GEOS-Chem Newsletter, Summer 2014

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The dates for IGC7 are now set!

We are pleased to announce that the **7th International GEOS-Chem Meeting (aka IGC7)** will take place at Harvard University from May 4-7, 2015. You will find the latest information about the IGC7 meeting at our web site **meeting.geos-chem.org**. As the meeting date draws closer, we will update the site with information about hotels, registration, and the list of oral and poster presentations.

The GEOS-Chem Steering Committee met on June 5, 2014

Please take a moment to read the minutes from the latest GCSC telecon. The next GCSC telecon will take place in August or September 2014, date TBD.

GEOS-Chem v9-02 wrap-up

We officially released GEOS-Chem v9-02 on 03 Mar 2014

The GEOS-Chem v9-02 public release (03 Mar 2014) includes several important updates:

- New soil NOx emission module
- Several updates for the Mercury simulations
- New POPs simulation
- Structural updates to facilitate running GEOS-Chem within the GEOS-DAS
- Several chemistry and emission updates (including AEIC aircraft emissions)
- Removal of NOx-Ox partitioning
- Improved HO2 uptake by aerosol
- Support for GEOS-FP met fields
- Many fixes for technical issues

We invite you to visit the *GEOS-Chem v9-02* wiki page for the most up-to-date information about GEOS-Chem v9-02. Please visit our *GEOS-Chem v9-02 benchmark history* wiki page for information about the 1-month and 1-year benchmarks used to validate GEOS-Chem v9-02.

GEOS-Chem v9-02 was the first version of GEOS-Chem in which we solicited feedback from users during a period of public comment. This allowed GEOS-Chem users to download and test a provisional release of v9-02. During the period of public comment, which lasted approximately

1 month, GEOS-Chem users identified several minor issues with the specialty and nested-grid simulations. The GEOS-Chem Support Team fixed these issues before the official release of v9-02 on 03 Mar 2014.

We recommend that all GEOS-Chem users migrate to v9-02 as soon as possible. If you have not yet downloaded v9-02, then follow the instructions in Chapter 2 of the GEOS-Chem Online User's Guide.

We have fully integrated the TOMAS microphysics package into v9-02

The TOMAS aerosol microphysics package has been reincorporated into GEOS-Chem v9-02. TOMAS now has 4 options (12, 15, 30, 40 size bins) and is now fully parallelized. Furthermore, TOMAS is more tightly incorporated into GEOS-Chem than in previous versions.

Benchmark simulations performed by Jeff Pierce and his group at Colorado State show that TOMAS in GEOS-Chem v9-02 performs comparably to previous simulations done with the older GEOS-Chem version v8-02-02. For more information, please see these validation plots on our *TOMAS aerosol microphysics* wiki page.

We would like to acknowledge the TOMAS team for their recent contributions: Peter Adams (Carnegie Mellon), Jeff Pierce, Sal Farina, Steven D'Andrea, Robin Stevens (all @ Colorado State), and Marguerite Marks (Carnegie Mellon).

We updated the *List of New Developments* and *Narrative Description* for v9-02

The GEOS-Chem Steering Committee has updated the *GEOS-Chem Narrative* and the *New GEOS-Chem Developments* web pages for GEOS-Chem v9-02. The *GEOS-Chem Narrative* provides a quick reference for papers to cite in describing the model. The *New GEOS-Chem Developments* lists updates of sufficient recent vintage—most of them for v9-02—that we recommend offering co-authorship to developers if they are significant for your paper.

We remind all GEOS-Chem users and developers to be generous in citations and co-authorships for GEOS-Chem developers. It is good practice and is key to our success as a community. See the *Credits and References* web page for more information.

We were not able to correct all identified issues before the release of GEOS-Chem v9-02

A few issues were still unresolved by the time GEOS-Chem v9-02 shipped on 03 Mar 2014. For a complete list, please see our *Currently unresolved issues in GEOS-Chem* wiki page.

We have been able to fix some of these issues—such as coding bugs and typographical errors—in our development version GEOS-Chem v10-01. For example, the `input.geos` file that shipped with v9-02 contained an incorrect molecular weight. We added the proper molecular weight to the `input.geos` file in version GEOS-Chem v10-01. We also informed the GEOS-Chem users so that they could apply the proper molecular weight to their copies of the `input.geos` file.

Other unresolved issues from v9-02 reflect areas of active research.

We issued a patch after the release of v9-02 in order to fix a problem with acetone photolysis

After the release of GEOS-Chem v9-02, we were informed of a problem with the computation of the photolysis rate of acetone, aka J(ACET). The implementation of acetone photolysis in GEOS-Chem v9-02 and prior versions (dating back to 2009) neglected the strong pressure dependency for wavelengths > 300 nm, as reported in the JPL 10-6 recommendation. We invite you to read the complete description of the problem on our *FAST-J photolysis mechanism* wiki page.

