GEOS-Chem Newsletter
Fall 2016 Edition

GEOS-Chem Support Team
07 November 2016

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GEOS-Chem Steering Committee news

Meeting minutes 04 November 2016

The GEOS-Chem Steering Committee met by conference call on Friday 04 November 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.

IGC8 will take place from May 1-4, 2017

The 8th International GEOS-Chem Meeting (IGC8) will take place at Harvard University from May 1-4, 2017. Mark your calendars! More information will be forthcoming.

GEOS-Chem v11-01 Development Overview

GEOS-Chem v11-01 development is wrapping up. We are aiming to have the v11-01 public release by the end of calendar year 2016. The FlexChem chemical solver has been added to GEOS-Chem, and we are currently making sure that the chemical production and loss diagnostics are working properly.

All of the legacy SMVGEAR code has been completely removed from GEOS-Chem. We expect that these updates will cause GEOS-Chem to perform much more efficiently than before. This will also make it much easier to add species and customize your own chemistry mechanisms.

We are continuing to develop the **GCHP development kit ("Dev Kit")**, which is available for you 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. To date, the GCHP Dev Kit has been installed on both Harvard and Dalhousie computers, where further testing and debugging is ongoing. More information on the GCHP Dev Kit is included below.

GEOS-Chem v11-01g

GEOS-Chem v11-01g was approved on 28 September 2016. This version introduced the FlexChem chemical solver package into GEOS-Chem. Please see the following links for complete information about the validation of GEOS-Chem v11-01g:

1. *Approval form for 1-month benchmark simulation v11-01g*
2. *Results for 1-year benchmark simulation v11-01g-Run0*

v11-01g Feature	Type	Submitted by

FlexChem
• Replacing SMVGEAR with a clean and flexible implementation of KPP
• Removing legacy SMVGEAR code and input files, including:
  o Removing 1-D array indices (`JLOOP, KLOOP,` etc.)
  o Removing `globchem.dat, mglob.dat`
  o Removing the distinction between tracers and species
	Science	Mike Long (Harvard)
		GCST

Update 4x5 soil Hg files and Hg simulation photoreduction and soil emission coefficients	Science	Jenny Fisher (Wollongong)
Parallelization bug fixes for GEOS-5 Hg simulations	Bug fix	Bob Yantosca (GCST)
Bug fixes for HEMCO, including: • Fix missing pointer in call to HCO_CalcVertGrid • Fix bug preventing HEMCO from writing restart files more than once per run • Diagnostic fix for zero biomass burning emissions when QFED is used	Bug fix	Christoph Keller (NASA GSFC) GCST

v11-01g Feature	Type	Submitted by
NetCDF Output Phase 2: • Use netCDF restart files for Hg simulation	Structural	Lizzie Lundgren (GCST)
Restore the tagged CO specialty simulation • Use HEMCO to split CO emissions into tagged tracers • Restore tagged CO unit tests	Structural	GCST
Updates for High Performance GEOS-Chem (GCHP) Dev release, includes: • Prevent segmentation fault in HEMCO that can happen with Intel Fortran Compiler v12 or newer	Structural & Bug fix	Seb Eastham (Harvard) GCST
Do not nullify local pointers in the same line where they are declared	Structural	Bob Yantosca (GCST)
Improved species indexing • Removed `tracerid_mod.F` from GEOS-Chem	Structural	GCST

GEOS-Chem v11-01h

GEOS-Chem v11-01h was approved on 11 Oct 2016. Please see the following links for complete information about the validation of GEOS-Chem v11-01h:

1. *Approval form for 1-month benchmark simulation v11-01h*
2. *Results for 1-year benchmark simulation v11-01h-RnPbBe*

v11-01h Feature	Type	Submitted by
Fix to remove moisture signature in dry mixing ratio	Bug fix	Meemong Lee (JPL) Richard Weidner (JPL) Lizzie Lundgren (GCST) Kevin Bowman (JPL)
Modifications for running nested Asia simulations with MERRA-2	Structural	Melissa Sulprizio (GCST)
Bug fixes for the dry deposition diagnostic when using TURBDAY	Bug fix	Bo Zhang (NIA/NASA Langley)

