when running simulations with GEOS-5</a>	v11-01j	Science	Jenny Fisher (Wollongong)	Delivered to GCST (Apr 2016)
<a href="#">Updates to TOMAS Jeagle sea salt extension</a>	v11-01j	Science	Jack Kodros (Colorado State)	Delivered to GCST (Jul 2016)
Halogen chemistry updates	TBD	Science	Tomás Sherwen (York) Johan Schmidt (Harvard) <a href="#">Oxidants and Chemistry WG</a>	Will go in after FlexChem
<a href="#">Updating chemistry rate constants based on JPL Publication 15-10</a>	TBD	Barron Henderson (U. Florida) Mat Evans (U. York)	Science	Will go in after FlexChem

<a href="#">Set ACTA and HCOOH to active</a>	TBD	Bug fix	Katie Travis (Harvard)	Delivered to GCST
<a href="#">NetCDF Output Phase 3a: Output diagnostics in NetCDF format</a>	TBD	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>	TBD	Bug fix	<a href="#">GCST</a> , Christoph Keller	In progress
<a href="#">PAN updates</a>	TBD	Science	Emily Fischer (CSU)	Delivered to GCST, partially implemented into development code
<a href="#">Monthly mean surface methane distributions</a>	TBD	Science	Lee Murray (NASA GISS/LDEO)	Awaiting code from developer
<a href="#">Ocean ammonia emission inventory</a>	TBD	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>	TBD	Science	Xuan Wang (MIT)	Delivered to GCST

## Structural Updates

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### Removal of the distinction between “tracers” and “species”

**Advected tracers** in GEOS-Chem are those species which are subject to transport, cloud convection, boundary layer mixing, wet deposition and dry deposition. Historically, advected tracers are read from restart files in volume mixing ratio ( $v v^{-1}$ ), are then converted to kg, and undergo several unit conversions throughout GEOS-Chem.

**Chemical species** are those species that are listed as reactants or products (either of gas-phase or photolysis reactions) in one of [GEOS-Chem's chemistry mechanisms](#). Chemical species, which traditionally have been read from a separate restart file, are stored in the SMVGEAR solver array CSPEC and have units of  $\text{molec cm}^{-3}$ .

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 short that they never get transported outside of the confines of the grid box where they are created.

For compatibility with the legacy SMVGEAR solver, GEOS-Chem has been constrained to store advected tracer concentrations [mixing ratio or kg] in a separate array from the chemical species concentrations [molec cm<sup>-3</sup>]. This duplication of storage substantially increases the amount of memory needed to run a GEOS-Chem simulation.

Recent new developments allow us to lift this restriction:

- [The GEOS-Chem species database](#) (introduced in [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 stores logical flags that denote whether each species is advected, is dry deposited, or is wet scavenged.
- [FlexChem](#) (which is being added to [v11-01g](#)) is a clean and computationally efficient implementation of the KPP chemical solver. As such, FlexChem does not rely on any of the legacy SMVGEAR infrastructure.

As a result of these developments, the distinction between advected tracers and chemical species now becomes a little more blurred. We can now speak of everything as a GEOS-Chem "species". Some species are advected, some are dry-deposited, and some are wet-deposited, and some belong to one of the KPP chemical mechanisms. As described in the following section, removing the distinction between "tracers" and "species" will allow us to remove legacy code that currently prevents optimal GEOS-Chem execution.

## Removal of the `State_Chm%Tracers` array

Due to SMVGEAR's legacy infrastructure, those chemical species that are also advected (e.g. NO, O<sub>3</sub>, CO, ISOP, etc.) actually get stored twice in GEOS-Chem.

1. The `State_Chm%Tracers` array holds the concentrations of these advected species in varying units: v v<sup>-1</sup> or kg in v10-01 and prior versions, and mostly kg kg<sup>-1</sup>dry air, but also kg, v v<sup>-1</sup>, or kg/m<sup>2</sup>, in v11-01.
2. The `State_Chm%Species` array holds the concentrations of non-advected species in molec cm<sup>-3</sup>.

