

Consideration of HOMs in α - and β -pinene SOA model

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Secondary organic aerosol (SOA) is the major burden of the atmospheric organic particulate matter with 140–910 TgC yr⁻¹ (Hallquist et al., 2009). SOA particles are formed via the oxidation of volatile organic carbons (VOCs), where the volatility of the VOCs is lowered due to the increase in their functionalization as well as their binding ability. Therefore, gaseous compounds can either nucleate to form new particles or condense on existing particles. The framework of SOA formation under natural conditions is very complex, because there are a multitude of gas-phase precursors, atmospheric degradation processes and products after oxidation. A lacking understanding about chemical and physical processes associated with SOA formation makes modeling of SOA processes difficult, leading to discrepancy between measured and modeled global SOA burdens.

The present study utilizes a parcel model SPACCIM (SPECTral Aerosol Cloud Chemistry Interaction Model, Wolke et al., 2005) that couples a multiphase chemical model with a microphysical model. For SOA modeling a further development of SPACCIM was necessary. Therefore, two components are added (i) a gas-phase chemistry mechanism for the VOC oxidation and (ii) a partitioning approach for the gas-to-particle phase transfer. An aggregated gas-phase chemistry mechanism for α - and β -pinene was adapted from Chen and Griffin (2005). For the phase transfer an absorptive partitioning approach (Pankow, 1994) and a kinetic approach (Zaveri et al., 2014) are implemented. Whereby the kinetic approach serves some advantages. The organic aerosol can be resolved in different size sections, whereby the particle radius is involved in the partitioning equations. The phase state of the organic material and the reactivity of the organic compounds in the particle-phase directly influence the modeled SOA yields.

Recently, highly oxidized multifunctional organic compounds (HOMs) were found in the gas phase from lab and field studies. They are also known as extremely low-volatile organic compounds (ELVOCs) (Ehn et al. 2014). The importance of HOMs for the early aerosol growth makes them indispensable in SOA modeling. Thus, we included HOMs in our model framework. The measurements from the institute's own smog chamber LEAK are used as a base for model evaluation and process analysis, especially since HOMs were lately identified from LEAK data (Mutzel et al., 2015). The presentation will provide a sensitivity study for the kinetic approach as well as a comparison of measured and modeled SOA yields.

References:

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