GEOS-Chem v11-01i

GEOS-Chem v11-01i was approved on 19 Oct 2016. Please see the following links for complete information about the validation of GEOS-Chem v11-01i:

1. *Approval form for 1-month benchmark simulation v11-01i*
2. *Results for 1-year benchmark simulation v11-01i-RnPbBe*

v11-01i Feature	Type	Submitted by
Fix bug in GEOS-FP/MERRA/MERRA-2 re-evaporation calculation	Bug fix	Virah Shah (UW) Bo Zhang (NIA) Hongyu Liu (NIA/NASA Langley)

GEOS-Chem v11-01j

GEOS-Chem v11-01j is currently under development as of this writing. This version will contain the following features:

1. Update to HEMCO v2.0.003
2. Support for the GNU Fortran compiler
3. Several user-submitted bug fixes and emissions updates

v11-01j Feature	Type	Submitted by
Fix for TOMS/HEMCO to address strange cycle in OH output	Bug fix	Barron Henderson (U. Florida)
Correct bug in units of EDGAR v4.2 SO2 emissions	Bug fix	Jaegun Jung (Ramboll Environ)
Prevent biofuel emissions from being double counted in EDGAR v4.2	Bug fix	GCST
Fix for monthly stratospheric P/L rates in HEMCO	Bug fix	Christoph Keller (NASA GSFC)
Fix bug in the GMI stratospheric production rates for HCOOH	Bug fix	Eloise Marais (Harvard) Xin Chen (UMN)
Fix bug in NOx diurnal scale factors	Bug fix	Brian Boys (Dalhousie) Christoph Keller (NASA GSFC)
Update HEMCO from version 1.1.016 to version 2.0.003	Structural	Christoph Keller (NASA GSFC)
Add option for QFED & FINN emissions in the Hg simulations	Science	Jenny Fisher (Wollongong)
Use TOMS ozone for all years when running simulations with GEOS-5	Science	Jenny Fisher (Wollongong)
Updates to TOMAS Jeagle sea salt extension	Science	Jack Kodros (Colorado State)
0.1° x 0.1° CAC emissions	Science	Aaron van Donkelaar (Dalhousie)
Replace RETRO C3H8 emissions with emissions from Xiao et al.	Science	Emily Fischer (CSU)
Add PM2.5 diagnostic	Structural	Melissa Sulprizio (GCST)
Add support for the GNU Fortran compiler	Structural	Seb Eastham (Harvard) Bob Yantosca (GCST)
Fix minor issues in the specialty simulations discovered by the GNU Fortran compiler	Bug fix	Bob Yantosca (GCST)
Set ACTA and HCOOH to active	Bug fix	Katie Travis (Harvard)
Fix KPP's prod/loss diagnostic to account for reactions where there is cycling between species within a chemical family	Bug fix	Mike Long (Harvard)

Priorities for future development

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

Proposed development of GEOS-Chem v11-2, in order	Authors
Chemistry updates	
Updating chemistry rate constants based on *JPL Publication 15-10*	Barron Henderson (U. Florida) Mat Evans (U. York) Oxidants and Chemistry WG
PAN updates	Emily Fischer (CSU)
Halogen chemistry updates	Tomás Sherwen (York) Johan Schmidt (Harvard) Oxidants and Chemistry WG
Enhance default GEOS-Chem simple SOA	Aerosol Working Group Chairs
Update density of BC to 1.8 and add absorption enhancement factor in input.geos	Xuan Wang (MIT)
Update isoprene chemistry	Katie Travis (Harvard), Kelvin Bates (Caltech)
Add aqueous isoprene uptake to SOA scheme	Eloise Marais (Harvard)
Monthly mean surface methane distributions	Lee Murray (NASA GISS/LDEO)
Emission updates	
Including EDGARv4.3 in HEMCO	Chi Li (Dalhousie)
EPA-derived BC/OA emissions over US (1990-2012)	David Ridley (MIT)
Dalhousie updates to emissions: historical Canadian emissions, default US emissions to NEI after 2011, ammonia from Arctic birds	Dalhousie
Ocean ammonia emission inventory	Fabien Paulot (NOAA/GFDL)
Lightning update	Katie Travis (Harvard)
Deposition/surface updates	
Fix to direct/diffuse radiation	Katie Travis (Harvard)
Species Database Phase 3: • Harmonizing Henry's Law coefficients across wet and dry deposition	GCST
Updated organic deposition	Katie Travis (Harvard) Jenny Fisher (U. Wollongong)

