

GEOS-Chem Newsletter

Winter 2017 Edition

GEOS-Chem Support Team
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News from the GEOS-Chem Steering Committee

Latest GCSC meeting minutes

The GEOS-Chem Steering Committee (GCSC) met on November 30, 2017. We invite you to [read the meeting minutes](#).

The next GCSC meeting will take place on **February 22, 2018 at 5:30 PM ET (22:30 UTC)**.

GEOS-Chem Vision Documents

Daniel Jacob wrote:

Dear GEOS-Chem users: I am attaching two recent presentations on GEOS-Chem model development that may be of interest to you:

1. [A presentation by myself on current/future directions for GEOS-Chem](#)
2. [A presentation by Bob Yantosca on the development of NetCDF diagnostics](#)
(NOTE: Please also see the "NetCDF diagnostics update" section in this newsletter)

These presentations have been reviewed and approved by the GEOS-Chem Steering Committee. A central component of our vision is that even as we bring the software architecture of GEOS-Chem into the 2020s, we are committed to continuing to serve atmospheric chemists who want a simple, readily accessible, and stable model architecture for their science applications. So in particular:

1. *Although we are very excited by GCHP, **there is absolutely no plan to retire GC-Classic for the foreseeable future**, and development of GC-Classic and GCHP will proceed together;*
2. *Although NetCDF diagnostics are a massive improvement, **the current diagnostics will be preserved in v11-02 of the model** to be released in early 2018.*
3. ***We continue to prioritize scientific development of GEOS-Chem above all else!** [V11-02](#) will include updated SOA and isoprene chemistry, comprehensive tropospheric-stratospheric halogen chemistry, new flux diagnostics to enable regional mass balances, updated emission inventories and kinetics, and many other user-contributed scientific improvements.*

Thank you for your continued support of GEOS-Chem! Daniel

GEOS-Chem Asia Meeting, May 2018

We are excited to announce that the **first regional GEOS-Chem Asia meeting (GCA1) will be held on May 21-23, 2018** at [Nanjing University of Information Science and Technology \(NUIST\)](#).

The international GEOS-Chem community has been gathering every two years at Harvard for [International GEOS-Chem meetings \(IGC\)](#) to share results and set directions for model development. The goal of GCA1 is to provide a supplementary venue for the Asian community to stay informed about model developments and initiate collaborations. GEOS-Chem users and the broader community outside Asia are also warmly invited to attend. We plan to conduct GCA meetings in alternate years with the flagship IGC meetings.

Hong Liao (NUIST) will be the GCA1 meeting organizer. The registration process will go live this December on the GCA1 website: http://geos-chem.org/meetings/2018_GCA/.

GEOS-Chem Europe Meeting, September 2018

Mat Evans wrote:

After the last Steering Committee meeting Daniel, myself and Paul Palmer at Edinburgh have had a discussion over organizing a European GEOS-Chem meeting in a similar vein to the Asian one to be held in Nanjing. This seems like a good idea and Edinburgh can host. The suggestion has been...September 2018.

We will keep you posted as more information becomes available.

Desupporting Obsolete Meteorological Fields

Daniel Jacob wrote:

Dear GEOS-Chem user:

I write to address some confusion about the different GEOS meteorological datasets produced by NASA GMAO and used by GEOS-Chem.

The two main data archives that you should use for your GEOS-Chem simulations are:

1. The operational data stream from the GEOS Forward Processing (0.25° x 0.3125°, 72 levels) starting in 2012, which should be called [GEOS-FP](#);
2. The consistent [MERRA-2](#) reanalysis for 1979-present (0.5° x 0.625°, 72 levels).

GEOS-Chem also supports older GEOS data sets including [GEOS-4](#), [GEOS-5](#), and [MERRA](#). **These are of inferior quality and GMAO does not want us to use them.** They can still be useful to characterize model transport errors or the effects of different met fields for the same year, but should not be used for any other applications.

While GEOS-4, GEOS-5, MERRA and GCAP (legacy 4° x 5° resolution data only) are desupported starting in GEOS-Chem [v11-02d](#), **we would like to reassure everyone that the GEOS-5 and MERRA data will be preserved on the Dalhousie shared data archive (rain.ucis.dal.ca) for the foreseeable future.** You will still be able to access the entire GEOS-5 and MERRA data archives at Dalhousie for use in your existing projects.

GEOS-Chem v11-02 Development Overview

The sections below detail the new features recently or soon-to-be added to GEOS-Chem v11-02. We anticipate publicly releasing GEOS-Chem v11-02 in early 2018.

NOTE: v11-02c, v11-02d, etc. denote intermediate stages of GEOS-Chem development, which are evaluated with 1-month and/or 1-year benchmarks.

GEOS-Chem v11-02c

GEOS-Chem v11-02c introduced some long-awaited updates to the isoprene and SOA chemistry mechanisms, as well as fixes for minor issues and several structural updates.

