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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Modelling non-equilibrium secondary organic aerosol formation and evaporation with the aerosol dynamics, gas- and particle-phase chemistry kinetic multi-layer model ADCHAM" *by* P. Roldin et al.

Anonymous Referee #1

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This paper submitted by Roldin et al. entitled as 'Modelling non-equilibrium secondary organic aerosol formation and evaporation with the aerosol dynamics, gas- and particle-phase chemistry kinetic multi-layer model ADCHAM' describes development and application of a new numerical model for aerosol formation and aging in smog/environmental chambers, especially focusing on influence of particle phase on chemistry. The model includes state-of-the-art knowledge on wall loss of particle and

gas species in smog chambers, gas phase chemistry, and multiphase aerosol chemistry to simulate important experiments in recent publications. Overall, quality of the paper is good, and I personally enjoyed reading the manuscript. The manuscript is suitable for publication in Atmospheric Chemistry and Physics after addressing the following comments. Some parts of the paper were not easy to follow, although the research itself looks very good. I strongly suggest the authors to read the manuscript carefully, and ask a third person for an opinion to improve the presentation quality of the manuscript if necessary.

Comments P775L21 'In the future, we intend to use this knowledge, to develop the ADCHEM model (Roldin et al., 2011a). ADCHEM is a 2-D-Lagrangian model for Aerosol Dynamics, gas phase chemistry and radiative transfer which has been used for urban plume studies (Roldin et al., 2011b). One of the main purposes with ADCHEM is to improve the sub-grid scale aerosol particle representation in large-scale chemistry transport models (e.g. Bergstrom et al., 2012). In the first version of ADCHEM aging of the organic com- pounds in the atmosphere was simulated with a non-equilibrium 2-D-VBS approach. The 2-D-VBS method treats the oxidation of organic compounds in a simplified way by generalized OH reactions rates, functionalization and fragmentation patterns (Jimenez et al., 2009; Roldin et al., 2011a and Donahue et al., 2011).'

Future perspective of the study is the main focus of the paragraph; however, this paragraph is located at introduction. Please consider to move this paragraph to the last part of the manuscript.

P777L2 'homogeneous nucleation'. Please clarify how homogeneous nucleation rates for organic compounds were parameterized in the model.

P779 equation 1 Please cite an appropriate reference for the equations. In addition, please clarify unit of all the parameters.

P780L10 'In this article we either treat all SOA (monomers + oligomers + organic salts) as one phase or as two completely separated phases.' It was not clear how phase

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separation was treated in the model. Please clarify it.

P781-784 Section 2.2.3 introduces many parameters to describe wall losses of both particles and gas phase species. The authors have conducted a sensitivity study on those values in section 3.4. I was unable to understand how the values of those parameters in section 2.2.3 were determined until reading section 3.4. I suggest to rearrange the manuscript so that readers will be able to follow the story smoothly.

P789 R1a-R6 Please clarify how the reaction constants were determined.

P794 equation 18 Please clarify how the value for mass accommodation coefficient was determined.

P801L26 'In this work we model the organic salt formation between ammonium and carboxylic acids as a process occurring in the particle surface layer and particle bulk and not in the gas phase.' It was not clear why the authors have made this assumption, after telling 'part of the ammonia uptake could be attributed to reactive uptake of NH3 and organic acids from the gas phase (Kuwata and Martin, 2012).'

P810L21 'Experimental evidence suggests that there are no substantial diïňĂerences in chemical composition of α-pinene SOA particles upon evaporation in thermodenuders' I am not sure if it is true. For instance, Kuwata et al. (2011) has demonstrated that chemical composition of α-pinene SOA particles after evaporation is different from original particles.

Figure S1 Change the ordinate to logarithmic scale, since the figure is mapped by dN/dlogDp.

Figures S4, and S6 Add units for ordinates.

Reference Kuwata, M., Chen, Q., and Martin, S. T.: Cloud condensation nuclei (CCN) activity and oxygen-to-carbon elemental ratios following thermodenuder treatment of organic particles grown by a-pinene ozonolysis, Phys. Chem.Chem.Phys, 13, 14571–14583, 10.1039/c1cp20253g, 2011.

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