Remove dependence of species drydep on HNO3 drydep	Katie Travis (Harvard) Jenny Fisher (U. Wollongong)
Update SO2 scavenging in convective updrafts for consistency	Duncan Fairlie (NASA/LARC)
Sedimentation of stratospheric aerosols	Seb Eastham (Harvard)
Structural updates	
Uniformity of units	Lizzie Lundgren (GCST)
NetCDF Output Phase 3a: Output diagnostics in NetCDF format	GCST
NetCDF Output Phase 3b: Updates to eliminate differences between single and multi-segmented GEOS-Chem runs	GCST Christoph Keller
Hg/POPs	
PCB simulation	Carey Friedman (MIT) Helen Amos (Harvard)
Hg code updates (chemistry, ocean, land)	Hg and POPs Working Group
Surface ocean Hg boundary conditions from MITgcm	Hannah Horowitz (Harvard)
Expansion of model capabilities	
Additional modifications for FlexChem, including: • Rebuild the pre-built chemistry mechanisms (Standard, Tropchem, UCX, SOA, SOA-SVPOA) with Kppa • Add capability for custom chemistry mechanism by building KPP on-the-fly in GEOS-Chem	Mike Long (Harvard) GCST
FlexGrid: Use HEMCO I/O and regridding capabilities to read and regrid met fields	Jiawei Zhuang (Harvard) Jintai Lin (PKU)
Merge standard simulation with specialty simulations for OVOC, acids, aromatics, dicarbonyls, terpenes	Dylan Millet (UMN) Xin Chen (UMN)
Nested CO2, CH4, Hg, TOMAS, adjoint, etc.	Nested Model Working Group

Defer to v11-3 unless ready in time	
Global evaluation of using LWC and IWC from met fields for wet scavenging	Hongyu Liu (NIA/NASA LARC) Bo Zhang (NIA)
Kz eddy mixing scheme	Karen Yu (Harvard)
Updated VBS	Rokjin Park (SNU)
Benchmark of stratosphere simulation	Dylan Jones (U. Toronto)
Not prioritized for v11-2 (can be revisited at IGC8)	
Python GEOS-Chem output processing and visualization package	Benoît Bovy (U. Liège-Belgium)
Sea salt emission from sea ice	Jiayue Huang (UW)
Re-evaluation of SST dependence of sea salt emissions	Jiayue Huang (UW)
MOSAIC implementation	Sebastian Eastham (Harvard)
Update MODIS LAI fields through 2015	Barron Henderson (UF)
Lightning NOx chemistry parameterization	Alicia Gressent (MIT)
A snow NOx source from deep snowpack	Maria Zatko (UW) Becky Alexander (UW)

New data directories for v11-01

The following HEMCO data directories have been added and/or updated for GEOS-Chem v11-01. Once the GEOS-Chem v11-01 public release ships, you will need to download these data directories to your system.

Inventory	What was added?	When added?	Directory
Aerocom volcano emissions	Now split into separate eruptive and degassing emissions	v11-01b	HEMCO/VOLCANO/v2015-02/
DMS seawater conc.	Update to Lana climatology	v11-01b	HEMCO/DMS/v2015-07/
POPs simulation	Updates for secondary emissions and GCAP met	v11-01c	HEMCO/POPs/v2015-08/
GFED4 biomass	Update to GFED v4.1	v11-01d	HEMCO/GFED/v2015-10/
MASKS	New file: EMEP_mask.geos.1x1.20151222.nc (Do not zero emissions at 30N)	v11-01f	HEMCO/MASKS/v2014-07/
Restart Files	NetCDF restart files (moved here from the Unit Tester repo)	v11-0f	ExtData/NC_RESTARTS
FINNv1 biomass	Data processing scripts	v11-01g	HEMCO/FINN/preprocess/ FINN_preprocess.tar.gz
CAC Canadian anthro	0.1° x 0.1° data files	v11-01j	HEMCO/CAC/v2016-09/
Timezones	New file: timezones_1x1.edit.nc (Fix ocean values in timezones mask file)	v11-01j	HEMCO/TIMEZONES/v2015-02/
GMI	New file: gmi.clim.HCOOH.geos5.2x25.20160912.nc (Fix bug in GMI rates for HCOOH)	v11-01j	HEMCO/GMI/v2015-02/
MASKS	New file: USA_LANDMASK_NEI2011_0.1x0.1.20160921.nc (Do not zero Canadian and Mexican emissions)	v11-01j	HEMCO/MASKS/v2014-07/
TOMS/SBUV O3 columns	Barron Henderson reprocessed TOMS/SBUV data in order to fix a strange cycle in OH output when running GEOS-Chem with GEOS-5 meteorology.	v11-01j	HEMCO/TOMS_SBUV/v2016-11/