Please see the following links for complete information about the validation of v11-02c:

- [Approval form for 1-month benchmark simulation v11-02c](#) (Approved 07 Sep 2017)
- [Results for 1-year benchmark simulation v11-02c-Run0](#) (Approved 21 Sep 2017)

v11-02c Feature	Submitted by	Type
Enhance default GEOS-Chem simple SOA	Sal Farina (Colorado State) Aerosols WG Chairs	Science

v11-02c Feature	Submitted by	Type
Updates to isoprene and monoterpene chemistry	Katie Travis (MIT) Jenny Fisher (U. Wollongong) Eloise Marais (U. Birmingham) Christopher Chan Miller (Harvard) Kelvin Bates (Caltech) Rebecca Schwantes(Caltech)	Science
Add aqueous isoprene uptake to SOA scheme	Eloise Marais (U. Birmingham)	Science
Carbon balance (fix C creation)	Sarah Safieddine (MIT)	Bug fix
Fix bugs for EOH and MGLY following implementation of PAN updates in v11-02a	Melissa Sulprizio (GCST)	Bug fix
Update HEMCO from v2.0.004 to v2.1.001	Christoph Keller (NASA GMAO)	Structural
<p>HEMCO updates:</p> <ul style="list-style-type: none"> • Add a HEMCO-standalone run directory for benchmarking purposes • Now use YYYYMMDDhhmm for time stamp values • Add error trap in to avoid a segmentation fault when the DustGinoux extension is turned off 	Christoph Keller (NASA GMAO) Andy Jacobson (NOAA) Paulo Tuccella (L'Aquila)	Structural
<p>Fixes for several minor issues:</p> <ul style="list-style-type: none"> • Bug fixes for the ND50 timeseries diagnostic • Fixed an incorrect format statement in input_mod.F • Add MERRA2 to #if and #elif statements where it had been omitted • Bug fixes for Hg emissions • Fix bug in species definitions for marine POA simulation • Fix diagnostic bugs in the SOA-SVPOA simulation 	Chris Holmes (Fla. State) Chris Holmes (Fla. State) Jiawei Zhuang (Harvard) Amanda Giang (MIT) Katie Travis (MIT) Katie Travis(MIT)	Bug fix

v11-02c Feature	Submitted by	Type
Fixes for the TOMAS simulation: <ul style="list-style-type: none"> • Fixes for TOMAS simulation in v11-02c • Fix typo in wetscav_mod.F for TOMAS30 • Remove a couple of array temporaries and an out-of-bounds error 	Sal Farina (Colo. State) Jack Kodros (Colo. State) Bob Yantosca (GCST)	Bug fix
Fix STE flux diagnostics and add to benchmark procedure	Melissa Sulprizio (GCST)	Bug fix & Benchmarking
Initial structural modifications for netCDF diagnostics: <ul style="list-style-type: none"> • Introduce Headers/State_Diag as a stub module (for now) • Add a registry object into State_Met, State_Diag, and State_Chm in order to obtain a pointer to any module variable (or slice) by looking up its name • Add new module Headers/registry_mod.F90 which contains derived types and routines for registering module variables. 	Bob Yantosca (GCST)	Structural
Combine timestep settings in input.geos in a Timesteps menu	Melissa Sulprizio (GCST)	Structural
Update CO data used in 1-year benchmark plots	Jenny Fisher (U. Wollongong)	Benchmarking

GEOS-Chem v11-02d

GEOS-Chem v11-02d will introduce a new halogen chemistry mechanism (cf. [T. Sherwen et al. ACP, 16, 1161-1186, 2016](#)) and remove support for the following met field products: GCAP (legacy 4⁰ x 5⁰ resolution data only), GEOS-4, GEOS-5, and MERRA.

As of this writing we are awaiting approval of the v11-02d benchmarks.

v11-02d Feature	Submitted by	Type
Halogen chemistry updates	Tomás Sherwen (York) Johan Schmidt (Harvard) Seb Eastham (MIT) Lei Zhu (Harvard) Oxidants and Chemistry WG	Science
Sulfur oxidation by reactive halogens	Qianjie Chen (UW)	Science

v11-02d Feature	Submitted by	Type
Add bug fixes for GLYX, MGLY, IEPOX, and IMAE heterogeneous chemistry	Sebastian Eastham (MIT)	Bug fix
Update CH4 latitude bands for 2014-2016	Katie Travis (MIT)	Science
Remove support for GCAP, GEOS-4, MERRA, GEOS-5	Melissa Sulprizio (GCST)	Structural
Timestamp HEMCO diagnostics filename with start time rather than end time	Lizzie Lundgren (GCST)	Structural
Structural updates for netCDF diagnostics	GCST	Structural

GEOS-Chem v11-02e

GEOS-Chem v11-02e will introduce more chemistry updates, including updates for [stratospheric chemistry with UCX](#).

