Secondary Organic Aerosol modeling with GECKO-A

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GECKO-A: Systematic generation of Organics Oxidation schemes

- Systematic computer assisted auto-generation ⇒ Extremely detailed chemical mechanisms.
- Experimental data first. No available data ⇒ Structure Activity Relationships.
- Oxidation of most primary compounds of atmospheric interest.
- Typically ~ $10^6$ species and ~ $10^7$ reactions.
- Mechanisms are integrated in a boxmodel.

- We can use the boxmodel in an eulerian or lagrangian setup.
- We can test new mechanistic pathways in ideal test cases (sensitivity tests).
- We can simulate all kinds of “local” experiments (i.e. we can assume homogeneity of the system): lab, smog chambers experiments.
- We can simulate field campaign cases, typically urban plumes.
Comparison with Experimental Data

What is a good experimental data set for GECKO-A?

- Well constrained environmental parameters (T, P, HR, dilution, hv, injection flux, ...).
- Sensitivity tests! It is possible that GECKO-A won’t get the absolute value right, but will get a similar response to changing T, RH, COV/NOx, ...

Limitations

- Some compounds classes cannot be handled: amines, PAH, alkynes
- Particles are assumed to be inert, monodisperse, liquid and homogeneous.
What quantities can be tracked?

If you can measure it, and if there is a way to estimate it from knowing the molecular composition, we can do a comparison.

- **Molecular Weight**
- **Vapor Pressure / Solubility**
- **Dry Glass Transition Temperature** (Shiraiwa et al. 2017)
- **Per-particles diversity** (Riemer & West, 2013)

- **atomic ratios**