Further complicating matters, each time chemistry is called, GEOS-Chem copies the non-advected chemical species concentrations (in molec cm<sup>-3</sup>) from the `State_Chm%Species` array to an internal SMVGEAR array named CSPEC. Not only does GEOS-Chem have to allocate additional memory to the CSPEC array, the constant copying of data between the two arrays incurs computational overhead. This extra memory and overhead can adversely affect GEOS-Chem simulations, particularly when running at extremely fine resolution (e.g. 1/4° nested or global grids).

In [v11-01](#), we replace the obsolete SMVGEAR chemistry solver a new, clean implementation of the KPP chemical solver which we call FlexChem. This is necessary to obtain the best performance when running GEOS-Chem in high-performance computing environments. As a result, we no longer need to preserve the SMVGEAR method of having to store advected species separately from the non-advected species.

Starting in v11-01g, we use a single array field to store GEOS-Chem species concentrations. We preserve the `State_Chm%Species` array and remove all references to the now-obsolete `State_Chm%Tracers` and `CSPEC` arrays. The appropriate unit conversions will be applied to the concentrations stored in `State_Chm%Species` so as to closely preserve the behavior of prior GEOS-Chem versions. This work is nearing completion as of this writing.

## Removal of the STT Pointers and Select Input\_Opt Variables

In [v11-01g](#) we also remove references to the local variables named `STT` that point to the `State_Chm%Tracers` array. For example, we will remove instances of code such as:

```
STT => State_Chm%Tracers
```

And replace these with

```
Spc => State_Chm%Species
```

The name `STT` no longer has a relevant meaning in GEOS-Chem. It originally came from the old Harvard-GISS CTM from which GEOS-Chem was originally built.

Going forward, we shall now use `Spc` as an alias for `State_Chm%Species`. This abbreviation makes it more apparent that `Spc` is pointing to the GEOS-Chem chemical species array.

We are also removing several `Input_Opt` variables that are no longer necessary with the species database. These include `TRACER_MW_G`, `TRACER_MW_KG`, `XNUMOL`, and `TCVV`.

## Retirement of `tracerid_mod.F`

In [v10-01](#) and prior GEOS-Chem versions, the location of each advected tracer in the `State_Chm%Tracers` array was stored in an integer variable (e.g. `IDTNO`, `IDT03`, `IDTCO`, etc.) located in the module `GeosCore/tracerid_mod.F`. These `IDT*` variables were initialized in routine [TRACERID](#), which was called during the initialization phase of GEOS-Chem.

The `SMVGEAR` chemistry solver kept another set of indices. These integer variables (e.g. `IDOH`, `ID03`, `IDISOP`, etc.) denoted the position of each species in the `SMVGEAR` master chemical concentration array (aka `CSPEC`). They were defined in routine [SETTRACE](#), also located in module `GeosCore/tracerid_mod.F`.

The integration of `FlexChem` into v11-01g has now rendered these `IDT*` and `ID*` indexing variables obsolete. The `KPP` chemical solver computes its own set of index variables that denote the position of each species in the `KPP` chemical mechanism matrix. This means that the prior indexing scheme is now incompatible with `FlexChem`. Furthermore, the `KPP` species indexing has been incorporated into the [GEOS-Chem species database](#). The species database is now used to obtain the position of each species in the list of advected species, dry-deposited species, wet-deposited species, and `KPP` chemical species.

In June 2016, several members of the Jacob research group at Harvard participated in the first ever GEOS-Chem Code-A-Thon resulting in the complete removal of `GeosCore/tracerid_mod.F` from v11-01g.

## Addition of the Ind\_() function for species indexing

In GEOS-Chem v11-01g we have added a new function that performs a fast name-to-index search. This work was also done as part of the Code-A-Thon that took place in June 2016.

Function Ind\_() (located in Headers/state\_chm\_mod.F90) can be used to look up the position of a species in the State\_Chm%Species array given the species name. Here is a simple example of how you can use this function:

```
SUBROUTINE MySub( ..., State_Chm, ... )

  !%% MySub is an example of the new indexing scheme %%

  ! USE statements
  USE GIGC_State_Chm_Mod, ONLY : Ind_

  ! Local variables
  INTEGER :: id_O3, id_CO

  ! Find tracer indices with function the Ind_() function
  id_O3 = Ind_ ( 'O3' )
  id_CO = Ind_ ( 'CO' )

  ! Print species concentrations
  IF ( id_O3 > 0 ) THEN
    print*, 'O3 at (23,34,1) : ', State_Chm%Species(23,34,1,id_O3)
  ENDIF
  IF ( id_CO > 0 ) THEN
    print*, 'CO at (23,34,1) : ', State_Chm%Species(23,34,1,id_CO)
  ENDIF

END SUBROUTINE MySub
```