v11-02e Feature	Submitted by	Type
Sync GEOS-FP files on Harvard ftp with files at Dalhousie	GCST	Bug fix
Update density of BC to 1.8 and add absorption enhancement factor in input.geos	Xuan Wang (MIT)	Science
Monthly mean surface methane distributions	Lee Murray (NASA GISS/LDEO)	Science
Remove initial stratospheric 2D mixing ratio option	Seb Eastham (Harvard)	Science
UCX stratospheric water boundary condition update	Chris Holmes (UC Irvine) Seb Eastham (Harvard)	Science
Use monthly mean stratospheric prod/loss rates from UCX simulation for all species	GCST	Science
Metal catalyzed oxidation of SO2 (as a switch)	Viral Shah (UW) Becky Alexander (UW)	Science

v11-02e Feature	Submitted by	Type
Spatially varying OM/OC	Sajeev Philip (Dalhousie/NASA Ames)	Science
Add bug fixes for aerosols	Jingyuan Shao (UW)	Bug fix
Remove MONX from chemical mechanisms	Sam Silva (MIT)	Bug fix
Diagnostic for correcting ozone from the height of the lowest model level to the surface	Structural	Katie Travis (MIT)

Priorities for Future Development

Beyond v11-02e, there are many updates that are currently listed as “in the pipeline” for inclusion into GEOS-Chem. Prioritization of these updates will be set by the GEOS-Chem Steering Committee, based on the recommendations of the Working Group chairs. If you would like to weigh in on prioritization of the updates please contact your Working Group chairs. For a list of these updates, please see [the "in the pipeline" table of the GEOS-Chem v11-02 wiki page](#).

Implementation of NetCDF Diagnostics in GEOS-Chem

Overview

[GEOS-Chem v11-02](#) will contain structural updates to archive diagnostic quantities to netCDF output. **The existing “binary punch” diagnostics will be preserved in the public release of v11-02.**

NetCDF has now become the de-facto standard file format for atmospheric and climate models worldwide. Unlike the existing [binary punch \(aka “bpch”\) file format](#), netCDF files can be written to and read from disk very efficiently in high-performance computing (HPC) environments. There are also several free and open-source software packages for visualizing and manipulating netCDF data files.

Development of the netCDF diagnostic infrastructure within GEOS-Chem is currently in progress. Bob Yantosca has created [an overview presentation about the new netCDF diagnostics for v11-02, included in the GEOS-Chem Vision documents, which summarizes the initial validation process](#). He has also set up a wiki page entitled [List of diagnostics for v11-02](#) in which you will find more information, including a list of names for each diagnostic quantity. Lizzie Lundgren is leading the GCHP diagnostics development effort.

Design Details

Here are some important points about the structure of the netCDF diagnostics in GEOS-Chem:

1. The new netCDF diagnostic package in GEOS-Chem “Classic” is designed to mimic how the diagnostics already work in [GEOS-Chem with the High-Performance Option](#) (aka “GCHP”).
 - GEOS-Chem “Classic” uses the same diagnostics input file (called HISTORY.rc) as GCHP does, with some minor modifications.
 - The netCDF diagnostics in both GEOS-Chem “Classic” and GCHP are “array” based rather than “point” based. This means that the diagnostics are designed to store data on a grid rather than as individual points along a flight track or satellite path.
2. We do not plan on introducing netCDF diagnostic features into GEOS-Chem “Classic” that are not also present in GCHP.
 - For example, we will not have the ability to save out a series of points like the ND40 planeflight diagnostic (ASCII output) or ND48 point timeseries diagnostic (bpch output) in the new netCDF diagnostic package.
 - That being said, we will “grandfather in” the ND40 planeflight diagnostic for GEOS-Chem “Classic”. We will either keep it in ASCII format, or replace it with equivalent functionality, such as NOAA’s ObsPack code.
3. At present, the netCDF diagnostic output in GEOS-Chem “Classic” can archive global fields.
 - It would be easy to add in the capability to save a subset of fields (e.g. a horizontal region of the world).
 - We plan to delay implementation of this until after all of the diagnostics required for benchmark simulations have been implemented as netCDF output.
4. Many of the emissions diagnostics in GEOS-Chem are archived by the [HEMCO emissions component](#), and are manually written to bpch output.
 - The new netCDF diagnostics will not attempt to save diagnostic quantities that can already be archived by HEMCO.
 - These HEMCO-based diagnostics will be saved to the HEMCO_diagnostics*.nc netCDF files.
5. For now the units of the new netCDF diagnostics will remain same as the existing diagnostics, as this will facilitate validation.
 - We propose that we implement area-independent units (e.g. [kg/m²/s] or [kg/m³/s], depending on the type of the diagnostic) at a later date (perhaps in the version following v11-02).
 - Area-independent diagnostics will facilitate using GEOS-Chem to use any type of grid (e.g. GCHP cubed-sphere).

- Area-independent diagnostics will also be consistent with the units of diagnostic outputs from the [HEMCO emissions component](#).
 - Area-independent diagnostics facilitate comparing GEOS-Chem output on different types of grids (cubed-sphere vs. lat-lon).
6. The user will be able to request time-averaged or instantaneous diagnostic collections, with a specified archival frequency.
- Time-averaged collections will get updates from the various arrays in GEOS-Chem once per dynamic (aka “heartbeat”) timestep by default. This is 10 minutes for most GEOS-Chem simulations and it mimics the behavior of GCHP. However, it has implications for binary vs. netCDF diagnostic reproducibility. This is discussed in more detail in a later section.

