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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Kinetic modeling of Secondary Organic Aerosol formation: effects of particle- and gas-phase reactions of semivolatile products" *by* A. W. H. Chan et al.

Anonymous Referee #2

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This study expands on Kroll et al. (2005) and presents a framework for analyzing laboratory SOA data that includes kinetic and equilibrium terms. The behavior of the model is first explored in this paper by analyzing different combinations of processes. The model is then applied to analyze data from several smog chamber reaction systems. An important recommendation of this work is that since aerosol yields can depend on the initial amount of precursor, experimental conditions need to be selected with care to represent ambient conditions.

Simplified, empirical relationship can sometimes capture the important processes of a complex system. The authors seem to be proposing such empirical models for the sev-

eral reaction systems in Figure 11-13. However, in the concluding section, the authors pointed out that “it is not generally possible to infer the precise mechanism of SOA formation solely on the basis of SOA growth data.” To gauge the utility of the model, therefore, it may be useful to explore the uncertainties of the fitted parameters and whether different variations of the model can perform equally well given the parametric uncertainties.

The use of the term “pseudo first order” in the text and appendix is unorthodox and confusing for students trained in kinetics. Chemical engineers typically refer to reaction kinetics of A+B as pseudo first order when one of the reactants is in excess and the rate (k[A][B]) can be written as k’[B] because the change in [A] is negligible. In this case, the kinetics of a second order reaction is written as the product of k’, [A], and the mole fraction of A. Even though k’ has the unit of inverse time, the rate should still depend (implicitly) on the squared concentration of A. Is an assumption being made that the mole fraction is roughly constant? If so, please state and justify.

Interactive comment on Atmos. Chem. Phys. Discuss., 7, 7051, 2007.