Structural Updates

Recap of structural updates added in v11-01

We have added many structural updates into GEOS-Chem v11-01 in order to pave the way for the new FlexChem chemical solver. These updates were covered in depth in past editions of the GEOS-Chem newsletter. Please view the following links for more information about each update.

1. Implementation of the GEOS-Chem Species Database
2. Standardization of physical properties for GEOS-Chem species
3. Removal of the distinction between "tracers" and "species", as well as removal of the `State_Chm%TRACERS` array
4. Retirement of `tracerid_mod.F`
5. An updated method for GEOS-Chem species indexing
6. Migration of restart files from binary punch to COARDS-compliant netCDF format

Added support for the GNU Fortran compiler

Bob Yantosca (GCST) and Seb Eastham (Harvard) have added support for the GNU Fortran compiler into GEOS-Chem v11-01. GNU Fortran, which is free and open-source, may be an attractive alternative to the more expensive Intel and PGI compilers for some users.

GNU Fortran has proved to be a useful debugging tool, as it is able to flag non-standard Fortran code very readily. But this strictness comes at a price. At present, GEOS-Chem can only compile with GNU Fortran version v4.4.7 and v4.8.2, which are older versions. GNU Fortran v5.x.x and v6.x.x cannot compile GEOS-Chem successfully, as they object to some of the legacy code in the ISORROPIA module.

Please see our *GNU Fortran compiler* wiki page for the most up-to-date information about the implementation of GNU Fortran into GEOS-Chem.

Chemistry Updates

FlexChem milestones

The following table lists recent milestones that were achieved in the implementation of the new FlexChem chemical solver since August 2016:

Task	Developer	Status
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 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 Aug 2016
Store species background concentrations values previously stored in `globchem.dat` in the species database	Lizzie Lundgren	Completed Aug 2016
Attach the new KPP prod/loss output to the GEOS-Chem prod/loss diagnostic (ND65)	Melissa Sulprizio	Completed Aug 2016
Remove `State_Chm%Tracers` and use species concentrations in `State_Chm%Species` instead	GCST	Completed Aug 2016
Validate FlexChem with v11-01g benchmarks	GCST	1-month benchmark: Approved 14 Sep 2016 1-year benchmark: Approved 28 Sep 2016
Fix P/L diagnostics to ignore cycling reactions	GCST	Ongoing
Rebuild Standard, Tropchem, UCX, SOA, SOA-SVPOA chemistry mechanisms with Kppa	GCST	Slated for v11-02
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	Slated for v11-02
Update GEOS-Chem documentation and user manual for v11-01	GCST	To be done prior to v11-01 public release

As of this writing, the remaining FlexChem development work is to restore the production and loss diagnostics (see below).

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 restore this diagnostic so that it will generate production and loss for families like Ox, NOx, and NOy.

Declare ACTA and HCOOH as active species in GEOS-Chem chemical mechanisms

Katie Travis reported an error in the v10-01 `globchem.dat` file—the master chemical mechanism for SMVGEAR. Both ACTA and HCOOH had been set to inactive (`I`), but they undergo chemistry and should have been set to active (`A`).

In v11-01j, we will add Katie's fix into the FlexChem/KPP master equation file and rebuild the KPP solver code accordingly.