Naming Convention for GEOS-Chem Diagnostic Quantities

As part of the migration to netCDF diagnostics we are overhauling the diagnostic names to improve usability. The naming convention for GEOS-Chem diagnostic quantities (netCDF only) is described below.

1. Diagnostic names may only consist of letters, numbers, and single underscores for consistency with both the [COARDS](#) and [CF](#) netCDF conventions.
2. Diagnostic names are case-insensitive. However, we recommend using “camel case” (i.e. mixed upper and lower case) to improve readability (e.g. ProdBCPI from BCPO),
3. “CHEM_” (case-insensitive) must precede the array name when archiving an array field from the State_Chm object. (e.g. CHEM_Species_NO, CHEM_AeroAreaSulf)
4. “MET_” (case-insensitive) must precede the array name when archiving an array field from the State_Met object (e.g. MET_U10M, MET_T, MET_TROPP).
5. Single underscores may only be used in these instances:
 - Separating the prefixes “CHEM_” and “MET_” from the rest of the variable name, as described above.
 - Separating the diagnostic name from a wildcard or tag that can be included in a wildcard (e.g. SpeciesConc_NO or SpeciesConc_?ADV?).
6. You can use wildcards to request a subset of species or bins instead of having to list each diagnostic name individually. Below is a preliminary set of wildcards:
 - ?ADV?: Advected species
 - ?AER?: Aerosol species
 - ?ALL?: All GEOS-Chem species
 - ?DRY?: Dry-deposited species

- ?FIX?: Inactive (aka "fixed") species in the KPP chemical mechanism
- ?GAS?: Gas-phase species
- ?KPP?: KPP species
- ?PHO?: Photolyzed species
- ?VAR?: Active (aka "variable") species in the KPP chemical mechanism
- ?WET?: Wet-deposited species
- ?DUSTBIN?: Dust bins

We invite you to visit our [List of diagnostics for v11-02 wiki page](#) to view a complete list of diagnostic names, and the corresponding legacy "binary punch" diagnostic that each netCDF diagnostic corresponds to.

Configuring NetCDF Diagnostic Output

Below is a sample HISTORY.rc file that is used to request netCDF diagnostic output from a GEOS-Chem "Classic" simulation. The format is based upon the diagnostic file specification developed by GMAO for use in GEOS-5 and is similar to that used in GCHP.

```
COLLECTIONS: 'inst',
             'avg',
             ::
inst.filename: './GEOSChem.inst.%y4%m2%d2.nc4',
inst.frequency: 060000,
inst.duration: 240000,
inst.mode: 'instantaneous',
inst.fields: 'SpeciesConc_?ADV?', 'GIGCchem',
             'Met_T', 'GIGCchem',
             'DryDepVel_?DRY?', 'GIGCchem',
             'WetLossLS_?WET?', 'GIGCchem',
             ::
avg.filename: './GEOSChem.avg.%y4%m2%d2.nc4',
avg.frequency: 000100 000000,
avg.duration: 000100 000000,
avg.mode: 'time-averaged',
avg.fields: 'SpeciesConc_?ADV?', 'GIGCchem',
            'Met_PEDGE', 'GIGCchem',
            'Jval_?JVN?', 'GIGCchem',
            'WetLossLS_?WET?', 'GIGCchem',
            'OHconcAfterChem', 'GIGCchem',
            ::
```

In this HISTORY.rc file, we are requesting two collections, or types of netCDF file output.

1. The first collection (**inst**) is **instantaneous (aka timeseries) output** with a **6-hour frequency**. A new file will be created **every 24 hours**.
2. The second collection (**avg**) is **time-averaged output**. Data will be updated at the dynamic timestep (= 10 minutes for most GEOS-Chem simulations) by default and **averaged into monthly-mean output**. A new file will be **created at the start of each new month**.
3. **The diagnostic quantities (aka “fields”)** listed after the “fields” tag are archived in each collection. These diagnostic quantities must follow the naming convention described in the previous section.
 - a. For GEOS-Chem “Classic” simulations, you may use wildcards to request sets of diagnostics. For example, instead of listing SpeciesConc_NO, SpeciesConc_O3, SpeciesConc_PAN, SpeciesConc_CO, etc. individually, you can simply use SpeciesConc_?ADV? to request all of the advected GEOS_Chem species.
4. The “GIGChem” text is only relevant for GCHP and will be ignored for GEOS-Chem “Classic” simulations.

For more examples, please see [Bob Yantosca’s netCDF diagnostics overview presentation](#). We will also add more documentation to the GEOS-Chem wiki in the coming weeks.

