Secondary Organic Aerosol modeling with GECKO-A

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GECKO-A: Systematic generation of Organics Oxidation schemes

- Systematic computer assisted auto-generation $\Rightarrow$ Extremely detailed chemical mechanisms.
- Experimental data first. No available data $\Rightarrow$ 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.

Teflon wall

CO_2

...

Aqueous Phase

Henry's law

OVOC 2

Organic Aerosol

OVOC 1

Raoult's law

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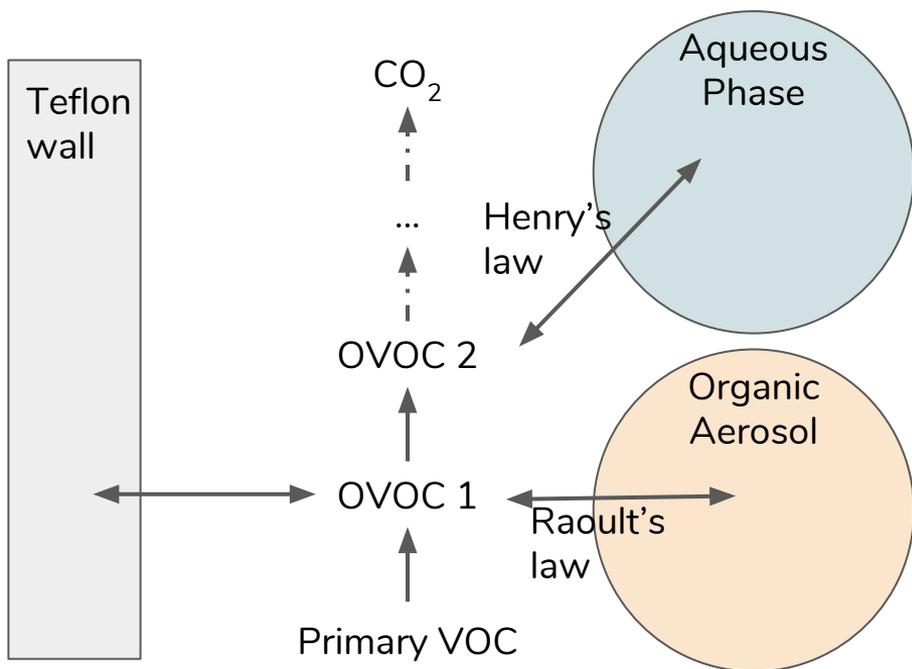
- We can use the boxmodel in an eulerian or lagrangian setup.
- We can test new mechanistic pathways in ideal test cases (sensitivity tests).
- We can simulate all kinds of "local" experiments (*i.e.* we can assume homogeneity of the system): lab, smog chambers experiments.
- We can simulate field campaign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

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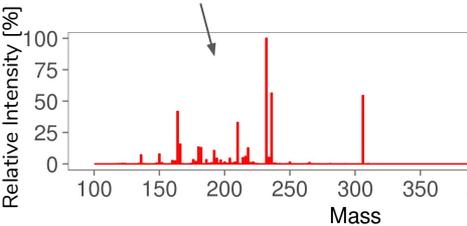
Vapor Pressure / Solubility
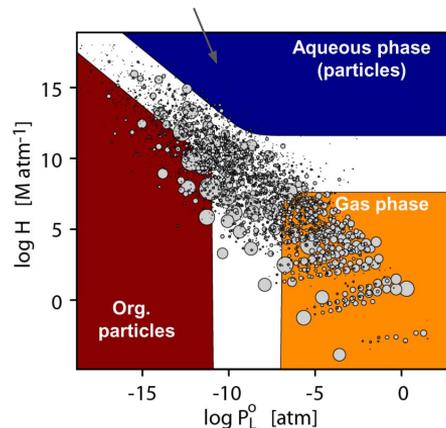
Dry Glass Transition Temperature
(Shiraiwa et al. 2017)
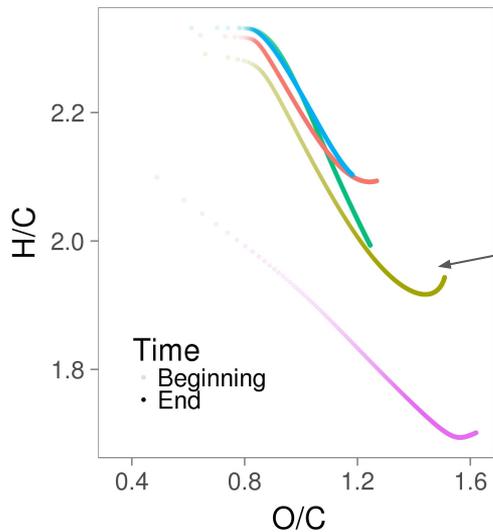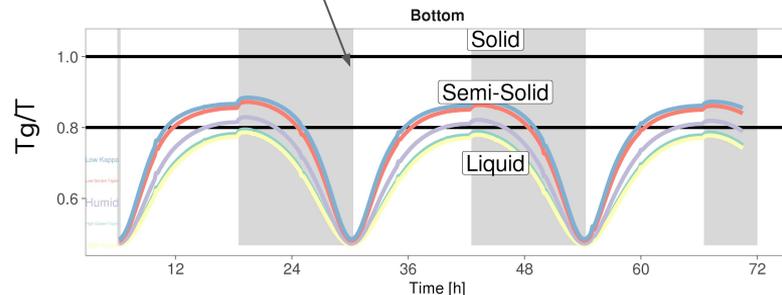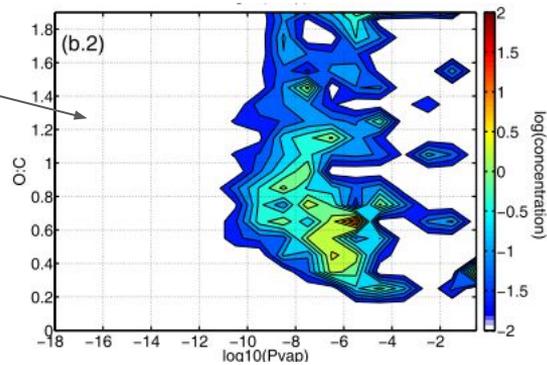
Per-particles diversity
(Riemer & West, 2013)

atomic ratios