The GECKO-A Explicit Chemical Model
A Developing Community Resource

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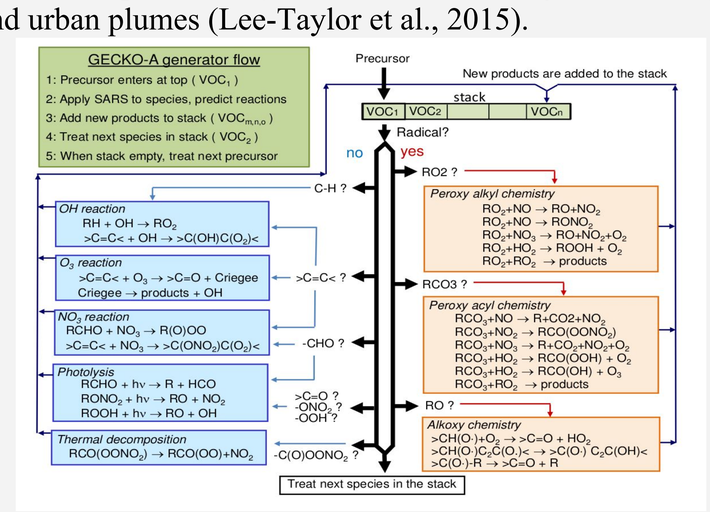
What is GECKO-A?

Based on available experimental data coupled to a set of rules and estimation methods used for unknown species, GECKO-A can generate completely **explicit mechanisms** for organic compounds of atmospheric interest (Aumont et al., 2005). It has been successfully applied to simulate chamber experiments (La et al., 2016; McVay et al., 2016) and urban plumes (Lee-Taylor et al., 2015).



The Library

In a first step of making GECKO-A a community resource, we are currently building a comprehensive library of hyper-explicit **boxmodel outputs** for an extensive list of precursors of atmospheric interest under a variety of standard chemical scenarios. This library is **available online** to the research community.
This library might be useful for multiple purposes:

- Informing chamber experiments by providing expected major constituents of gas phase VOCs.
- Providing an explicit reference to evaluate mechanism reduction efforts for 3D models.

Setup

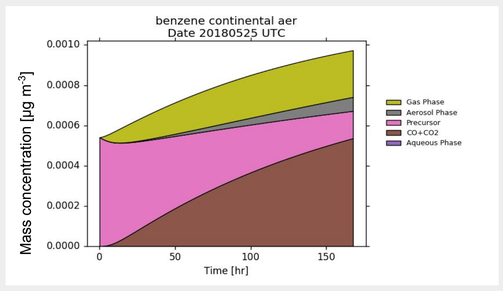
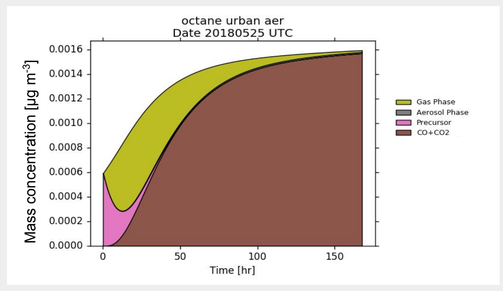
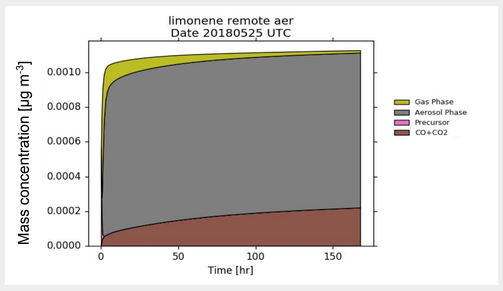
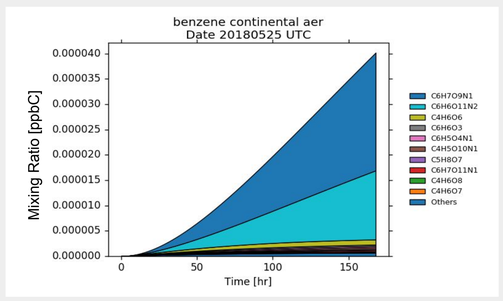
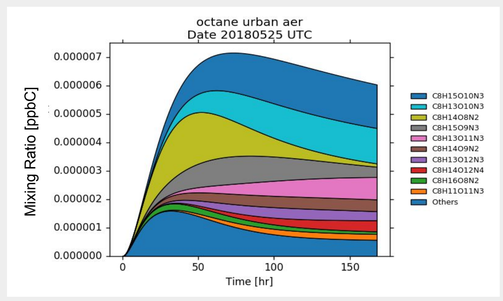
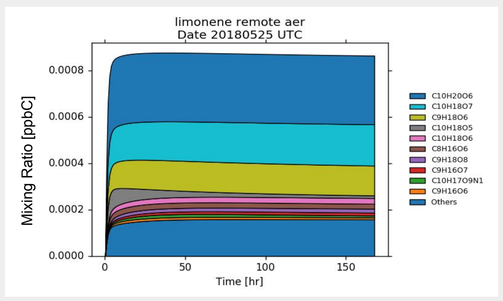
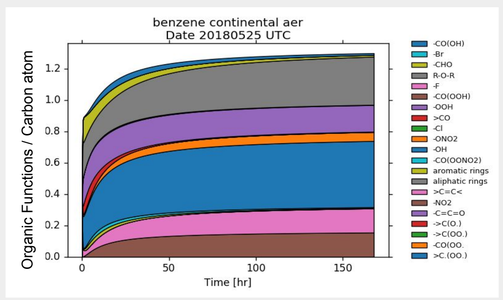
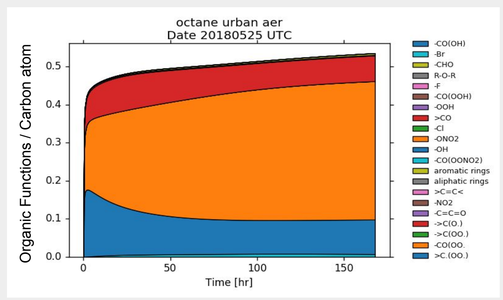
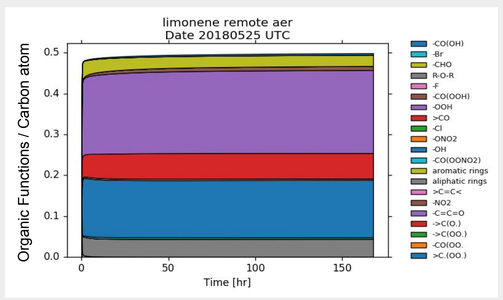
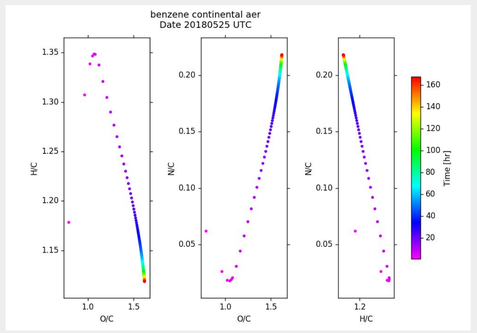
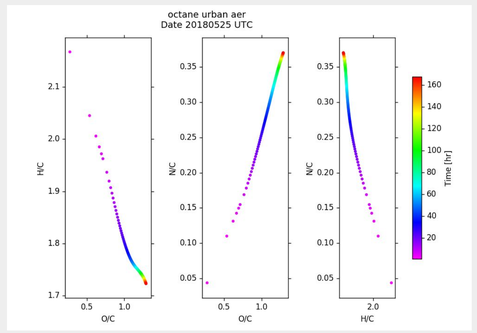
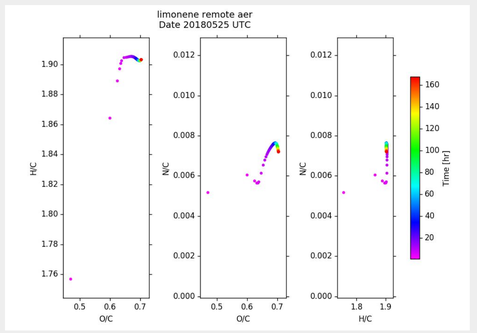
Primary hydrocarbons of anthropogenic and biogenic origin are included in the library.
The list is **open to new additions**.