The Ind\_() function by default will return the species index (i.e. the [ModelId](#) value in the GEOS-Chem species database). You may also tell Ind\_() to return other species indices by passing an optional second argument. For example:

```
AdvectId = Ind( 'HN03', 'A' ) ! Position in list of advected species
DryDepId = Ind( 'HN03', 'D' ) ! Position in list of drydep species
WetDepId = Ind( 'HN03', 'W' ) ! Position in list of wetdep species
KppFixId = Ind( 'HN03', 'F' ) ! Position in list of KPP inactive species
KppVarId = Ind( 'HN03', 'V' ) ! Position in list of KPP active species
```

The Ind\_() function will return -1 if a species does not belong to any of the above lists.



## Migration of restart files from binary punch to netCDF file format

In [v11-01f](#) and [v11-01g](#) we completed the replacement of the traditional GEOS-Chem restart files in [binary punch format](#) with netCDF format restart files. With the removal of tracers, the restart files now contain all GEOS-Chem species concentrations which are archived in mixing ratio units ( $v v^{-1}$  dry air) and saved to netCDF restart files named `GEOSChem_restart_YYYYMMDDhhmm.nc`.

GEOS-Chem species are saved to the netCDF restart file by name instead of by separate category and species number fields. This removes the former restriction of having to list all of the species for a given GEOS-Chem simulation in sequential order. It will also make it easier to add new species to a restart file, which can be done using open-source netCDF tools (e.g. NCO, CDO).

Other relevant restart quantities (e.g. ocean mercury fields for the Hg specialty simulation) are now saved to the same netCDF restart file where the GEOS-Chem species concentrations are archived.

For the v11-01 public release, we will provide tools that you can use to convert an existing binary punch format restart file to the new netCDF format. This will let you adapt your restart files from older GEOS-Chem simulations into the proper format for v11-01.

**NOTE:** Because the HEMCO emissions component is a separate code module, all HEMCO restart quantities (e.g. soil NO<sub>x</sub> parameters) will continue to be saved to the separate HEMCO restart file named `HEMCO_restart.YYYYMMDDhhmm.nc` file. Therefore, the new GEOS-Chem restart files do not replace the existing HEMCO restart files.

**ALSO NOTE:** As of this writing we have not yet migrated the Global Terrestrial Mercury Model (GTMM) restart file from binary punch to netCDF format.

## Chemistry Updates

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### FlexChem milestones

The following table lists recent milestones that were achieved in the implementation of the new FlexChem chemical solver since the last GCSC meeting (16 May 2016):

Task	Developer	Status
Merge FlexChem with other <a href="#">v11-01g</a> updates and bug fixes	Bob Yantosca	Completed 17 May 2016
Remove family tracer fields of the <code>Input_Opt</code> object, namely: <code>TRACER_N_CONST</code> , <code>TRACER_CONST</code> , <code>TRACER_COEFF</code> , <code>ID_EMITTED</code> . These were only used by SMVGEAR and are now obsolete.	Bob Yantosca	Completed 18 May 2016
Create mapping vectors in the <code>State_Chm</code> object to store the ID numbers of species that are advected, dry-deposited, wet-deposited, and/or included in the KPP chemical mechanism	Bob Yantosca	Completed 19 May 2016

