Understanding formation of small acids from multiphase processing of isoprene epoxydiols

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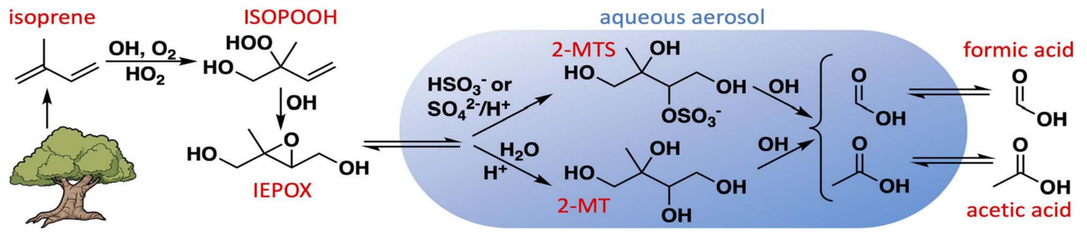
1. Background and motivation

Heterogeneous processing of IEPOX forms small acids



[Bates et al., 2023]

- FA and AA can contribute to atmosphere acidity, alter the oxidative capacity and impact the formation of cloud droplet.
- Via heterogeneous production of small acids, oVOCs are being underestimation in the GEOS-Chem model.
- Model need to be improved to better constrain IEPOX heterogeneous reactions, addressing oVOCs underestimation and refining global ozone budgets.

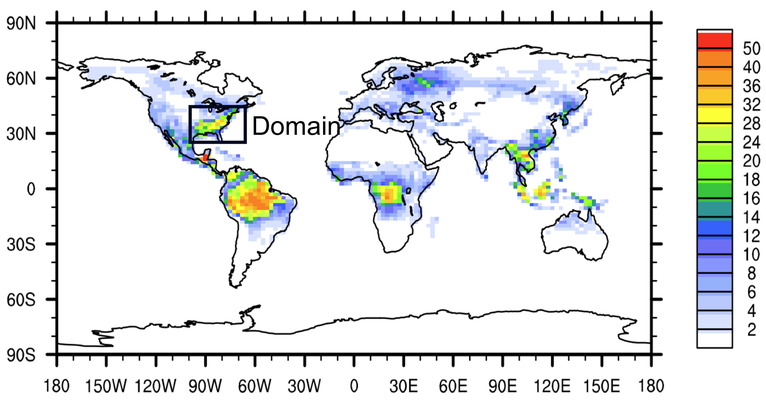
2. Research Methods

GEOS-Chem

We use:

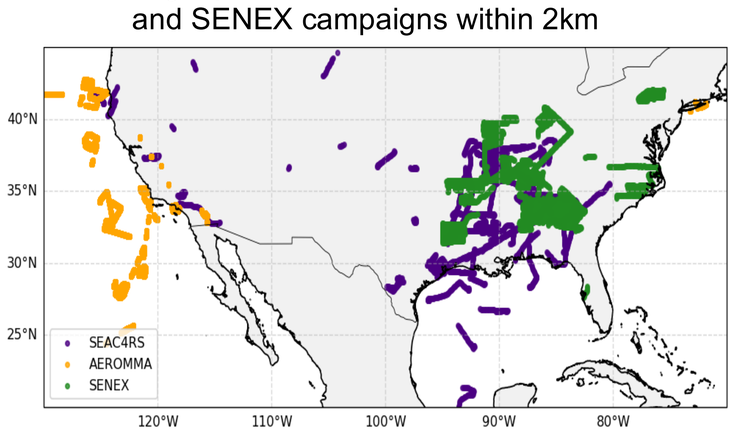
- GEOS-Chem model v14.5.0 nested grid simulations (0.25°×0.3125°) and global simulations (4°×5°)
- Aircraft observations from NASA aircraft campaigns (AEROMMA, SEAC⁴RS, SENEX)
- We use CIT-CIMS to measure isoprene oxidation products; use AMS to measure aerosol composition; use NOAA Iodide CIMS to measure small acids.

