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Simulation of Aerosol Formation in Alpha-pinene Oxidation Experiments with a Quasi-Explicit Model

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A detailed model is presented for the oxidation of the monoterpene alpha-pinene and the associated formation of Secondary Organic Aerosols (SOA). It is based on a quasi-explicit mechanism for the oxidation of alpha-pinene down to the formation of primary products, developed on objective grounds using advanced quantum theoretical methods, and on a simplified representation for the further oxidation of the products. Gas/particle partitioning follows a kinetic representation with coefficients from vapor pressures calculated using a dedicated group contribution method.

This model is evaluated against a large number of laboratory experiments. The simulated and observed SOA yields agree to within a factor of 2 in most cases for photo-oxidation experiments (Capouet et al. 2008, JGR vol.113, in press).

We also present new results for the simulation of dark ozonolysis experiments. The level of agreement between modeled and experimental yields is found to be highly dependent on the experimental conditions, such as initial alpha-pinene concentration, temperature and use of OH-scavenger. For experiments with high temperature and low initial alpha-pinene concentrations, the SOA yield is sometimes strongly underestimated.

The role of known shortcomings in the degradation mechanism is discussed. The influence of heterogeneous and particle phase reactions is also estimated. In particular we evaluated the role of association reactions between aldehydes and hydroperoxides in the particle phase, based on laboratory measurements for the (forward and backward) reaction rates in different solvents. These reactions are found to have a significant

impact in several low-NOx ozonolysis experiments.