Remove all 1-D loop indexing variables (JLOOP, KLOOP, KTLLOOP, JLOP, IXSAVE, IYSAVE, IZSAVE) that were used by SMVGEAR	Melissa Sulprizio	Completed 19 May 2016
Remove SMVGEAR input files (globchem.dat, mglob.dat) and associated subroutines (readchem.F, reader.F)	Melissa Sulprizio	Completed 30 Jun 2016
Remove tracerid_mod.F and related tracer ID flags (IDTxxxx, IDxxxx) from GEOS-Chem.	Jacob Group Code-A-Thon	Completed 24 Jun 2016
Use the GEOS-Chem species database to retrieve species index from species name	GCST	Completed 24 Jun 2016
Remove tracers from restart files and read/write restart file species only	Lizzie Lundgren	Completed 12 Jul 2016
Create unit conversion routines for species that mimic existing routines for tracers or convert to/from molecules/cm3	Lizzie Lundgren	Completed 25 Jul 2016
Add State_Chm variable to track species units throughout GEOS-Chem (State_Chm%Spc_Units)	Lizzie Lundgren	Completed 25 Jul 2016
Remove the remaining family tracers (ISOPN, MMN, CFCX, HCFCX). Henceforth, FlexChem will only work with individual species.	Melissa Sulprizio	Completed 28 Jul 2016
Move the non-advected species initial unit conversion of background values from INIT_FLEXCHEM (called during chemistry) to READ_GC_RESTART (called during restart file read)	Lizzie Lundgren	Completed 4 Aug 2016
Store species background concentrations values previously stored in globchem.dat in the species database	Lizzie Lundgren	Completed 11 Aug 2016
Rebuild Standard, Tropchem, UCX, SOA, SOA-SVPOA chemistry mechanisms to use the new prod/loss functionality in KPP (i.e. FLUX on)	Melissa Sulprizio	Completed 13 Jul 2016
Attach the new KPP prod/loss output to the GEOS-Chem prod/loss diagnostic (ND65)	Melissa Sulprizio	Completed 11 Aug 2016
Remove State_Chm%Tracers and use species concentrations in State_Chm%Species instead	GCST	In progress
Rebuild Standard, Tropchem, UCX, SOA, SOA-SVPOA chemistry mechanisms with <a href="#">Kppa</a>	GCST	TBD
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.	GCST	TBD

Validate FlexChem with additional debugging, unit testing, and benchmarking	GCST	TBD
Update GEOS-Chem documentation and user manual for v11-01	GCST	TBD

We are confident that FlexChem is working as it is designed to. Most of the remaining work involves removing of the legacy infrastructure that remains from the SMVGEAR solver.

## New production and loss diagnostics

Mike Long implemented prod/loss structure parsing in the KPP source code. The pre-built [chemistry mechanisms](#)—Standard (aka “benchmark”), UCX, TropChem, SOA, and SOA-SVPOA—were built with this new prod/loss diagnostic turned on. The prod/loss rates from KPP can now be saved out in GEOS-Chem via the traditional ND65 diagnostic.

At present, the new prod/loss diagnostic output in KPP is not yet complete. We are working to resolve the following issues:

1. The current implementation of the prod/loss diagnostics computed production and loss for individual species but not for families (i.e. P(Ox), L(Ox), P(BrOx), L(BrOx), etc.). We are currently building this capability into the KPP chemical solver code in v11-01g.
2. The prod/loss diagnostic as it stands now is somewhat inefficient. The code is set up so that KPP calculates the prod/loss of ALL species, even though a user may only want prod/loss rates for a few species. This likely adds considerable memory overhead. Making this code more efficient is a priority for future development.

## Emissions updates

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GEOS-Chem users have submitted updates that will fix minor errors in the current emissions configuration. These are listed below.

### Correct bug in units of EDGAR v4.2 SO2 emissions

Jaegun Jung wrote:

*EDGAR v4.2 SO2 – A README file and HEMCO configuration file say that the file has a unit of kgSO2 while in the emission netcdf file header shows kg(S). I calculated annual emission rate by creating HEMCO diagnostic output file. The value that I have is about 40 – 50 % from what is reported in the [EDGAR in GEOS-Chem PDF](#).*

*But, when I multiply by  $Mw(SO_2)/Mw(S)$ . It gets much closer within 10%. So I am pretty sure that the README and HEMCO configuration file are wrong.*

To fix this bug, the SULFUR2SOX scale factor (scalID 62) should be added to the EDGAR v4.2 SO2 and SO4 entries in the HEMCO configuration file HEMCO\_Config.rc. For example:

0 EDGAR\_S02\_1A1a\_6C ... C xy kg/m2/s S02 11/42/31/62 1 2

etc. We will correct this issue in the HEMCO configuration files that ship with the GEOS-Chem v11-01 public release.