	anthropogenics								biogenics			
	n-pentane	n-hexane	n-heptane	n-octane	n-decane	n-dodecane	benzene	toluene	isoprene	α-pinene	β-pinene	limonene
# Species	3.9×10^3	7.8×10^3	1.4×10^4	2.0×10^4	5.0×10^4	1.0×10^6	1.9×10^3	4.0×10^3	8.9×10^2	2.2×10^5	1.6×10^5	1.1×10^5
# Reactions	3.0×10^4	5.7×10^4	1.0×10^5	1.5×10^5	3.5×10^5	7.2×10^5	1.5×10^4	3.0×10^4	5.6×10^3	1.5×10^6	1.1×10^6	7.9×10^5

	Remote	Remote Continental	Continental	Polluted Continental	Urban
NO_x [ppb]	0.02	0.025	0.5	2	20
CO [ppb]	120	120	150	200	300
NMHC K_{OH} [s^{-1}]	0	1	6	9	13
CO + NMHC K_{OH} [s^{-1}]	0.7	1.7	6.9	10.2	14.8
HCHO [ppb]	0	0	2	5	10

NO_x fixed
NO/NO_2 allowed to vary
NMHC: surrogate to constrain VOC/NO_x ratio
All simulations: O_3 = 40 ppb, CH_4 = 1850 ppb, T = 298 K, RH = 70%, sza = 45°, SOA seed = 10 μg m^{-3}
1 ppt of the precursor is introduced when steady state is reached

Example Plots

	continental benzene	urban octane	remote limonene
Organic Carbon phase distribution			
Main isomers contribution to the aerosol phase			
Organic moieties distribution in the aerosol phase			
Van Krevelen Diagrams in the organic aerosol phase			

Developing the GECKO-A community resource

In parallel with sharing standard GECKO-A results, we envision several possible levels of cooperation between the GECKO-A development team and the overall community.

- We will keep adding precursors and scenarios to the library based on the community needs.
- In closer collaborations with experimental teams, we are able to provide detailed simulations results in a format easily exploitable with software generally used by experimentalists (Matlab, Igor, R, …).
- We are figuring out how to setup community tutorial workshops to train autonomous new GECKO-A users.
- We are aiming towards sharing the full GECKO-A codebase with the community to start a community oriented development process.

To support these future GECKO-A developments, knowledge of the community's needs and expectations from hyper-explicit modeling tools is crucial. We are open to suggestions and collaborations!

https://www.acom.ucar.edu/gecko/output-library.shtml

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References

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