Differences Between Binary and NetCDF Diagnostic Values

One of the design decisions GCST must resolve is the update frequency for accumulating values when archiving time-averaged diagnostics. This decision has implications for reproducibility between binary and netCDF diagnostics, compatibility with GCHP, and the distribution of diagnostics in output files. GCST seeks feedback from GCSC on this issue.

The considerations are as follows:

1. Each netCDF diagnostic collection (e.g. time-averaged) uses a common update frequency for accumulated values.
 - To enable inclusion of all diagnostics within a single output file (single collection) the update frequency is the heartbeat, or minimum timestep (usually dynamic), of the model run.
 - This is consistent with the MAPL History component in GCHP, upon which the GEOS-Chem “classic” History component is based, and allows simple compatibility between GEOS-Chem “classic” and GCHP diagnostic infrastructure.
2. In contrast, binary diagnostics use multiple update frequencies.
 - Many binary diagnostics use the chemistry timestep (20 min for most simulations) as the update frequency rather than the heartbeat. For example, the ND45 species concentration diagnostic is updated on each chemistry timestep.

3. Switching to use of a single update frequency for all diagnostics will result in differences between the binary and netCDF time-averaged diagnostic values for certain diagnostics.
 - For example, the species concentration diagnostic will be updated after every dynamic timestep, different from the binary ND45 which updates every other dynamic timestep. This will result in non-negligible differences.

The GCST recommends that the time-averaged diagnostic quantities in GEOS-Chem "Classic" be updated on each "heartbeat" timestep despite these differences. This is so the diagnostic infrastructure mimics the behavior of the History component in GCHP and allows for output of all time-averaged diagnostics in a single file.

Status of netCDF Diagnostics

We invite you to view the presentation [NetCDF diagnostic validation in GEOS-Chem "Classic"](#) by Bob Yantosca and the GCST, which summarizes the initial validation process.

Plans For Recreating Specialty Diagnostics

ND40 Planeflight Diagnostic

Tomas Sherwen (York) wrote:

Please could I ask if there is a position on/plan for restoring the chemical rate tracking (REA_??) functionality of the planeflight diagnostic?

In v11-01/ v11-02d REA_?? has been deactivated due to [FlexChem](#).

I use this functionality (and I suspect many others do) for tracking rates (e.g. JNO2) along plane/ship/station tracks/timeseries at instrument resolution.

Melissa Sulprizio (GCST) replied:

Yes, we will eventually restore the chemical rates in the planeflight diagnostic. One issue is that we're currently developing netCDF diagnostics and that will mess up the planeflight diagnostics even more. Bob wrote to the GCSC:

For the "planeflight" diagnostic, we will investigate using a separate package (such as NOAA ObsPack, as recommended by Andy Jacobson at IGC8) that can more efficiently store point data. Then new diagnostic package we are developing works well for array data but not as well for point data.

Once the netCDF diagnostics are in place, we will reconsider how to fix/update planeflight_mod.F. If you need these diagnostics in the meantime, you should be able to hack it into the chemical mechanism by adding dummy species to the reactions you want to track and then rebuilding the mechanism based on [these](#)

[instructions](#). In flexchem_mod.F90, you can then obtain the rate from KPP using the C array (e.g. Rate = C(ind_NEWSPC) / DT to get molec/cm3/s).

Mat Evans (York) replied:

I've had a quick look at obspack. I'm not sure its well suited to our needs.

I personally don't see much need to update the plane flight files. They are easy to understand at the moment and easy to manipulate being in ascii. The biggest problem at the moment is that the rate constants have fallen out of them because of the move to FlexChem. If we can get that sorted I don't think there is a pressing need to update the format.

ND48 Station Diagnostics

We will keep the current ND48 station diagnostics (bpch format) in [GEOS-Chem v11-02](#) until we can find a suitable replacement.

Jenny Fisher (U. Wollongong) wrote:

It seems we are losing compatibility for both ND48 (station) and ND51 (satellite) diagnostics. These are probably the two my group uses most frequently (and replacing with e.g. hourly output everywhere will require a lot of extra disk space). If we are going to have regional subsetting of diagnostics available, then ND48 can probably be dealt with by subsetting down to the level of a single box – but ND51 is harder.

ND49 Instantaneous Timeseries Diagnostic

The legacy ND49 diagnostic in GEOS-Chem saves diagnostic quantities to binary punch files as instantaneous output, with a user-specified frequency.

Any GEOS-Chem diagnostic quantity can be archived to netCDF output as an instantaneous collection. For detailed instructions, please see [this post on our List of diagnostics for v11-02 wiki page](#).

ND50 24-hr Average Timeseries Diagnostic

The ND50 “binary punch” diagnostic in GEOS-Chem saves diagnostic quantities to binary punch files as daily-averaged output.

Any GEOS-Chem diagnostic quantity can be archived to netCDF output as a time-averaged collection with a 24-hour frequency. For detailed instructions, please see [this post on our List of diagnostics for v11-02 wiki page](#).