Dynamics and wet deposition updates

Added fix to represent moisture correctly in GEOS-Chem air quantities

GCST member Lizzie Lundgren (Harvard) discovered that v10-01 tracer unit conversions between [v/v] and [kg] did not accurately handle moisture in their use of moist air mass with dry air molecular weight. Updates to fix this issue and other moisture-related discrepancies discovered during the update implementation were introduced in GEOS-Chem 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. We traced this phenomenon to lack of moisture handling within transport. Tracer mass was distributed relative to moist rather than dry air pressure and therefore preferentially pooled within grid boxes that contained more water vapor mass.

Meemong Lee and Richard Weidner (JPL) issued a JPL Publication detailing a transport moisture fix for the Adjoint model addressing this issue. Their adjoint fix consisted 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) adapted JPL's Adjoint fix to the GEOS-Chem forward model in GEOS-Chem v11-01h. The GEOS-Chem v11-01h implementation does the following:

1. Corrects the transport mass distribution problem by using dry surface air pressures in advection
2. Preserves the moisture updates incorporated into v11-01a, including 3D dry and moist air pressures
3. Preserves inert tracer mass conservation by using dry air mass derived from dry surface pressure in species unit conversions and mixing ratio updates

See the Moisture Updates in v11-01 wiki page for details of the v11-01a and v11-01h moisture updates. Changes specific to the updates in v11-01h are discussed in the Transport section of that page. Important changes to highlight with this fix are as follows:

1. The dry air mass per level calculated using the dry surface pressure is close but not exactly the same as the dry air mass calculated using the legacy method. Both methods produce valid approximations of level mass, but **using dry air mass derived from the new dry surface pressure is required for species unit conversions to ensure mass conservation**. This is because species are advected in units of mass mixing ratio, with dry air mass in the denominator. Retaining the same global species mass before and after advection, therefore, requires unit conversions that use a dry air mass definition consistent with that used in advection.
2. **The new dry surface pressure should NOT be used for constructing vertical profiles of dry and moist air pressures**. The dry air pressure derived from dry surface pressure and GMAO vertical grid parameters A and B would not reflect an accurate height profile and

cannot be used to derive a moist pressure height proxy. For this reason, 3D pressures (State_Met variables PEDGE, PEDGE_DRY, PMID, and PMID_DRY) are still constructed using the v11-01a method with GMAO wet surface pressures in combination with specific humidity.

Lizzie's updates were validated in v11-01h with a 1-month "standard" benchmark as well as a 1-year Rn-Pb-Be benchmark. V11-01h was approved on 11 Oct 2016.

Added fix for GEOS-FP, MERRA, and MERRA-2 re-evaporation calculation

In the August 2016 GEOS-Chem newsletter, we wrote about a wet deposition update submitted by Viral Shah (U. Washington). This update corrects for an error in the re-evaporation of precipitation when running GEOS-Chem simulations with the GEOS-FP ("forward processing"), MERRA, or MERRA-2 meteorology.

Viral's update was added to v11-01i, and was validated with a 1-month "standard" benchmark simulation and a 1-year Rn-Pb-Be benchmark simulation.

Viral recently wrote us to give his assessment of the results:

> *Thank you for sharing the v11-01i benchmark results. I have no objections to them.*
>
> *I have looked at the new Pb210 budget, and see that the changes in the wet deposition fluxes are equal to what I had obtained in my runs while testing the fix.*
>
> *Currently, the re-suspension of aerosols and highly soluble gases (species for which washout is treated as a kinetic process) is not performed when running GEOS-Chem with GEOSFP/MERRA fields. This fix corrects that. Thus there is a widespread increase in the concentrations of these species at the surface and to a smaller extent at 500 hPa. There is also an increase in species (or decrease for a few species) with low solubility likely because they are connected chemically to the species that are directly affected by the fix. The relative increases seem fairly large (factor of 2), but for the most part the highest ratios are in places with low concentrations. I suggest members of the Steering Committee also take a look at the benchmark plots.*

GEOS-Chem v11-01i was approved on 19 Oct 2016.

