Molecular corridor based approach for predicting phase state of secondary organic aerosols

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The formation and aging of secondary organic aerosols (SOA) proceed through multiple steps of chemical reaction and mass transport in the gas and particle phases, which is challenging for the interpretation of field measurements and laboratory experiments as well as accurate representation of SOA evolution in atmospheric aerosol models. Particle phase state (e.g., liquid, semisolid, or amorphous solid) is important in gas-particle interactions inluding formation and evolution of SOA as well as activation to cloud droplets and ice crystals.

We found that organic compounds with a wide variety of functional groups fall into molecular corridors, characterized by a tight inverse correlation between molar mass and volatility (Fig. 1) [1,2]. Based on the concept of molecular corridors, we develop parameterizations as a function of molar mass and O:C ratio to predict glass transition temperature of SOA, which is a key property for determination of particle phase state. Utilizing the atmospheric chemistry model EMAC and an SOA module ORACLE [3], a global prediction of SOA phase state will be presented.

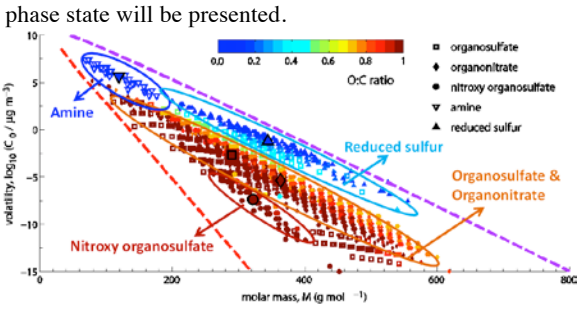

Figure 1. Molecular corridors of volatility vs. molar mass for nitrogen and sulfur containing compounds in ambient air [2].

[1] Shiraiwa et al. (2014) *Atmos. Chem. Phys.*, **14**, 8323-8341. [2] Li et al. (2015) *Atmos. Chem. Phys. Discuss.*, **15**, 27877-27915.
[3] Tsimpidi et al. (2014) *Geosci. Model Dev.*, **7**, 3153-3172.