ND51 Satellite Diagnostic

Aaron van Donkelaar (Dalhousie) wrote:

I wanted to double check about how the satellite-overpass diagnostic (ND51) was being included. There was some mention of it within the [\(netCDF diagnostic\) presentation](#), but I wasn't clear to me how the time-averaged netcdf collection could be made to output something similar to the current ND51.

My main concern was that ND51 samples between two defined local times once each day. From what I understood of the time-averaged collection via netcdf, it could be set to regularly sample between a defined interval of time (e.g. every six hours), but I didn't understand how this could be set to sample between, say, 10am-12pm local time each day. Neither local time, nor once per day seemed an option.

Apologies if I've just misunderstood, but I thought I should check that an ND51-type output would still be possible.

Bob Yantosca (GCST) replied:

At this time we don't yet have a good substitute for the ND51 satellite timeseries diagnostics. We may be able to replicate this with some type of satellite simulator package, but that remains to be seen as of yet. Right now we are focusing our efforts on implementing the netCDF diagnostics that are required for benchmarking. (Specialty diagnostics will be added later.)

We have designed the netCDF diagnostics for GEOS-Chem "Classic" to replicate the behavior of the diagnostics in GCHP. Having the diagnostics work the same way in both configurations of GC facilitates benchmarking and comparing GC "Classic" to GCHP. It also makes it easier for users to switch between GC "Classic" to GCHP. But GCHP does not allow for local-time diagnostics. GCHP relies on the MAPL library, and its diagnostic package (aka "History") only allows for instantaneous or time-averaged output.

One could save e.g hourly timeseries, along with a local time field, to netCDF, and apply the local time comparison in post-processing. This would be doable but it would also end up generating a ton of output.

The good news is that we will preserve the bpch diagnostics in v11-02 (I need to update the wiki better to reflect that). We will not remove the bpch diagnostics until we have found a suitable replacement for the local-time diagnostics. So for the time being you can still rely on ND51.

Plans to Implement Better Flux Diagnostics

Chris Holmes has suggested a plan to improve the diagnostics which compute the flux of species due to advection, convection, and PBL mixing in GEOS-Chem. He writes:

It's a pretty basic idea: track the change in burden (moles) of species S within a [vertical] region R due to each process P. After each month, or other user-defined interval, write the burden change to the log file or elsewhere.

- $\text{Number of diagnostics} = (\text{Number of Regions}) * (\text{Number of Species to track}) * (\text{Number of processes to track})$

For a start:

1. Number of regions = 3
 - Within the PBL
 - Within the troposphere
 - Within the whole column,
2. Number of species = 1
 - O3
 - Users could add more if they wish.
3. Number of processes to track = 7
 - 'Emission', 'Chemistry', 'Advection', 'PBL', 'Convection', 'DryDep', 'WetDep'

For each diagnostic,

1. Qualitative definition:
 - Burden change (moles) for species S in region R due to process P
2. Quantitative definition
 - Units: moles or moles/s
 - # of dimensions: 2 (number of longitudes * number of latitudes).
 - Precision: single real*4

The GEOS-Chem Support Team is planning on implementing these new flux diagnostics, probably in GEOS-Chem v11-02f. The flux diagnostics will be 2-dimensions on a horizontal grid to enable output in both GEOS-Chem "classic" and GCHP. There will be a separate diagnostic name for each vertical region, process, and species, and all flux diagnostics will be configurable with species wildcards.

Other structural updates

Returning errors to the main program level

In v11-02d we are overhauling how error trapping is done in GEOS-Chem, concurrently with the implementation of netCDF diagnostics.

When an error occurs in a GEOS-Chem simulation, the simulation often halts in the routine where the error occurred. This is usually not an issue for GEOS-Chem “Classic” simulations, which only run on a single node of a computer system. But this can be a problem for GCHP simulations, which can run on multiple nodes. A GCHP simulation that encounters an error could potentially halt on one node but continue to execute on all other nodes.

A better way to handle errors is to immediately exit the routine where the error occurred and propagate a “failure” status all the way up to the main program level. The simulation can then be terminated gracefully from the main level. This would ensure that a GCHP simulation would halt on all nodes on which it is running.

This effort is being done in a piecemeal process. At present only a few modules (input_mod.F, convection_mod.F, wetscav_mod.F) have been converted to return errors to the main level. We will continue to add this functionality in further v11-02 development.

