

GEOS-Chem Chemistry Working Group Update 2022-02-23

Working group co-chairs: Mat Evans, Barron Henderson, Lu Hu, and Jingqiu Mao

Version Updates

- 13.3 includes:
 - Kelvin Bates introduced new Aromatic and ethene/ethyne (C2) chemistry, the CH3O2+OH reaction
 - Jonathon Moch added hydroxymethanesulfonate (HMS) chemistry.
 - Tomas Sherwen updated iodine nitrate hydrolysis
 - Bug fixes and minor changes to heterogeneous chemistry (Viral Shah and Chris Holmes)
- 13.4 includes
 - sulfate production moved to into KPP.
 - Some chemical bug fixes for high acidity Henry's laws some chemistry. Some minor changes/bug fixes in the heterogeneous chemistry.
 - Bob highlighted Viral's Hg chemistry has been ported to KPP and will be included in 13.4.0. This mechanism will undergo further validation by the Hg & POPs working group. Other specialty simulations will be ported to KPP in the future.
- Ongoing ozone low bias issue, particularly at remote clean regions, but also causing problems over the UK.

Other highlights from the community

- Jingqiu Mao's recent paper on lightning oxidants (doi:10.1029/2021GL095740)
- Jenny Fischer let us know that Maria Paula Perez-Peña (CC'd) has a relevant paper in ACPD on tropospheric H2: <https://acp.copernicus.org/preprints/acp-2021-1052/>
 - Adding a tropospheric H2 simulation capability to GEOS-Chem. We had this ages ago but it wasn't maintained. Chris Holmes has I believe done some work with H2 in the stratosphere. In this work, Maria Paula has made H2 an active species in the standard chemistry mechanism and added relevant sources & sinks (and evaluated against obs).
 - Testing the impact on H2 of some new aldehyde photochemistry that has been discovered in lab experiments.
- Will Porter has "shared our 12.9.3 KPP implementation of the Chen et al. DMS oxidation mechanism with Becky's group along with some other collaborators"
 - moving it into 13.4 alongside the other sulfur improvements for testing soon (weeks).

Development priorities

http://wiki.seas.harvard.edu/geos-chem/index.php/GEOS-Chem_model_development_priorities

Extend UCX into the mesosphere	Sebastian Eastham (MIT) Eric Fleming (NASA GMAO)
Stratospheric HCN chemistry	Armin Kleinbohl (JPL) Debra Weisenstein (Harvard, retired)
* Adaptive chemical solver (as option)	Mike Long (Harvard) Haipeng Lin (Harvard)
** Implement H2 chemistry in UCX	Chris Holmes (FSU)