We have since applied a fix for acetone photolysis to GEOS-Chem v9-02. Katie Travis produced these plots comparing SEAC4RS aircraft observations to GEOS-Chem output before and after the fix to acetone photolysis. The fix improves J(ACET) from the GEOS-Chem v9-02 public release, but there are still some discrepancies due to uncertainties in both the measurements and model.

If you are currently using GEOS-Chem v9-02, please follow these instructions to obtain a fresh copy of the code with the fix for acetone photolysis applied!

We would like to acknowledge Sebastian Eastham (MIT), Jingqiu Mao (Princeton), Katie Travis (Harvard), and Chris Chan Miller (Harvard) for their assistance in resolving this problem.

GEOS-Chem v10-01 development

We corrected several minor issues in v10-01

GEOS-Chem v10-01a introduced a fix to reduce the dry deposition surface resistance when using the Olson 2001 land map. This development came out of the research being done by our SEAC4RS team, consisting of Patrick Kim, Karen Yu, Lei Zhu, Natasha Goss, and Katie Travis (all @ Harvard), and Jenny Fisher (U. Wollongong).

In GEOS-Chem v10-01b, we corrected an error in the `input.geos` file (wrong molecular weight for PROPNN). We also now use the MAP_A2A regridding algorithm to regrid the TOMS overhead ozone columns from 1^o x 1^o resolution.

In GEOS-Chem v10-01d, we fixed a typo in the chemical mechanism input file, a parallelization error in the 0.5^o x 0.666^o nested-grid simulation, and a minor bug in the dry deposition diagnostic.

We added a stratospheric chemistry capability to v10-01

We have integrated the UCX strat-trop chemical mechanism into GEOS-Chem v10-01c. With the UCX mechanism, GEOS-Chem can finally perform detailed online chemistry in the

stratosphere. UCX accounts for several stratospherically-important species, such as the CFCs and HCFC's.

The 1-month benchmarks for v10-01c were approved on 29 May 2014. But the 1-year benchmarks for v10-01c are still running as of this writing. We expect them to have finished by the second week of June 2014.

We would like to acknowledge Sebastian Eastham (MIT), Debra Weisenstein (Harvard), and Steven Barrett (MIT), who are the authors of the UCX mechanism and source code.

We updated the photolysis mechanism in v10-01

The implementation of UCX into GEOS-Chem necessitated the replacement of the FAST-J photolysis mechanism with FAST-JX version 7.0. FAST-JX (written by Oliver Wild and Michael Prather) can simulate photolysis in the stratosphere better than FAST-J can. FAST-JX also contains more up-to-date photolysis rates than those contained in FAST-J.

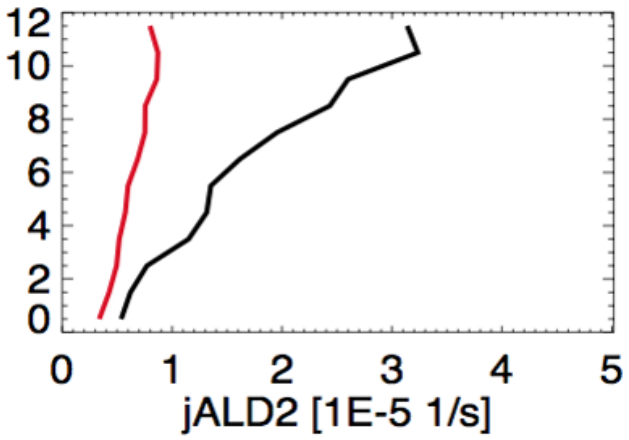
For more information on the differences between FAST-J and FAST-JX, we invite you to read our newly-updated *FAST-J photolysis mechanism* and *FAST-JX v7.0 photolysis mechanism* wiki pages.

We would like to acknowledge Sebastian Eastham (MIT) for implementing FAST-JX v7.0 into GEOS-Chem. Furthermore, Jingqiu Mao (Princeton), Chris Chan Miller (Harvard), and Katie Travis (Harvard) provided invaluable assistance in validating the photolysis for acetone and several other VOC species.

We are still researching the photolysis rates of some VOC species in v10-01

Jingqiu Mao writes:

> We know that carbonyl nitrate should be photolyzed much faster than the current rates in FAST-JX v7.0, according to this paper. But updates in this rate should also be combined with updates in the OH rate in order to better reproduce the experimental results from chamber studies. This seems more like a research question, so we decided to leave this to our SEAC4RS research team.
>
> We also saw large discrepancies between **observed** and **modeled** J(ALD2), as shown in this plot (on the next page) by Chris Chan Miller:



This discrepancy is very likely due to the lack of pressure dependence on the quantum yield. But Michael Prather didn't include this pressure dependence in any of the FAST-JX versions. So this remains as a problem in all GEOS-Chem versions, including GEOS-Chem v10-01c. We are currently investigating.

