Notes and outcomes from the GC Chemistry Working group telecon on the 13th March 2019

People on the call

Will Porter, Chris Holmes, Dylan Millet, YingYing Yan, Eloise Marias, Jintai Lin, Tzung-May Fu, Daniel Jacob, Kelvin Bates, Xin Chen, Mat Evans

Action points

- ▫ Chris Holmes, Becky Alexander, and Erin McDuffie to update heterogeneous NOy parameterization
- ▫ Chris Holmes, Eloise Marais to discuss differing calculations of surface area within the model
- ▫ Yingying Yan, Jintai Lin, Will Porter, Mat Evans to include aromatic chemistry into standard version of the model.

Notes

NO_y Heterogeneous chemistry

Chris Holmes has been working on updating the NOy heterogeneous chemistry with an aim of improving of better representing the reactive uptake on clouds. However, he has explored updating the NOy uptake of NO_2, NO_3 and N_2O_5 to aerosols and circulated a document with recommendations for the gamma values.

Erin McDuffie has a new parametrization for the uptake of N_2O_5 onto organic and SNA aerosol (McDuffie et al., et al., JGR, 2018) which is ready to be included into the model. Uptake onto sea-salt is unchanged. How this impacts uptake for non-seasalt chloride needs to be checked.

Becky Alexander has previous raised concerns that the NO_2 and NO_3 uptake parameters were too high leading to excessive uptake. Chris's updates will lower these gamma values.

It was suggested that a single update to the model with the new parameters for NO_2, NO_3 and N_2O_5 from Chris and Erin. Chris, Erin and Becky to work together on this.

Work on heterogenous HONO production is ongoing in Harvard and will be brought forwards into the standard model when appropriate.

Concerns were raised about the differing calculations of surface area within the model. Chris and Eloise to discuss.

Aromatic hydrocarbons.

There has be interest and work in aromatic chemistry in GC over the last decade - SOA production, di-carbonyls etc. More recently, Will Porter has explored the impact of aromatics in the model (Porter et al., Atmos. Env., 2017). Yingying Yan has recently described implementing the SAPRC-11 scheme into

GEOS-Chem (Yan et al., GMD, 2019). Peter Ivatt (York) has implemented the RACM-2 scheme into GEOS-Chem (unpublished).

It was felt that including a "full" aromatic scheme (benzene, toluene, xylene) into the standard chemistry scheme would be beneficial but there were concerns about the computational cost. Porter et al., 2017 reported a significant (~15%) increase in run-time, however the more recent work (Yan and Ivatt) suggested much smaller increases (~5%). It was therefore felt that inclusion of the aromatics would lead to a useful increase in model capability with a limited increase in computational burden. A number of choices need to be made: which scheme to include, which emissions to use and how to they relate to the current VOC emissions, deposition parameters of degredation products, wiring up diagnostics (RO2 etc), ensuring pull through to the SOA schemes. Will Porter, Yinying Yan, Jintai Lin and Mat Evans will discuss these choices and ensure pull through of this work into the standard code.

Biogenic hydrocarbons.

Kelvin Bates is working on updates to the isoprene chemistry based on work coming out of CalTech. This will be included into the standard model when appropriate

Other organics

Kelvin has an ethylene scheme and it was felt that this should be placed into the standard model when appropriate.

A 'universal' offline chemistry version of the model would allow the transport and tracer chemistry of a large number of hydrocarbon than we currently have to be explored. Development for this is in progress from the GCST.

The connection between the gas phase chemistry and the SOA chemistry can be a little clunky. Some of the SOA scheme deals with the chemistry in carbon_mod.F whereas it could be in the chemistry integrator. It was felt that in the future trying to move more of the aerosol precursor chemistry into the chemical integrator would make the model clearer to understand.

Halogen chemistry

Wang et al. (accepted in ACP) has added full tropospheric chlorine chemistry in the model consistent with SSA and with the rest of tropospheric and stratospheric halogen chemistry. This is ready to go in the standard model and does not break ozone, but this is because the BrO is lower than observed (it has been this way ever since we added HOBr+S(IV)). Zhu et al. (ACPD, in revision) has taken the Wang et al. scheme and made some improvements that greatly improve free tropospheric BrO. But it leads to very high BrO in the extratropics in winter and could possibly break ozone - Lei will investigate. We could include the Wang et al. chemistry now in the standard code and have in this manner a complete treatment of halogen chemistry in the model. We could then wait for Lei's updates to be implemented at a later stage.

General discussion

Concerns were raised about the number of different simulations we are supporting. The creation of a 'universal' offline chemistry version of the model should be able reduce the number of different simulations

supported. The issue will be raised at iGC9. The would be the possibility of writing a narrative to guide for users to help their choice of version.