Chemistry Updates

Halogen chemistry mechanism

In GEOS-Chem v11-02d, we plan on introducing the halogen chemistry scheme of Tomas Sherwen et al (cf. [ACP, 16, 12239-12271, 2016](#)) into the GEOS-Chem. From the abstract:

We present a simulation of the global present-day composition of the troposphere which includes the chemistry of halogens (Cl, Br, I). Building on previous work within the GEOS-Chem model we include emissions of inorganic iodine from the oceans, anthropogenic and biogenic sources of halogenated gases, gas phase chemistry, and a parameterised approach to heterogeneous halogen chemistry. Consistent with Schmidt et al. (2016) we do not include sea-salt debromination. Observations of halogen radicals (BrO, IO) are sparse but the model has some skill in reproducing these. Modelled IO shows both high and low biases when compared to different datasets, but BrO concentrations appear to be modelled low. Comparisons to the very sparse observations dataset of reactive Cl species suggest the model represents a lower limit of the impacts of these species, likely due to underestimates in emissions and therefore burdens. Inclusion of Cl, Br, and I results in a general improvement in simulation of ozone (O₃) concentrations, except in polar regions where the model now underestimates O₃ concentrations. Halogen chemistry reduces the global tropospheric O₃ burden by 18.6 %, with the O₃ lifetime reducing from 26 to 22 days. Global mean OH concentrations of 1.28×10^6 molecules cm⁻³ are 8.2 % lower than in a simulation without halogens, leading to an increase in the CH₄ lifetime (10.8 w) due to OH oxidation from 7.47 to 8.28 years. Oxidation of CH₄ by Cl is small ($\sim 2\%$) but Cl oxidation of other VOCs (ethane, acetone, and propane) can be significant ($\sim 15\text{--}27\%$). Oxidation of VOCs by Br is smaller, representing 3.9 % of the loss of acetaldehyde and 0.9 % of the loss of formaldehyde.

We have also added oxidation of sulfur by reactive halogens (cf. Qianjie Chen et al GRL, 10.1002/2017GL073812, 2017):

Sulfur and reactive bromine (Bry) play important roles in tropospheric chemistry and the global radiation budget. The oxidation of dissolved SO₂ (S(IV)) by HOBr increases sulfate aerosol abundance and may also impact the Bry budget, but is generally not included in global climate and chemistry models. In this study, we implement HOBr + S(IV) reactions into the GEOS-Chem global chemical transport model and evaluate the global impacts on both sulfur and Bry budgets. Modeled HOBr mixing ratios on the order of 0.1–1.0 parts per trillion (ppt) lead to HOBr + S(IV) contributing to 8% of global sulfate production and up to 45% over some tropical ocean regions with high HOBr mixing ratios (0.6–0.9 ppt). Inclusion of HOBr + S(IV) in the model leads to a global Bry decrease of 50%, initiated by the decrease in bromide recycling in cloud droplets. Observations of HOBr are necessary to better understand the role of HOBr + S(IV) in tropospheric sulfur and Bry cycles.

Halogen chemistry will be turned on by default in all GEOS-Chem mechanisms (even in the “tropchem”, or tropospheric-only simulation).

Bug fixes for heterogeneous chemistry

This update will be included in [v11-02d](#).

Sebastian Eastham wrote:

There's a bug in the v11-02c het rate code. In KPP/Standard/gckpp_HetRates.F90, many of the dedicated routines (e.g. HetIMAE) loop over NAERO. The loop looks like

```
Do N=1,NAERO
  ! [Comment]
  If (N==8) Then
    XSTKCF = [number]
  End If

  If (N == 13) Then
    ADJUSTEDRATE = XAREA(N)*XSTKCF
  Else
    ADJUSTEDRATE = ARSL1K( XAREA(N), XRADI(N), XDENA,
                          XSTKCF, XTEMP, (A**0.5_FP) )
  End If

  Het_IMAE = Het_IMAE + ADJUSTEDRATE
End Do
```

The problem here is that every aerosol after aerosol 8 is inheriting the sticking coefficient from aerosol 8. Crucially, this includes SOAS – so the fact that the simple SOA tracer is missing could affect this. GCC is artificially increasing the het rate on all aerosols because of this bug, whereas GCHP is not. Fixing this would be as simple

as inserting either $XSTKCF = 0.0$ or $XSTKCF = B$ at the start of the loop, where I've written ! [Comment]. The question of which is correct is really a science question (probably $XSTKCF = B$, although I'd ask the original authors). However, what's definitely true is that one of these two options needs to be put in or the result of the calculation will be wrong.

Fixing this bug is likely to change SOA burdens in both GCC and GCHP. In `gckpp_HetRates`, the following routines are definitely affected:

- `HetGLYX`
- `HetMGLY`
- `HetIEPOX` (forms SOAIE)
- `HetIMAE` (forms SOAME)

The other het routines look like they have the correct form (either by a "header" of $XSTKCF = B$, or because they have an `If...Elseif...Else...End` clause that catches all possible values of N and sets $XSTKCF$ accordingly).

Melissa Sulprizio replied:

The solution is to set $XSTKCF = TINY(1e0)$ where ! [Comment] is in the code snippet above, following what is done in Eloise Marais's version of `calcrate.F`.

Update CH4 latitude bands for 2014-2016

The last year of latitudinal CH4 concentration data (based on CMDL flask observations) was 2013. (Data is provided in 4 [latitude bands](#): 90°S-30°S, 30°S-0°N, 0°N-30°N, 30°N-90°N.) [Katherine Travis](#) has updated the subroutine `get_global_ch4.F` with additional years of latitudinal CH4 data from 2014 thru 2016. These data will be added to v11-02d.

