Improved understanding of southeast US isoprene SOA using ground (SOAS), aircraft (SEAC$^4$RS), satellite (MODIS, OMI), and model (GEOS-Chem) data

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SEAC$^4$RS STM
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Default decoupled GEOS-Chem isoprene SOA scheme

Use fixed yields ($\alpha_i$), despite large variability in chamber studies:

Lab results for OA < 20 $\mu$g m$^{-3}$

Yields colored by relative humidity

In GEOS-Chem $\alpha_i$ is $\sim$3% at 10 $\mu$g m$^{-3}$.

Realized yields are lower
Isoprene Emissions and SOA yields in GEOS-Chem

Very low yield (~1%) in the southeast US

High yields not coincident with isoprene emissions

High yields where there is biomass burning (high pre-existing aerosol; low temperatures).

\[
\text{Yield} = \frac{\Delta \text{SOA}}{\Delta \text{isoprene}}
\]
By interpolation, SEAC$^4$RS-derived isoprene OA yield is 3%.

SEAC$^4$RS OA-HCHO relationship provides total isoprene SOA yields. Obtain additional information from AMS-derived isoprene SOA components.
New GEOS-Chem isoprene SOA parameterization

Develop a mechanism that couples gas and aerosol phases
Better understand the processes that lead to isoprene SOA formation

Reversible partitioning of semivolatile precursors retained for ISOP+OH and removed for ISOP+NO₃

Fixed $\gamma$ for carbonyls
Gaston et al. [2014]
parameterization for others.
Large uncertainty is $H_{eff}$
Isoprene OA precursors in GEOS-Chem

GEOS-Chem branching ratios:
Southeast US (Jun-Aug)

[Ng et al., 2008; Rollins et al., 2009]

[Lee et al., 2014]

[Eddingsaas et al., 2010; Gaston et al., 2014]

[Jacobs et al., 2014]

[Lin et al., 2013; Riedel et al., 2015]

[Krechmer et al., 2015]

[Liggio et al., 2005; Fu et al., 2008; Nguyen et al., 2013; Sumner et al., 2014]
GEOS-Chem isoprene OA during SEAC4RS

Vertical profile of AMS-derived IEPOX-SOA and GEOS-Chem IEPOX-SOA

Relatively uniform distribution throughout the boundary layer

Slight model overestimate likely caused by gas-phase overestimate in IEPOX, but also likely due to uncertain uptake dynamics.

IEPOX-SOA data provided by P. Campuzano-Jost
IEPOX-SOA is \(~2\) \(\mu g\) m\(^{-3}\) during SOAS. ISOPOOH-SOA is an order of magnitude lower.

GEOS-Chem captures temporal variability during SOAS. GEOS-Chem IEPOX-SOA sensitive to effective Henry’s constant \((H_{eff})\)
Large decline in anthropogenic emissions, so consider 2 time periods. **Coincident** enhancements in AOD and HCHO [Veefkind et al., 2011], but AOD includes ubiquitous inorganic aerosols.

Interpret relationship between satellite AOD and formaldehyde with the GEOS-Chem CTM. Test effect of sulfate mass loading on isoprene OA yields using top-down approach.
Satellite-derived isoprene OA yields

Points are monthly mean 2x2.5 degree data colored by tropospheric column NO₂.

**Top panel:** Satellite AOD-HCHO

**Middle:** GEOS-Chem semivolatile partitioning with and without isoprene SOA

**Bottom:** GEOS-Chem with irreversible uptake of isoprene SOA and 2 different yields

GEOS-Chem AOD-HCHO relationship has little sensitivity to changes in the underlying isoprene SOA
Concluding Remarks and Future Work

- Isoprene OA yields are ~3% from fitting relationship between observed OA and HCHO over the SEAC4RS domain.
- Resolved isoprene OA components during SEAC4RS and SOAS campaigns provide constraints on isoprene SOA formation.
- Test model simulation of aerosol-phase IEPOX organosulfate using PALMS IEPOX-organosulfate measurement.
- Satellite-derived yields limited by low AOD sensitivity to isoprene SOA yields.
- Replace monoterpene SOA volatility basis set scheme with monoterpene SOA formation that couples the gas and aerosol phases.
- Estimate the contribution of individual isoprene SOA components to the isoprene SOA budget using GEOS-Chem.