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Interactive comment on “Modeling kinetic partitioning of secondary organic aerosol and size distribution dynamics: representing effects of volatility, phase state, and particle-phase reaction” *by* R. A. Zaveri et al.

Anonymous Referee #1

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Review of “Modeling kinetic partitioning of secondary organic aerosol and size distribution dynamics: representing effects of volatility, phase state, and particle-phase reaction” by Zaveri et al., submitted to ACPD.

General remarks: This is a well written paper that extends the model for kinetic gas-particle partitioning to include particle-phase diffusion and chemical reaction. The paper also provides evaluation of the theoretical framework of this model with implementation in MOSAIC and comparison of results to a finite-difference solution. Further,

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growth dynamics of the Aitken and accumulation mode particles are studied at several combinations species volatility, particle-phase diffusivity and particle-phase reaction rate constant. Although the model is immensely complex, and requires number of parameters that are very hard to derive from experiments, the model evaluation advances scientific understanding of kinetic partitioning of SOA and can act as a template to design future SOA formation algorithms for implementation in 3-D Eulerian models. I recommend publishing the manuscript in ACP only after taking into account the following minor changes/additions

Specific comments 1. One of the major drawbacks of the model is the failure to account for SOA formed through aqueous-phase pathways (Carlton et al, Atmos. Chem. Phys., 13, 10203-10214, 2013). This can be particularly important in areas such as Eastern US and other urban centers where sulfate-rich conditions increase the particle-phase liquid water and subsequently aqueous-phase SOA. This should be highlighted as one of the limitations of the current proposed framework for inclusion in 3-D Eulerian models.

2. Although the paper focuses on the interplay between organic solute volatility, particle-phase diffusivity and particle-phase reactivity, some discussion on previous studies using accommodation coefficients to impose kinetic constraints on SOA formation arising from mass-transfer during phase transition would be helpful to set up a broader context of the current formulation (Bowman et al., Atmospheric Environment 31, 3921âĂŤ3931; Saathoff et al., Atmos. Chem. Phys., 9, 1551–1577, 2009; Parikh et al., Atmospheric Environment 45 (5), 1126-1137).

3. A major limitation of this model is the requirement of size-dependent diffusion parameters and kinetic rate constants for actual particle-phase chemical reactions (the specification of such reactions is still incomplete). Also several combinations of species volatility, particle-phase diffusivity and particle-phase reaction rate constant can lead to the similar aerosol size distributions, making it difficult to verify the parameters experimentally – particularly requiring size distributions of isolated SOA chemical species

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that are formed as products of particle-phase reactions. The burden of acquiring parameters for the model for it to be implemented in larger-scale models is very high – this caveat should be stressed and the focus of the summary and implications section should be on key scientific findings from the model, rather than suggesting it can be implemented in larger-scale models.

Interactive comment on Atmos. Chem. Phys. Discuss., 13, 28631, 2013.