July 2000 global emission of ISOP simulated with MEGAN 2.1 using CLM4 (micro-moles/m²/hr)



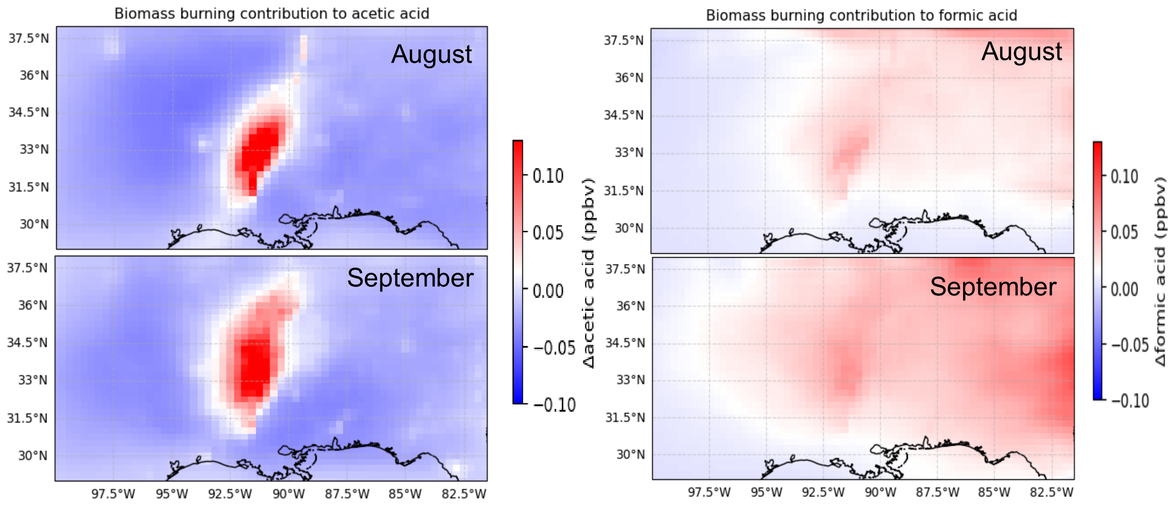
[Guenther et al., 2012]

Flight paths of SEAC4RS, AEROMMA, and SENEX campaigns within 2km



3. Impact of biomass burning on concentrations of small acids in 2013 SEAC⁴RS

The analysis focuses on model simulations within the lower troposphere (altitudes below 2 km). The contribution of biomass burning is moderate.



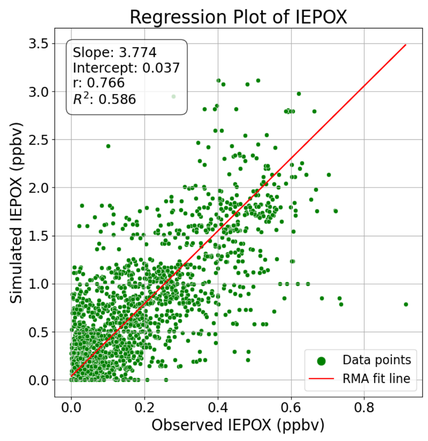
Acetic acid:

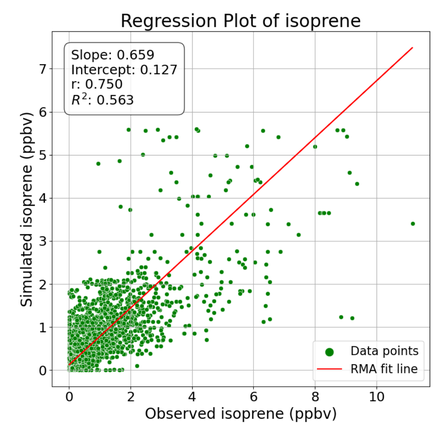
- August: Local enhancement near source, slight regional decrease (-0.013 ppbv, -3.4%)
- September: Even weaker effect (-0.004 ppbv, -1.2%)