## Prevent biofuel emissions from being double counted

EDGAR v4.2 includes biofuel emissions in their 1A4 category. From [the EDGAR website](#):

*EDGAR Factsheet - Energy: Combustion in 1A4*

*Stationary combustion in residential, commercial and public services, agriculture, forestry, fisheries and other sectors.*

However, in the default HEMCO configuration file (`HEMCO_Confi g. rc`) that source is only being added to HEMCO Category 1 (i.e. anthropogenic emissions). Instead the `EDGAR_*_1A4` entries should be changed from:

0 EDGAR\_NO\_1A4 ... NO 1/40/25/30 1 2

to:

0 EDGAR\_NO\_1A4 ... NO 1/40/25/30 1/2 2

in order to reflect that this source includes both anthropogenic and biofuel emissions. Otherwise, GEOS-Chem double counts biofuel emissions by including both EDGAR's 1A4 source and the Yevich and Logan biofuel emissions. This should only impact South America, Africa, Russia, and Australia because biofuel emissions over the other regions are zeroed to account for the fact that the existing regional inventories (BRAVO, CAC, NEI2011, EMEP, MIX) already include biofuel emissions.

This fix will be added to the HEMCO configuration files that ship with GEOS-Chem v11-01 public release.

## Fix bug in CH4 emissions

The CH4 emissions appear to be too low (by  $\sim 1e11$ ) in [v10-01](#) and later versions. There is likely a unit conversion bug that was introduced by [HEMCO](#). We will fix this issue in GEOS-Chem v11-01.

## Dynamics updates

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### Removal of moisture signature from tracer concentrations in dry mixing ratio

Prior to GEOS-Chem v11-01, tracer conversions between  $[v v^{-1}]$  and  $[kg]$  did not accurately handle moisture when using moist air mass and dry air molecular weight. [Updates to fix the moisture issue and related discrepancies](#), including problematic inert tracer mass conservation, were introduced in [v11-01a](#).

Validation of the v11-01a moisture corrections revealed an additional moisture handling issue in advection. Inert tracer dry mixing ratio maps contained patterns resembling the moisture signature in the atmosphere. GCST member Lizzie Lundgren attributed this phenomenon to lack of moisture handling within transport. Tracer mass is distributed relative to moist rather than dry air pressure and therefore preferentially pools within grid boxes that contain more water vapor mass.

Meemong Lee and Richard Weidner (JPL) issued a JPL publication detailing a transport moisture fix for the Adjoint model. Their adjoint fix consists of (1) deriving dry surface pressures from GMAO moist surface pressures and specific humidity, and (2) replacing moist pressures with dry pressures throughout the model.

Lizzie Lundgren (GCST) is adapting JPL's Adjoint fix to the GEOS-Chem forward model. The GEOS-Chem implementation corrects the transport mass distribution problem by applying JPL's fix to only transport and unit conversions and also preserves the moisture updates incorporated into v11-01a as well as inert tracer mass conservation. This will be the featured update of GEOS-Chem v11-01h, the first beta release following FlexChem.

## Other issues that will be resolved in v11-01

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### Fix to remove strange cycle in OH caused by TOMS overhead O3 errors

In v10-01, the TOMS O3 column data—which are passed to the FAST-JX photolysis mechanism when driving GEOS-Chem with GCAP, GEOS-4, or GEOS-5 meteorology—produced an unexpected artifact in OH concentrations.

Ben Brown-Steiner (MIT) wrote:

*I've been running [GEOS-Chem v10](#) "out of the box" (`geos5_2x25_tropchem`) and started to look at the daily output via the ND50 diagnostic (although this also happens with daily output to the main file)...Monthly averages look fine, and daily averages follow the long-term monthly behavior, but with a very weird cycle. At the 15th of each month, something just...stops. Certain species start to decay (e.g. OH) while others spike (e.g. O3).*

*I've attached a few plots demonstrating the strange behavior.*

*First is [global surface O3](#) (this is every day for a year, January - December, the plotted dates are wonky, please ignore).*

*Next is [surface OH](#), with a similar strange behavior.*

*I've also plotted POX at the [surface](#) and in the [upper atmosphere](#).*

*It seems that this happens most prominently over the oceans that over the land, and influences almost every tracer (NO, CO, PRPE, ISOP).*

*We don't know what's going on, but we suspect that it's not an emissions problem (as a similar pattern exists in the upper atmosphere). Perhaps something with radiation?*

*Do you know what's going on? Or point me to someone who does?*

Prior to v10-01, the TOMS overhead O3 columns were read from [binary punch](#) (aka “\*.bpch”) format files. In v10-01 and later versions, we converted the bpch files to netCDF files so that they could be read and regridded with HEMCO. Barron Henderson (U. Florida) and Jenny Fisher (U. Wollongong) discovered several issues with how the files were prepared, and how missing values were being treated in GEOS-Chem module `GeosCore/toms_mod.F`.

