

GEOS-Chem Steering Committee Telecon

23 February 2022

Attending/Missing:

Amos Tai, Andrew Schuh, Barron Henderson, Becky Alexander, Bob Yantosca, Chris Holmes, Christoph Keller, Daniel Jacob, Daven Henze, Dylan Jones, Dylan Millet, Eloise Marais, Fangqun Yu, Hong Liao, Jeff Geddes, Jeff Pierce, Jenny Fisher, Jingqiu Mao, Jintai Lin, Jun Wang, Kevin Bowman, Lee Murray, Liam Bindle, Lin Zhang, Lizzie Lundgren, Lu Hu, Lucas Estrada, Mathew Evans, Tzung-May Fu, Melissa Sulprizio, Prasad Kasibhatla, Pam Wales, Randall Martin, Sebastian Eastham, Yanxu Zhang, Yuxuan Wang, Clara Orbe

1. Updates to GCSC membership and responsibilities (Daniel, Randall)

- We welcome Clara Orbe to the GCSC as a new co-chair of the transport working group!
 - NASA GISS physical scientist with lots of overlap with GMAO doing transport analysis projects
- Daniel is stepping down as model scientist, Randall is stepping up to be the new model scientist. As Daniel says, it's time for a generational change and new ideas.
- Daniel is not going anywhere and the model will still be supported and developed by the teams at Harvard/ WashU
- Any nominations for steering committee members would be appreciated. An email will be sent asking for volunteers, but nominations tend to yield more interest.

2. Version 13.4.0 benchmark and what we do about ozone problem (Daniel)

- There are significant changes in sulfate that are due to the shift to KPP but they don't seem to break the model so OK.
- Ozone does not look good in the the southern hemisphere (too low) because of bromine chemistry
- BrO is still creeping up due to bug fixes.
- Should we release 13.4 and leave BrO as a research question?
 - Simple cure would be to disallow sea salt aerosol debromination
 - This would zero out heterogeneous chemistry reactions
 - There is precedent for doing this and was done in prior versions
 - With approval this is what we should do before releasing 13.4
 - Then we can have an option to turn it back on
- Eventually, we would like HBr to get deposited back into the ocean, but this requires further research

- Mat Evans: Ozone is about 10 ppb too low over the UK – hard to know where the problem is, but it is at the point where ozone is prohibitively too low for the model to be useful
 - Southern hemisphere has no ozone in springtime so we need to correct this at some point
- Daniel: We need to update the halogen chemistry – removing debromination will make the simulation at least reasonable
- Prasad: Is this an issue with other models?
- Barron: Yes this is also an issue at the EPA – they also tuned the bromine to get the ozone within acceptable levels
- CAM-Chem doesn't have ozone issues because they don't use halogen chemistry
- Christoph: We decided to do a 3 month release schedule, but does this force us to release a model that is hacked together?
 - Daniel: We have no obligation to release. We will go back to 1 month benchmark and zero out SSA debromination, then move on to a 1 year benchmark and will not release 13.4 until it is ready. We can't wait for a science fix to halogen chemistry because that may take a long time and in the meantime we want to release sulfur chemistry in KPP etc.

3. Plans for version 14.0 (Daniel, Lizzie)

- Version 14 will change the dimensionality of species arrays
- Lizzie: species conc array will change from 4d array to vector of 3d arrays
- This won't change outputs or inputs and only changes how source code looks. The change is motivated by wanting to store pointers to the 3d arrays in MAPL, which is not possible with the 4d array
- People with active development may need to resolve some conflicts, but the conflicts should not be difficult to fix
- Implementation of this feature will be delayed until after 13.4 is released

4. IGC10 plans (Randall)

- We have 68 registrants as of yesterday
- Looking to have a similar experience as previous IGC meetings at Harvard
- We will have interactive discussions for WG meetings and will try to have these at a time that is suitable across time zones
- 3 keynote speakers are confirmed
- We plan to have a full day of clinics prior to the rest of the conference. This is based on feedback that clinics at IGC9 were too short.
- Facilities are reserved for posters, presentations, etc
- Both on campus residences and off campus lodging are available –
- Randall urges people to consider the on campus residences as they are both convenient and WashU's residential housing is ranked #1 in the US

COVID Considerations:

- Meals that are provided can be eaten outside under a large overhang that should work nicely barring extreme weather
- The covid restrictions are not yet known, but current precautions on campus require indoor masking
- Currently planning to require participants to be fully vaccinated
- Jenny: Due to increased travel restrictions it may not be feasible to bring younger students and the time change can present challenges for attending the clinics virtually – will there be additional virtual clinics for attendees in different time zones?
- Potentially recording the meetings and making them available for all attendees
- Seb: good idea to record anyways
- Lizzie: we should be cognizant of which ones are interactive and these should be timed to reach the most people
- GCST may have youtube videos ahead of time for people to watch
- Could ask folks at WRF what they have done for their virtual clinics
- Kevin: Availability of rapid covid testing at IGC10? Randall will look into it
- Dylan Millet: Not planning to do remote presenters? Cap on in person attendees?
- Randall: We would like to prioritize in person experience so the preference is to have presentations restricted to in person. Not currently expecting a need for a cap because the capacity of the facility is 170, so quite large. Should allow us to spread out more than usual – expecting slightly less than IGC9 given travel restrictions – we will pay closer attention if we exceed 150 in-person registrants.
- Dylan Millet: Is there availability for digital lcd screens for posters that can be published using animations? Randall will look into it
- Daniel: Going to have WG meetings at a time that works for the virtual asian contingent
- Currently trying to secure travel funds – hoping to be able to support young scientists attending with their PIs

5. Working Group updates & perspectives:

a. Chemistry (Barron)

[*see accompanying slides for more detail](#)

- 13.3 chemistry updates:
 - Aromatic and ethene/ ethyne chemistry
 - Hydroxymethanesulfonate chemistry
- 13.4 chemistry updates:
 - Sulfate production moved to KPP
 - Viral's Hg chem is ported to KPP and is included in 13.4
 - Ongoing ozone low bias issue particularly in remote clean areas
- Jingqiu Mao's paper on lightning oxidants
- Maria Paula Perez-Peña has a relevant paper in acp tropospheric H2 simulation
- Dev priorities:

- Extend model chemistry to mesosphere
- Stratospheric HCN chemistry
- Adaptive solver
- H₂ chemistry
- Dylan Millet: Are HCN updates included in the troposphere? Barron: not sure whether it is just in stratosphere or not
- Dylan Millet is in process of adding HCN into the standard model for troposphere
- Lee: sulfate is in KPP – are there plans to bring other things into KPP? What is outside of KPP? kinetic SOA precursor chemistry is outside of KPP. Once that is in KPP we would have a comprehensive kinetic chemistry, need someone to do it
- Aerosol/cloud thermodynamics (ISORROPIA, VBS, cloud pH) would be separate and we would have a clean partition of modules between kinetics and thermo.
- Becky: Is alkalinity titration in KPP? Daniel: Yes! Integration into KPP will be in a paper soon.
- Eloise: [ACP paper showing an increased concentration of sulfate](#) – something to look out for since we increasingly have low sulfate – but putting sulfate chemistry in KPP is helping!

b. GCHP (Seb, Randall)

[*see accompanying slides for more detail](#)

Randall:

- GCHP parallelization is efficient on 10s of cores for coarse resolution and 1000s of cores for fine
- Stretched grid is available for fine resolution

Seb:

- Done:
 - Directly reading transport variables on cubed sphere
 - We have a year of GEOSFP mass fluxes at c720 since 3/11/2021 onward
 - One year of GEOS-IT data now available for testing, will eventually cover full record.
 - Using air mass fluxes instead of winds reduces error in vertical transport
 - Improved error logging using pflogger
 - New diagnostic of vertical air mass flux
 - Improved flexibility of diagnostic output
 - Ingestion of horizontal mass fluxes
- Amos Tai: We love the flexgrid, but have run into problems analyzing the output. Using gcpy works, but our group uses R – could the output of flexgrid be automatically turned into regular lat/lon grid to easily use R or other tools?
- Seb: This functionality is already available and is a feature inherited from GEOS. [More info available here.](#)
- Dylan Millet: Do we have stability between GCClassic and GCHP for long term simulations?

- We performed a 10 year comparison between gcclassic and gchp without divergence.
- Lee Murray: Yaml file updates will it all be in one file?
- Seb: Not expecting consolidation of all the files into a single file.