We improved the computational efficiency of GEOS-Chem in v10-01

Along with the UCX mechanism, we added several structural updates to GEOS-Chem v10-01c to remove computational bottlenecks. These include:

- We added support for the Tuning and Analysis Utilities (TAU). TAU allows you to generate profiles of GEOS-Chem execution, so that you can identify areas of code that are performing poorly.

- We were able to speed up computations in the Olson land map module by a factor of 100 by using TAU. We also reduced the time spent in an advection subroutine by a factor of 7.

- We reduced the memory footprint of the GMI stratospheric chemistry module by reducing the size of certain arrays from `REAL*8` to `REAL*4`.

- We removed inefficient subroutine calls in the GEOS-4 convection module, GCAP convection module, and Hg2 partitioning module.

We may be able to speed up the KPP chemical solver mechanism in v10-01

Mike Long has done some tests in speeding up the current implementation of the KPP chemistry solver. By using the Intel Math Kernel Library (aka MKL) instead of the default math libraries, Mike obtained a ~40% decrease in the time spent in the KPP chemical solver.

We are doing further testing. We hope to be able to add this as a compilation option into GEOS-Chem v10-01.

GEOS-FP update #1: Available met data at Dalhousie and Harvard

GEOS-Chem Support Team member Junwei Xu has been archiving the GEOS-FP met fields on the `rain.ucis.dal.ca` server at Dalhousie University. You may now download GEOS-FP data from April 2012 thru May 2014 for the following horizontal grids:

- 4^o x 5^o global
- 2^o x 2.5^o global
- 0.25^o x 0.3125^o nested grids:
    a. CH: China (70^o E – 140^o E; 15^o N – 55^o N)
    b. EU: Europe (15^o W – 40^o E; 32.75^oN – 61.25^o N)
    c. NA: North America (130^o W – 60^o W; 9.75^oN – 60^o N)
    d. SE: Southeast Asia (75^o E – 130^o E; 10^o N – 30^o N)

We are also storing the 4^o x 5^o global, 2^o x 2.5^o global and 0.25^o x 0.3125^o NA nested-grid data on the `ftp.as.harvard.edu` server at Harvard University.

GEOS-FP update #2: Archiving data at 0.25^o x 0.3125^o global resolution

Paul Palmer's group at U. Edinburgh will take the lead on processing the GEOS-FP met data to the full 0.25^o x 0.3125^o global resolution for input into GEOS-Chem. The GEOS-Chem Support Team will provide technical assistance to Paul's group.

The advent of the new supercomputer (and mass-storage unit) in the UK has generated a lot of interest in being able to run GEOS-Chem not only at the 0.25^o x 0.3125^o nested grids, but also at the 0.25^o x 0.3125^o global grid. The current (OpenMP-enabled) GEOS-Chem can probably only support a simple simulation with a few tracers (i.e. CO2, CH4, Hg) with the global 0.25^o x 0.3125^o GEOS-FP met before running into a memory limit. But the global 0.25^o x 0.3125^o data would be available for use with the new ESMF/MPI standalone Grid-Independent GEOS-Chem (aka GIGC) that is currently being developed. This would allow us to evaluate the performance of the ESMF/MPI standalone GIGC at the full global resolution of the GEOS-FP met.

Paul's group at U. Edinburgh will collaborate with other GEOS-Chem groups in the UK on this effort. We should have some 0.25^o x 0.3125^o global data in place by the time the ESMF/MPI standalone GIGC code is ready for use later this year.

Jintai Lin's group at Peking University has also started to work on a global 0.25^o x 0.3125^o degree simulation, to be run with GIGC. Jintai writes:

> It is very likely that by Oct 1 I can secure thousands of computation cores on a supercomputer to do this global high-res simulation. I now have one month of

> global high-res GEOS-FP met data to work with, thanks to the generous help of Junwei Xu at Dalhousie. I also have come up with some ideas to, for example, alleviate/solve the transport problem in the polar areas. I feel it is a good idea for Paul's and my group to develop the modeling capability together, instead of repeating the efforts.