These issues will be resolved prior to the v11-01 public release (currently slated for v11-01j). For more information about the fix, please see [this post on our FAST-JX v7.0 photolysis mechanism wiki page](#).

**NOTE:** GEOS-Chem simulations driven by GEOS-FP, MERRA, or MERRA-2 use the overhead ozone column field (TO3) contained in these met field products. Therefore, the errors described above do NOT affect the GEOS-Chem benchmark simulations (which use GEOS-FP meteorology).

## **Update to GEOS-FP re-evaporation calculation**

Viral Shah (U. Washington) has submitted a wet-deposition update to correct an error in the re-evaporation of precipitation when using GEOS-Chem with the GEOS-FP (“forward processing”) or MERRA-2 meteorology.

Viral wrote:

*The original code [in `GeosCore/wetscav_mod.F`] did not take into account the rate of re-evaporation of precipitation (GEOS-FP/MERRA field: REEVAPLSAN) when calculating the fraction of particles (and HNO3) re-suspended in a gridbox. The attached fix corrects this error.*

*Test simulations using this fix resulted in an annual lifetime for Pb210 of ~8.3 days for GEOS-FP and MERRA (simulation performed by Bo Zhang). Bo also found better correspondence with aircraft observations in the test simulations.*

*The specific changes included in the fix are:*

- a. Declare and initialize the REEVAP array to hold the re-evaporation rate, and*
- b. In the WETDEP\_MERRA routine, pass REEVAP instead of QQ to the DO\_WASHOUT\_ONLY routine to calculate the fraction of precipitation re-evaporating. This fraction (ALPHA) is now calculated as:  $(REEVAP * BXHEIGHT)/PDOWN$ .*
- c. REEVAP occasionally has negative values but with small magnitudes. We set these to zero.*

*I would like to acknowledge again the work of Bo Zhang and Hongyu Liu (both at National Institute of Aerospace) in evaluating the fix.*

This update is currently slated to be added to v11-01i (following the FlexChem and moisture fix updates).

## **Fix for monthly stratospheric P/L rates in HEMCO**

Brian Boys wrote:

*It appears that the current public release of GC is not updating monthly stratospheric P/L rates. I've read through strat\_chem\_mod and it says this is supposed to happen through HEMCO (there's no call to GET\_MONTH in strat\_chem). I suspect this b/c I've noticed a lack of stratospheric NO2 seasonality in year long runs, with stratospheric NO2 columns reflecting the simulation start month seasonality. Is it possible that the stratospheric P/L rates are set at the simulation start month and not updated?*

Christoph Keller responded:

*Thanks for reporting this. Does your HEMCO\_Config.rc have the following entries?*

```
* GMI_LOSS_NOx ... 2000/$MM/1/0 ...  
* GMI_PROD_NOx ... 2000/$MM/1/0 ...
```

*The GMI\_PROD/LOSS entries should all be:*

```
* GMI_LOSS_NOx ... 2000/1-12/1/0 ...  
* GMI_PROD_NOx ... 2000/1-12/1/0 ...
```

*The STRAT\_OH entry is (also) an error and should be fixed in the HEMCO configuration file. So the entry should be*

```
* STRAT_OH ... 2000/1-12/1/0 ...
```

*Instead of*

```
* STRAT_OH ... 2000/$MM/1/0 ...
```

*The difference between these two entries is that the current entry (2000/\$MM/1/0) reads the data only once (at the beginning) and then never updates it, whereas the correct entry (2000/1-12/1/0) updates the data every month – which is what we want.*

We will update the HEMCO configuration files that ship with GEOS-Chem v11-01. In the meantime, you can make the corresponding change in your current HEMCO configuration files.