Emissions updates

Add HEMCO v2.0.003 into GEOS-Chem

Christoph Keller (NASA/GMAO) has updated HEMCO from v1.1.016 to v2.0.003. He writes:

> *The updates in HEMCO v2 are mostly structural. The most important changes are:*
>
> ***1.*** *Bug fix in* `hcox_paranox_mod.F90` *(line 632): The deposition flux is now archived as absolute (i.e. positive) number. Without this fix, the merged code should give zero-diff to v11-01h.*
>
> ***2.*** *The timezones mask file should be updated to file* `HEMCO/TIMEZONES/v2015-02/timezones_1x1.edit.nc`
>
> *The current timezones mask file does not work properly in grid cells with large ocean overlap. The problem is that the ocean values are netCDF_FillValues that become zero within HEMCO. As a quick fix I updated the timezones file to use a value of –5000 in all ocean cells, which then forces HEMCO to determine the time zone based on longitude in those cells.*
>
> ***3.*** *HEMCO v2.0.003 now accepts scale factors for extension fields. For example, to uniformly scale GFED_TEMP by a factor of 2:*
>
> ```
> 111 GFED_TEMP $ROOT/GFED4/v2015-10/$YYYY/GFED4_gen.025x025.$YYYY$MM.nc DM_TEMP 1997-2014/1-12/01/0 C xy kgDM/m2/s * 1234 1 1
>
> ...
>
> 1234 GFED_TEMP_SCALE 2.0 - - - xy 1 1
> ```
>
> *This update requires that all HEMCO extension fields are evaluated on every emission time step. I don't expect this to have a notable impact on run time (and it didn't in my short test runs). However, if you find that it does slow down the benchmark simulation let me know and we can revert to version v2.0.002 (which does not include this update).*
>
> ***4. HEMCO v2 contains additional options to emit 2D fields across multiple vertical levels.*** For instance, to release 1.0 kg/m2/s of NO into levels 1-5, you can use:
>
> ```
> 0 NO_MULTILEVELS 1.0 - - xyL=1:5 kg/m2/s NO - 1 1
> ```
>
> *The emissions are then spread across the lowest 5 model levels based upon the model level thicknesses. Instead of specifying the model levels it is also possible to*

> *specify the altitude in meters or use PBL for the planetary boundary layer. For example, the following are all legal:*
>
> ```
>    0 NO_MULTILEVELS 1.0 - - xyL=1:2500m     kg/m2/s NO - 1 1  -
> > emits from surface level to 2500m
>
>    0 NO_MULTILEVELS 1.0 - - xyL=1000m:5000m kg/m2/s NO - 1 1  -
> > emits from 1000m to 5000m
>
>    0 NO_MULTILEVELS 1.0 - - xyL=500m:17     kg/m2/s NO - 1 1  -
> > emits from 500m to level 17
>
>    0 NO_MULTILEVELS 1.0 - - xyL=1:PBL       kg/m2/s NO - 1 1  -
> > emits from surface level to PBL top
> ```
>
> ***5.*** *From a coding perspective the HEMCO state object (`HcoState`) now has to be passed to each routine. `HcoState` contains all HEMCO related information (such as callback information for error messages). This update was needed to enable the execution of multiple HEMCO instances at the same time. This won't affect you unless you have to touch HEMCO related code.*

In addition, HEMCO v2.0.003 will contain several minor structural modifications for compatibility with the GNU Fortran compiler. For details, please visit these links:

1. List of modifications for GNU Fortran in HEMCO/Core modules
2. List of modifications for GNU Fortran in HEMCO/Extensions modules
3. List of modifications for GNU Fortran in NcdfUtil modules

We will bring HEMCO v2.0.003 into GEOS-Chem v11-01j.

Use Xiao anthropogenic C3H8 emissions by default; RETRO is too low

Emily Fischer (CSU) wrote:

> *(My graduate student) Zitely and I just looked at the C3H8 emissions totals for the globe. It looks like the default/ recommended emission inventory for C3H8 has been set to RETRO. Though we don't think the Xiao offline emission inventory is perfect, we do know that RETRO has C3H8 emissions are > 3 times lower than those in Pozzer et al. [2010], and should probably not be the default choice. We are working on a comparison between the model and the recent SONGNEX observations, so we should have a better recommendation for the US in a few months, but for now, I would recommend keeping Xiao as the default emission inventory when there are not US/Europe/East Asian regional inventories overwriting.*

This update,which only involves a change to the HEMCO configuration file, but no source code modifications, will be added into v11-01j.

