New Vapor Pressure Model EVAPORATION: Impact on Aerosol Predictions

S. Compernolle*, K. Ceulemans, J.-F. Müller (* steven.compernolle@aeronomie.be)

Belgian Institute for Space-Aeronomy

Ringlaan 3, 1180 Brussels, Belgium

I. Introduction

Vapor pressure p^0 of molecules is possibly one of the most important single-molecule properties regulating SOA formation. As this property is not measured for most molecules, it has to be estimated. However, the vapor pressure of polyfunctional molecules is poorly characterized, as is clear from the large variation in vapor pressure estimation by different methods. We recently developed the vapor pressure estimation method EVAPORATION (Estimation of VApor Pressure of Organics, Accounting for Temperature, Intramolecular, and Non-additivity effects), suited also for polyfunctional molecules (Compernolle et al., 2011).

II. EVAPORATION as web-application

This method is available on-line at http://tropo.aeronomie.be/models/evaporation_run.htm. Molecules can be inserted using the SMILES notation.

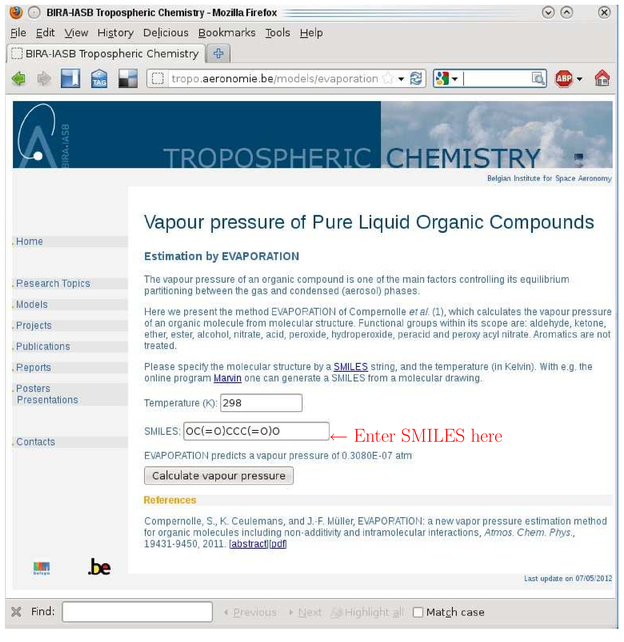


Figure 1: Snapshot of the site where EVAPORATION is hosted.

III. Comparing different vapor pressure methods: application to β-pinene oxidation products in BOREAM.

Following the work of Vereecken and Peeters (2012), the chemical oxidation mechanism BOREAM (Biogenic hydrocarbon Oxidation and Related Aerosol formation Model, Capouet et al., 2008) includes now also the oxidation of β-pinene, next to that of α-pinene.

Both EVAPORATION and SIMPOL (Pankow and Asher, 2008) return, on average, a lower p^0 for β-pinene oxidation products compared to the method of Capouet and Müller (2006).

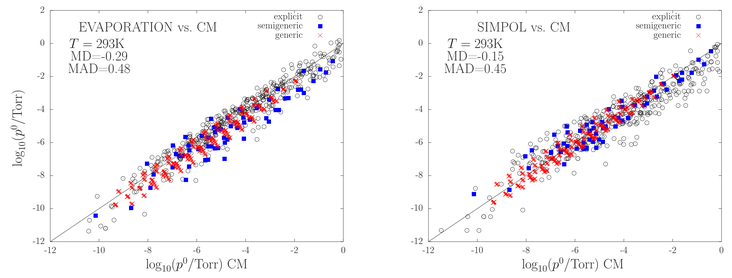


Figure 2: $\log_{10}(p^0/\text{Torr})$ of EVAPORATION (left) and SIMPOL (right) vs. the CM method.

To limit the number of species, BOREAM includes semigeneric and generic species, with no detailed structural information. Second-order effects, such as intramolecular interactions, of the vapor pressure methods were ignored for them.

IV. Smog chamber simulations: impact of vapor pressure model.

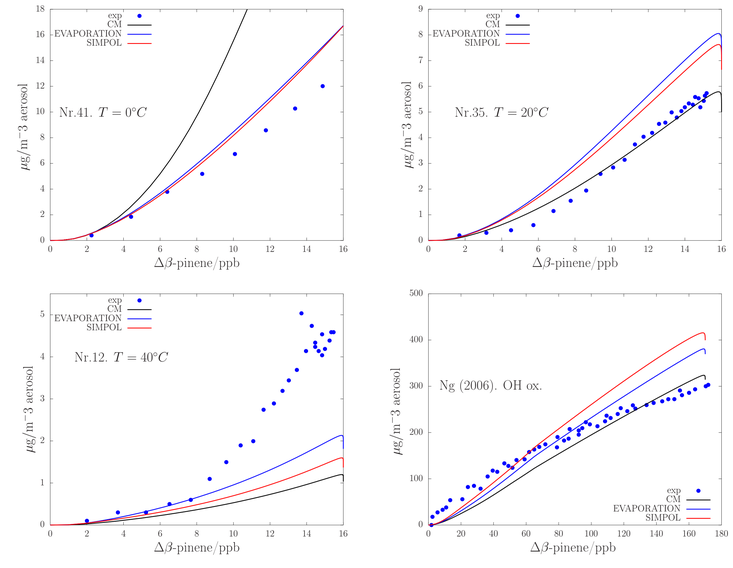
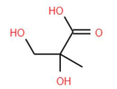
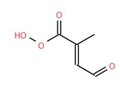
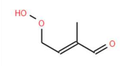
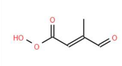
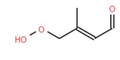
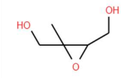


Figure 3: Simulations with BOREAM of β-pinene oxidation experiments from Pathak et al. (2008) (ozonolysis at different temperatures) and from Ng et al. (2006) (OH oxidation).

- The method of Capouet and Müller (2006) seems problematic at low temperature (0°C).
- Depending on the experiment type, either SIMPOL or EVAPORATION predicts the highest SOA.
- Choice of vapor pressure model cannot explain everything! (Cfr. $T = 40$°C exp. of Pathak.)

V. Estimated EVAPORATION vapor pressures of some atmospherically interesting compounds.

Molecule	structure	$p0$/atm	Molecule	structure	$p0$/atm
2-methyl-glyceric acid		6E-8	PACALD1		5E-5
HPALD1		4E-5	PACALD2		5E-5
HPALD2		4E-5	IEPOX		3.4E-6

References

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Pathak, R., Donahue, N. M., and Pandis, S. N., Environ. Sci. Technol., 42, 5081–5086, 2008.

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