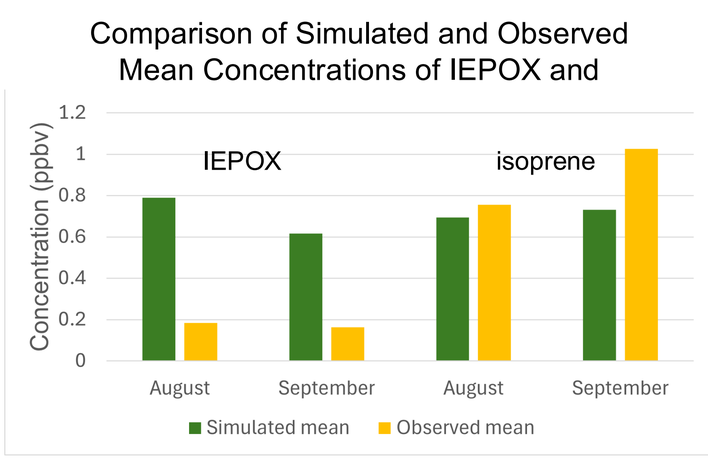
Formic acid:

- August: Widespread increase, regional mean +0.033 ppbv (+3.2%)
- September: Regional mean +0.050 ppbv (+4.6%)

4. Preliminary results about comparison between observation and simulation from SEAC⁴RS



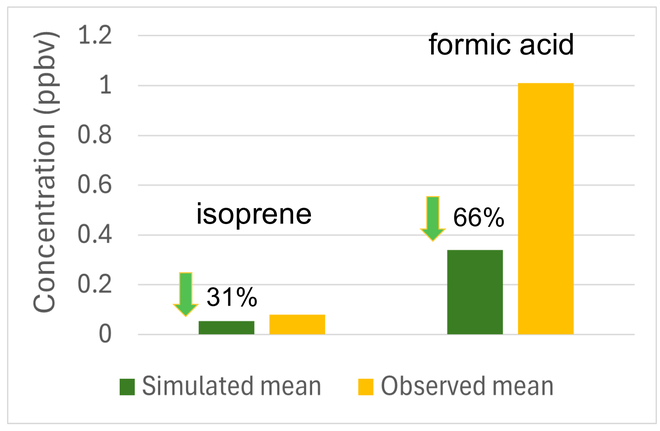


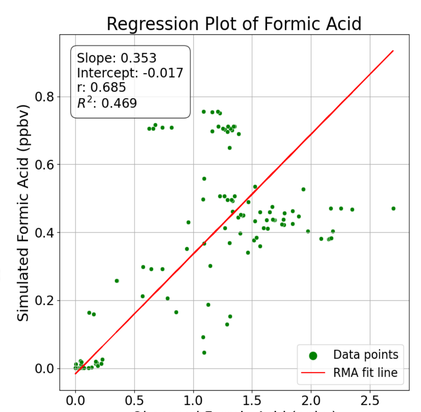


- For a single month, the model overestimates IEPOX, which consistent with the study of Vasilako in 2021.
- Based on the mean value of two months of IEPOX, the model overestimates 3.88 to 4.33 times.
- For isoprene, the model shows 10% difference in August, 29% underestimation in September.

5. Evaluation of isoprene and formic acid in June 2023 AEROMMA campaign

Comparison of Simulated and Observed Mean Concentrations of isoprene and formic acid





- Isoprene is slightly underestimated (31%) in the model compared to a large underestimate (66%) in formic acid.

6. Conclusions and ongoing work

- Biomass burning has negligible influence on acetic acid, but enhances formic acid, especially in September.
- Isoprene is slightly underestimated in the model compared to a large underestimate in formic acid and large overestimate in IEPOX .
- The initial comparison of the default model supports the need for a multiphase mechanism that would consume more IEPOX and produce more formic and acetic acid than the current model does.

Next step I will compare SENEX and other aircraft observations with the model simulations and add the multiphase conversions of IEPOX to small acids to address the large model bias and assess the influence of greater abundance of small acids on ozone.

References

1. Bates, K.H., Jacob, D.J., Cope, J.D., Chen, X., Millet, D.B. and Nguyen, T.B. (2023).*Environmental Science Atmospheres*, 3(11), pp.1651–1664. 2. Vasilakos, P., Hu, Y., Russell, A. and Nenes, A. (2021b). *Atmosphere*, 12(6), p.707. 3. Guenther, A.B., Jiang, X., Heald, C.L., Sakulyanontvittaya, T., Duhl, T., Emmons, L.K. and Wang, X. (2012). Geoscientific Model Development, 5(6), pp.1471–1492

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