HEMCO emissions component update

Christoph Keller has been implementing the Harvard-NASA Emissions Component (aka HEMCO) into GEOS-Chem. He writes:

> I have merged HEMCO into [my copy of] GEOS-Chem v10-01c.…The HEMCO configuration file…is in the run directory. It is set up to simulate a standard simulation (troposphere only). I just compared the results from a 1-month simulation against the standard run. I know that there is still an issue with the ParaNOx [ship plume model] … but apart from that it seems to me like HEMCO reproduces the emissions from the standard simulation within the expected deviation range.
>
> The next step will be to bring the UCX (strat-trop chemistry mechanism) input fields into HEMCO. As I realized, most of these data are boundary conditions and not emissions. I think it would be very easy to expand HEMCO in such a manner that it can also read and update boundary conditions.
>
> I haven't tested this version of HEMCO [i.e. in my copy of GEOS-Chem v10-01c] within an ESMF environment yet. There shouldn't be any problems with this, but I have to update the HEMCO – ESMF interface module.
>
> There are still some open structural questions that…mostly concern PBL mixing and diagnostics.
>
> I have implemented a new diagnostics scheme into HEMCO that allows generic diagnostics definitions and automatic output into netCDF files at a user-defined frequency. This makes it very easy to get emission fields (and any other variables) for different sources, species, etc. For now, the diagnostics have to be set within Fortran, but it would be easy to specify them through an input file.

We are currently merging Christoph's HEMCO code (based on v10-01c) into the GEOS-Chem source code repository. HEMCO is currently slated to be added to GEOS-Chem v10-01e. Once HEMCO has been validated in GEOS-Chem v10-01, we plan on adding the various emissions updates listed on the *GEOS-Chem model development priorities* wiki page. HEMCO will make adding these inventories a trivial process.

A version of HEMCO (based on the intermediate GEOS-Chem version v9-02l) has been successfully running within the GEOS-5 GCM on the NASA supercomputer Discover.

Lastly, the following paper has been accepted for final publication in GMD:

> Keller, C. A., Long, M. S., Yantosca, R. M., Da Silva, A. M., Pawson, S., and Jacob, D. J.: *HEMCO v1.0: A versatile, ESMF-compliant component for calculating emissions in atmospheric models*, Geosci. Model Dev. Discuss., **7**, 1115-1136, doi:10.5194/gmdd-7-1115-2014, 2014.

Grid-Independent GEOS-Chem (GIGC) update

We are testing the GIGC within the NASA GEOS-5 GCM

Mike Long has coupled the GEOS-Chem chemistry modules and HEMCO emission component with the NASA GEOS-5 GCM. He has run several test simulations using ~800 CPUs of the NASA Discover supercomputer. Mike's findings demonstrate that the GEOS-Chem chemistry module scales extremely well with an increasing number of CPUs.

Mike will write up his results in a journal article that will be submitted to GMD later this summer.

We are also working towards a standalone ESMF/MPI capable version of the GIGC

Our colleagues at NASA have been creating an ESMF-compliant version of the TPCORE advection module. Once this module is complete, we will interface this with our existing GEOS-Chem chemistry module and HEMCO emissions module. This will result in the creation of a new standalone GEOS-Chem that uses the same ESMF software infrastructure as the NASA GEOS-5 GCM, but can operate independently of the GCM (i.e. reading offline meteorology).

As of this writing, the ESMF-ized TPCORE advection module is still undergoing testing. We expect that this should be ready within a few weeks, if all continues to go well.

FLEXCHEM update

In preparation for the FLEXCHEM implementation in GEOS-Chem, we will have to rewrite how GEOS-Chem indexes tracers and species. Right now, GEOS-Chem uses a very historical method of integer variables in tracerid_mod.F (i.e. IDTO3, IDTCO, IDO3, IDNO, etc) that identify either an advected tracer or chemical species. But because FLEXCHEM will be able to add ANY chemical mechanism, we want to move away from this legacy code to a more flexible method using derived types. Mike Long is going to direct a "crowdsourcing" session at Harvard where several people will work on rewriting sections of code in parallel to implement this new indexing method.

At present there is no definite timetable when FLEXCHEM will be added into GEOS-Chem, other than it will follow HEMCO.

GEOS-Chem Unit Tester

We have a new tool that you can use to help find many common numerical errors and programming issues. The GEOS-Chem Unit Tester is an external package that can run several test GEOS-Chem simulations with a set of very strict debugging options. The debugging options are designed to detect issues such as floating-point math errors, array-out-of-bounds errors, inefficient subroutine calls, and parallelization errors.

The GEOS-Chem Unit Tester has become part of our standard validation protocol. We run a full set of unit tests before submitting each 1-month benchmark simulation. This ensures that common numerical errors will be found and fixed before the benchmark simulations are submitted.

We have recently added more unit tests for UCX, tagged Ox, tagged CO, POPs and TOMAS simulations. We have also modified the unit tester to display results from the individual unit tests in an easy-to-read web page format.

For complete instructions on how the GEOS-Chem Unit Tester can assist your debugging efforts, please see our *Debugging with the GEOS-Chem unit tester* wiki page.

Bob Yantosca
on behalf of the entire GEOS-Chem Support Team
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