Specialty simulation updates

Correct a unit conversion error in the tagged CO simulation

Beata Bukosa (U. Wollongong) wrote:

> *I was using the new Tagged_CO simulation in v11-01 … and it seems like the chemical loss isn't being applied to any of the tracers.*
>
> *I was running GEOS-Chem for the time period 2007- 2013 and … you will see that for the first year (2007) the values seem ~OK but after that the concentration is just rising like chemical loss isn't being applied at all.*
>
> *Also … the monthly average concentrations might be also wrong because of the same issue.*

Bob Yantosca replied:

> *I think I figured it out. HEMCO was bringing in the `GLOBAL_OH` field in kg/m3 but we were not converting it to molec/cm3 before using it. The fix is pretty simple. We just add a conversion factor. I added the lines in green, underneath these existing lines in routine `CHEM_TAGGED_CO`.*
>
> ```
> ! Factor to convert OH from kg/m3 (from HEMCO) to molec/cm3
> kgm3_to_mcm3OH = ( AVO / 17.0e-3_fp ) * 1.0e-6_fp
>
> . . .
>
>    ! Now impose a diurnal cycle on OH.
>    ! This is done in other offline simulations but was
>    ! missing from tagged CO (jaf, 3/12/14)
>    !
>    ! NOTE: HEMCO brings in OH in kg/m3, so we need to also
>    ! apply a conversion to molec/cm3 here. (bmy, 10/12/16)
>    OH_MOLEC_CM3 = ( OH(I,J,L) * kgm3_to_mcm3OH ) * FAC_DIURNAL
> ```
>
> *The problem was that `OH_MOLEC_CM3` was (in units of kg/m3) of order 1e-16, but should have much, much larger. So then we were multiplying the species by a number that was very close to 1, which resulted in minimal loss.*

Bug fix in Hg simulation: now call a subroutine after HEMCO is initialized

Jaegun Jung (Ramboll Environ) reported an error in the mercury simulation. When the in-plume reduction option (i.e. the `LRED_INPLUME` setting in the HEMCO configuration file) is turned on, GEOS-Chem dies with the following error:

```
================================================================================
GEOS-CHEM ERROR: Cannot get pointer to CFPP_NEI2005_Hg2!
STOP at DO_RED_INPLUME (mercury_mod.F)
================================================================================
     - CLEANUP: deallocating arrays now...
```

We determined that the error was happening because routine `DO_RED_INPLUME` (in module `GeosCore/mercury_mod.F`) was being called before the HEMCO configuration file was being read from disk. Because of this, the pointer `CFPP_NEI2005_Hg2`—which points to data from a file that is read by HEMCO—was uninitialized.

We fixed this issue by moving calling `DO_RED_INPLUME` from `SET_OPTIONS_FROM_HEMCO`, which is called on the first Hg chemistry timestep, after the HEMCO configuration file is read.

This update is being added to v11-01j.

Fixed several errors caused by uninitialized variables

While validating GEOS-Chem with the GNU Fortran compiler, we found and fixed several errors that were being caused by uninitialized or unallocated variables, in the following routines:

1. `OCEAN_MERCURY_READ` (in module `GeosCore/ocean_mercury_mod.F`)
2. `CHEM_POPGP` (in module `GeosCore/pops_mod.F`)
3. `SEASALT_CHEM` (in module `GeosCore/sulfate_mod.F`)
4. `INIT_SEASALT` (in module `GeosCore/seasalt_mod.F`)

All of these issues will be fixed in v11-01j.

MERRA-2 updates

MERRA-2 nested grids

Melissa Sulprizio (GCST) wrote:

> *There were several modifications needed to run nested grid simulations with MERRA-2. The source code updates for running MERRA-2 on the 0.5x0.625 nested NA and nested CH grids were included in v11-01e (approved 04 Jan 2016).*
>
> *The nested CH grid for MERRA-2 is defined as 10S to 55N and 60E to 150E. It therefore includes China, Southeast Asia, Japan, and India. In order to make it transparent to users that this domain has been expanded, the nested CH grid has been renamed to the nested AS grid for MERRA-2. This update was included in v11-01h (approved 11 Oct 2016).*

MERRA-2 global grids

Melissa Sulprizio (GCST) wrote:

> *The various "full-chemistry simulations" (i.e. those using the benchmark, UCX, SOA, and tropchem chemistry mechanisms) use emissions (e.g. lightning, dust) that have scale factors that must be tuned specifically for each met field product. The GCST has computed the dust and lightning scale factors using MERRA-2 met fields for 2009–2014. These updates were included in v11-01f (approved 16 Apr 2016).*
>
> *When the entire MERRA-2 coverage period (1980–present) has been processed, the lightning and dust scale factors for MERRA-2 will be adjusted as needed.*

Diagnostics updates

Bug fixes for the dry deposition flux diagnostic

After the initial 1-year Rn-Pb-Be benchmark simulations were completed for v11-01h, Hongyu Liu pointed out the 210Pb budget was not balanced. The imbalance was tracked to large values in the dry deposition flux diagnostic when using the TURBDAY mixing scheme. The issue does not impact simulations using the VDIFF mixing scheme.

Bo Zhang wrote:

> *The large drydep flux diagnostic term is likely caused by ignoring the difference between chemistry and convection timesteps. The drydep flux diagnostic is added up every convection step in `mixing_mod.F`:*
>
> ```
> AD44(I,J,DryDepID,1) = AD44(I,J,DryDepID,1) + FLUX
> ```
>
> *then it is divided by the chemistry scale in `diag3.F` before being saved into bpch. The chemistry and convection timesteps are 10 mins and 20 mins respectively, which leads to the issue.*
>
> ```
> ARRAY(:,:,1) = ( AD44(:,:,N,1) / SCALECHEM )
> ```
>
> *For non-local PBL, the difference is considered, but there is also a potential issue.*
>
> ```
> AD44(:,:,D,1) = AD44(:,:,D,1) + dflx(:,:,trc_id)      &
>               / TRACER_MW_KG(trc_id) * AVO * 1.e-4_fp &
>               * GET_TS_CONV() / GET_TS_EMIS()
> ```
>
> *Emission timestep is given the same value as chemistry in default, so this works fine, but it seems more appropriate to replace `GET_TS_EMIS()` by `GET_TS_CHEM()` because `SCALECHEM` is used eventually in `diag3.F`.*
>
> *My current fix is to add the term `GET_TS_CONV() / GET_TS_CHEM()` in the first equation in `mixing_mod.F`. In addition, the following lines update tracer concentrations and calculate drydep flux in `mixing_mod.F`. It seems that `FLUX` should be calculated first before the tracer conc gets updated (the second equation should come first).*
>
> ```
> ! Apply dry deposition
> State_Chm%Tracers(I,J,L,N) = FRAC *    &
>                              State_Chm%Tracers(I,J,L,N)
> ! Loss in kg/m2
> FLUX = ( 1.0_fp - FRAC ) * State_Chm%Tracers(I,J,L,N)
> ```

Bo's fixes were added into v11-01h. They were validated with a 1-year Rn-Pb-Be benchmark. These fixes did not impact the 1-month "standard" benchmark because the non-local PBL (VDIFF) mixing scheme is used in that simulation. V11-01h was approved on 11 Oct 2016.

GEOS-Chem High Performance update

You can now download the GCHP development kit!

We are continuing to develop the **GEOS-Chem High Performance Development Kit** (GCHP Dev Kit). 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").

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, meaning it is ready for testing but is not fully debugged; 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.

As of November 2016, we have made several modifications to the GCHP Dev Kit. The scripts that compile GCHP are now system-independent and much easier to use. GCHP is now compatible with both the OpenMPI and MVAPICH2 MPI libraries.

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. Please email the GEOS-Chem Support Team (geos-chem-support [at] as [dot] harvard [dot] edu) if you would like to take the GCHP Dev Kit out for a spin on your computer!

Conclusion

We are wrapping up GEOS-Chem v11-01 and hope to have a public release ready by the end of 2016. FlexChem has completely replaced the legacy SMVGEAR chemistry solver. Our last remaining FlexChem development item is to re-incorporate the chemical production and loss diagnostic.

We are currently working on v11-01j, which will be the last internal version before the public release. V11-01j will contain the most recent HEMCO version available, as well as several minor fixes and emissions updates. We will also add GNU Fortran compiler compatibility into v11-01j.

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, Lizzie, Mike, Junwei, Yanko)