## Fixed errors routine in DO\_STRAT\_CHEM

We discovered two errors in routine DO\_STRAT\_CHEM (located in the stratospheric chemistry module GeosCore/strat\_chem\_mod.F90), in the section where the Br<sub>y</sub> concentrations are set:

```
!$OMP PARALLEL DO &
!$OMP DEFAULT( SHARED ) &
!$OMP PRIVATE( NN, BEFORE, I, J, L, BryTmp ) &
!$OMP PRIVATE( LCYCLE )
DO NN=1,6
    . . .
    ! Is this Br2?
    ISBR2 = ( TRIM(Input_Opt%TRACER_NAME(Strat_TrID_GC(NN))) == 'Br2' )
```

The errors were:

1. The ISBR2 variable (highlighted in RED) is a scalar that gets assigned a value within a parallel loop. Therefore, it should be declared as PRIVATE to the loop.
2. The test to determine if the species is Br<sub>2</sub> used an incorrect algorithm. It returned FALSE even when the current species was indeed Br<sub>2</sub>.

The correct code should be:

```
!$OMP PARALLEL DO &
!$OMP DEFAULT( SHARED ) &
!$OMP PRIVATE( NN, BEFORE, ISBR2, L, J, I, LCYCLE, BryTmp )
DO NN = 1,6
    . . .
    ! Is this Br2?
    ISBR2 = ( Gc_Bry_TrId(NN) == id_Br2 )
```

We have now added the ISBR2 to the !\$OMP PRIVATE statement. We also now use a correct search algorithm that will properly denote if the current Br<sub>y</sub> species is Br<sub>2</sub>.

This fix will go into [v11-01g](#), along with the FlexChem update.

## 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 regrided 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).

## Future developments

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### Reading met fields via HEMCO and flexible grid definitions

Graduate student Jiawei Zhang (Harvard) plans to start working on a project to make it easier to define custom grids (global and nested) when using GEOS-Chem “Classic”. He writes:

*I have a version that can read netCDF metfields (GEOSFP and MERRA2) with HEMCO. This module is universal for different model resolutions and nested domains as the input metfield can be regrided and cropped online.*

*To further make the grid specification totally flexible, we [... can introduce...] run-time [grid] configurations. I know there are a couple of people building new nested simulations, like Africa, Australia and South America; but the code will get more and more redundant if the number of nested domains keeps growing.*

*Then, users will be able to use a single executable for all types of simulations [without having to recompile when changing the grid, met field type, or nest region]. For example, to switch [from a nested grid] to a global 4x5 simulation, [a user can] just modify the metfield path [and settings] in the HEMCO\_Config.rc configuration file.*

*Following this method we will immediately have these benefits:*

- 1) Developing a new nested simulation will be nothing more than preparing an input data set and tuning parameters. There will be nothing to modify in codes.*
- 2) One can easily run nested simulations over any sub-domains of archived metfields.*
- 3) It directly allows global 0.25/0.5 run if we have data, although only with OpenMP*

*It also opens doors for new resolutions and includes something that GCHP needs like setting parameters online.*

## Conclusion

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We are reaching the final stages of FlexChem development. The FlexChem solver has been integrated into GEOS-Chem and produces output that is consistent with the prior SMVGEAR solver.

Most of the work we have been doing this summer involved the implementation of important new structural updates and the removal of legacy infrastructure.

1. We have created a [GEOS-Chem species database](#) to store physical parameters and other relevant information for each species.
2. We have removed the obsolete [species indexing scheme](#) and replaced it with a new algorithm that is compatible with FlexChem.
3. We are removing the last vestiges of SMVGEAR and consolidating species concentrations into a single array in order to reduce the memory footprint of GEOS-Chem.
4. We have migrated GEOS-Chem's restart files from binary punch format to netCDF format.
5. We have removed the remaining family tracers from GEOS-Chem's chemistry mechanisms.

We believe that these updates will significantly improve GEOS-Chem's performance and flexibility.

We have been diligently validating and testing these wide-ranging modifications in order to ensure that we did not introduce any new errors along the way, or break any existing functionality. While this process often took longer than we had anticipated, we are confident that the end result will be a much more efficient, streamlined, and HPC-ready GEOS-Chem,

We are also confident that FlexChem will make it much easier for you to create new GEOS-Chem chemistry mechanisms for your research needs.

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)