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# Regional modeling of SOA formation under consideration of HOMs

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Secondary organic aerosol (SOA) is the major burden of the atmospheric organic particulate matter with about 140 – 910 TgC/yr (Hallquist et al., 2009). SOA particles are formed via the oxidation of volatile organic carbons (VOCs), where the volatility of the VOCs is lowered. 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 variety of gas-phase precursors, atmospheric degradation pathways and formed oxidation products. Up to now, atmospheric models underpredict the SOA mass. Therefore, improved regional scale model implementations are necessary to achieve a better agreement between model predictions and field measurements.
Recently, highly oxidized multifunctional organic compounds (HOMs) were found in the gas phase from laboratory and field studies (Jokinen et al., 2015, Mutzel et al., 2015, Berndt et al., 2016a,b). From box model studies, it is known that HOMs are important for the early aerosol growth, however they are not yet considered in mechanisms applied in regional models.
The present study utilizes the state-of-the-art multiscale model system COSMO-MUSCAT (Wolke et al., 2012), which is qualified for process studies in local and regional areas. The established model system was enhanced by a kinetic partitioning approach (Zaveri et al., 2014) for the gas-to-particle transfer of oxidized VOCs. The framework of the partitioning approach and the gas-phase mechanism were tested in a box model and evaluated with chamber studies, before implementing in the 3D model system COSMO-MUSCAT. Moreover, HOMs are implemented in the same way for the regional SOA modeling. 3D simulations were performed with an equilibrium partitioning and diffusion dependent partitioning approach, respectively.
The presentation will provide first 3D simulation results including comparisons with field measurements from the TROPOS field site Melpitz (51° 32’ N, 12° 54’ E, 87 m a.s.l.). Thereby, we will focus on two key issues influencing the SOA formation. Firstly, the increased SOA mass concentrations due to the consideration of HOMs from both isoprene and monoterpene oxidation is shown. Secondly, the influence of the particle phase diffusion coefficient on SOA formation will be presented, which is one of the key parameters in the newly implemented kinetic approach. The comparison of the equilibrium partitioning and diffusion dependent partitioning approaches reveals differences in the formed SOA mass.

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