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Kinetic modeling of secondary organic aerosol formation: effects of particle- and gas-phase reactions of semivolatile products

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Abstract. The distinguishing mechanism of formation of secondary organic aerosol (SOA) is the partitioning of semivolatile hydrocarbon oxidation products between the gas and aerosol phases. While SOA formation is typically described in terms of partitioning only, the rate of formation and ultimate yield of SOA can also depend on the kinetics of both gas- and aerosol-phase processes. We present a general equilibrium/kinetic model of SOA formation that provides a framework for evaluating the extent to which the controlling mechanisms of SOA formation can be inferred from laboratory chamber data. With this model we examine the effect on SOA formation of gas-phase oxidation of first-generation products to either more or less volatile species, of particle-phase reaction (both first- and second-order kinetics), of the rate of parent hydrocarbon oxidation, and of the extent of reaction of the parent hydrocarbon. The effect of pre-existing organic aerosol mass on SOA yield, an issue of direct relevance to the translation of laboratory data to atmospheric applications, is examined. The importance of direct chemical measurements of gas- and particlephase species is underscored in identifying SOA formation mechanisms.

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