[Lee Murray](#) will provide monthly mean CH4 concentration data from NOAA GMD flask observations. This update will be included in v11-02e. See [this post on our NOx-Ox-HC-aerosol wiki page](#) for more information.

Remove MONX from chemical mechanisms

This fix will be included in [v11-02e](#).

Sam Silva (MIT) wrote:

I was wondering why there were three monoterpene species in the chemical mechanism: MTPA (lumped alpha pinene), LIMO (lumped limonene) and then MONX (all monoterpenes).

MONX doesn't play with any of the monoterpene nitrate chemistry, it just is converted into 3 formaldehyde:

```
MONX = 3.000CH2O : GCARR(1.07E-05, 0.0E+00, 0.0);
```

It seems like having the MONX group (all monoterpenes) and the speciated lumped monoterpenes is an inconsistency. Ultimately, I'm interested in adding Glyoxal formation from monoterpenes, and it's not clear to me how to properly do that, given the three different species.

In v11-02a, we [introduced monoterpene chemistry during Emily's PAN updates](#). At that time MTPA was introduced. The [monoterpene chemistry was further modified and expanded upon](#) in v11-02c following Jenny's updates originally made for SEAC4RS.

Looking back at Emily's original PAN updates that she sent to us (based on v9-02h), it looks like MONX is a dead species in globchem.dat and the MONX -> 3CH2O reaction is not included. That may have been an oversight during the PAN updates implementation.

The MONX species will be removed from GEOS-Chem mechanisms in v11-02e, upon the recommendation given to us by Emily Fischer.

GEOS-Chem High Performance in the Standard Model

GEOS-Chem with the high performance option (GCHP) continues to be up-to-date with the standard model. GCHP features the same science as GEOS-Chem using the standard "classic" capability but operates on a cubed-sphere grid and is parallelized using a message-passing interface (MPI) implementation. GCHP improves upon GEOS-Chem "classic" by (1) enabling more accurate transport through elimination of the polar singularity inherent to lat-lon grids, and (2) providing efficient scaling across multiple machines making finer resolution global simulations possible.

As described previously, complete functionality of all GEOS-Chem diagnostics in GCHP is in development. We anticipate that all benchmark diagnostics will be fully functional in the GEOS-Chem v11-02 release. Colin Lee (Dalhousie) is assisting with GCHP diagnostic validation.

We have received a new version of MAPL from GMAO which has potential to improve I/O speed of GCHP. MAPL is a software interface used to streamline use of ESMF and contains much of the infrastructure upon which GCHP depends. The new MAPL version will be incorporated into GEOS-Chem v11-03.

As always, we encourage users to set up GCHP on their systems, join the GCHP Working Group, and provide feedback on user experience and model performance. [The GEOS-Chem HP v11-02 wiki page](#) lists version information as well as GCHP-specific features, bug fixes, and outstanding issues. We also have a GCHP Slack workspace for users to easily communicate with each other.

For more information on GCHP including tutorials and contact information, please see the [GCHP homepage](#) on the GEOS-Chem wiki.

GCPy: A new Python toolkit for GEOS-Chem

GCPy is a Python-based toolkit containing useful functions and routines for working with [GEOS-Chem](#), meant to update and replace the IDL-based [GAMAP](#) utility. GEOS-Chem user Daniel

Rothenberg (formerly MIT) led the development effort. GCPy aims to build on the well-established scientific python technical stack, leveraging tools like [cartopy](#) and [xarray](#) to simplify the task of working with model output and performing atmospheric chemistry analyses.

The GCPy package is comprised of two major components:

1. A library of functions, implementing some of the core chemistry and thermodynamic calculations in GEOS-Chem for use outside of the model.
2. Documentation including long-form articles, interactive notebooks, and short example snippets illustrating workflows using Python and GCPy.

If you would like to get started with GCPy, please view the [GCPy documentation and tutorials](#). For more information please contact the [GEOS-Chem Support Team](#).

Caveat: GCPy is still very much under development and is not 100% ready for widespread use. But we encourage interested users to start using GCPy and to provide feedback and/or contribute to its development.

For more information, please contact the [GEOS-Chem Support Team](#) or reach out to us on the [GEOS-Chem Wiki](#).

Conclusions

We anticipate releasing GEOS-Chem v11-02 in early 2018. The new version will contain important chemistry updates, particularly involving the SOA and halogen species, as well as structural improvements, such as the capability of outputting diagnostics in netCDF format. Binary diagnostics will continue to be available in GEOS-Chem v11-02.

Support for obsolete met fields will be removed from v11-02c. This will also allow us to eventually store a copy of the GEOS-Chem emissions and met field data on cloud-based storage.

GEOS-Chem with the High-Performance Computing option continues to be up-to-date with the standard GEOS-Chem model. We encourage interested users to take GCHP for a spin! Inclusion of diagnostics in GCHP output is in development and will be included in the v11-02 release.

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, Lizzie Lundgren, and Melissa Sulprizio
for the GEOS-Chem Support Team