6. Plan to move forward w/ the SF6 work and GCHP (Andrew, Clara)

- There is interest in running SF6 simulations
- We would like to diagnose why GCClassic is struggling in mid to higher latitudes
- We would like to use SF6 as a bridge between GEOS and GCClassic and a tracer for GCHP
- Contributing results from GCHP to Goddard
- SF6 emissions are somewhat difficult – decided the short term solution is a c90 simulation with EDGAR4.2 SF6 and interpolated wind advection
- Allows comparisons between previous runs of GCC and GEOS SF6 simulations
- Direct comparison with ATOM observations
- Higher resolution, flux advection, and better SF6 emissions can be revisited at a later time when possible
- Clara: Limitations of EDGAR4.2 simulations is a suggestion of underestimation in southeast asia and US
- Daniel: A lot of interest in this simulation at Harvard, MIT, and GMAO and would be willing to help with it

7. Effect of using air mass fluxes versus winds on vertical transport (Seb)

[*see accompanying slides for more detail](#)

- Ingesting mass fluxes in GCHP seems to improve GCHP
- Reduces vertical fluxes in stratosphere and increase in the troposphere
- Dylan Millet: What is the impact on stratosphere-troposphere exchange?
- Seb: We are working on it but I expect there is an effect. I think it will be a complex change.
- Mass fluxes is only available for GHCP because it is only available in the cubed sphere grid – we don't have a method to use it for lat lon framework or stretched grid – this may be a research question. .

8. Maintaining the tagged Ox simulation (Daniel)

- Simulation was broken when we retired tropchem - any reason to keep it alive?
- Several members say yes we should support this as a specialty simulation
- Lee: We could track production and loss in the stratosphere with tagged Ox in fullchem for people to track the simulation – which is common in CCMs
- Dylan Jones: A specialty simulation is not overly difficult to maintain once it is stabilized

9. Nested model problem in version 13.0, corrected in 13.1 (Daniel)

- A postdoc was struggling with bugs in Boundary Conditions that was a known bug in 13.0 and was fixed in 13.1. Spent a significant amount of time on this so we are adding a note in the newsletter that people using nested 13.0 to bump up to 13.1.

10. Cloud and benchmarking updates (Liam, Lucas)

[*see accompanying slides for more detail](#)

- Updates for benchmarking on GCClassic and GCHP on the cloud
- X.Y Benchmarks are still done manually on cannon
- We now have capacity to run automated alpha benchmarks of GCClassic on aws
- Automated alpha benchmarks for GCHP can be run on WashU's compute1 cluster
- X.Y benchmarks on aws and compute1 are in progress
- We have a framework for registering these tests so that the GCST can collaborate on testing GEOS-Chem, and execute different tests at different sites (AWS or Compute1 according to test costs and availability)
- The automation of benchmarking will improve the quality of benchmarking by reducing the amount of GCST time needed to run the simulations and allow for more time to scrutinize the outputted plots

11. GC data portal, BashDataCatalog, and new vertical mass flux diagnostic (Liam)

[*see accompanying slides for more detail](#)

- Updates on acquiring geoschem data from the WashU data portal
 - We are seeing a high amount of data consumed from it
 - We have seen periods of intermittent slowness
 - Trying to figure out what is causing the slowness
 - Appears to be from high usage
 - We ask that groups do not make a high volume of data downloads in parallel to ease the load of the server
- Bashdatacatalog will be released on Monday
- Top down approach to downloading data
- The GCST will generate X.Y specific catalog files that includes data collections used for each version
- Liam spent significant effort going through and cataloging the various data necessary for download
- Contact Liam directly if you have issues using bashdatacatalog
- New diagnostic in GCHP
- Seb: Bashdatacatalog – how does it handle optional inventories?
- Liam: Catalogs have a column for enabling different collections. You just need to enable/disable a specific inventory
- Jenny Fisher: Does bashdatacatalog allow you to specify a time period? Does it have a way to identify old data for removal?
- Liam: There is a date range argument for temporal datasets. Identifying old data is supported – there are commands that can be used to list old files.

12. Ending Remarks (Daniel)

- We will probably not have a steering committee before IGC10, but this will be discussed with Randall

- Thanks for attending and see everyone at IGC10!