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Atmospheric Chemistry and Physics
Discussions

Interactive comment on "Modeling the effect of non-ideality, dynamic mass transfer and viscosity on SOA formation in a 3-D air quality model" *by* Youngseob Kim et al.

Anonymous Referee #2

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This manuscript addresses the presentation of secondary organic aerosols in air quality model, specifically the non-ideality and viscosity of the particles. This is an important topic on the field of SOA studies and the topic is well suited for ACP. I find some points that should be addressed before publishing in ACP.

Specific comments:

Authors present organics with few surrogate compounds and this is understandable approach in 3D air quality model. There is no discussion in the manuscript about the effect of choice of the surrogate compounds on the results and I wonder if the authors could comment this little bit. First, how does the use of 21 surrogate compounds

(instead of the huge number of organics in the real atmosphere) affect the results regarding the non-ideality and the activity coefficient calculations; Is it expected that activity coefficients matter that much also when the particles consist of mixtures of much more compounds? Second, how does the choice of surrogate compounds affect the viscosity effect? For instance, monoterpene oxidation products seem to be missing low-volatility compounds (unless there is acidic aqueous phase). If the mass of low-volatility compounds was underestimated, wouldn't that lead to viscosity effect being overestimated?

There are some aspects in the description of dynamic calculations for viscous particles where some clarification would be helpful: 1) Eq. 7 seems to describe the diffusion in particle phase based on difference between equilibrium particle phase concentration and the actual particle phase concentration of compound i. Based on the given reference (Couvidat and Sartelet 2015), in eq. 7 the concentrations should be for each layer, not the total particle phase concentrations, right? 2) The equation in the given reference seems to be derived for a case where the particle phase concentration at the interface is constant (equilibrium with gas phase). This is not the case here if also condensation/evaporation is calculated dynamically. I wonder if the equation is correct to use here. 3) If the J_diff in eq. 5 is calculated for each layer as in the reference, then it is not clear which J_diff is used in eq. 10. for calculating J_tot. 4) Only two layers are used for calculations here. Is the model accurate with only two layers? In the given reference the model is evaluated only for three or more layers.

It is stated (P14, L20) that the aerosols are assumed internally mixed, but still different absorbing masses are used for hydrophilic and hydrophobic compounds. Are the two phases assumed to co-exist in a particle? How is this taken in to account in the dynamic approach where equations for spherically symmetrical cases are used (eq. 5-9)?

Figure 4 "Shrinking" part and related discussion on P14 L6-9: It is not clear how shrinking in this conceptual discussion is thought to happen. Could the authors clarify this? Especially confusing is the blue text about volatile compound A being stuck at the interface due to shrinking. In case of a net mass flux of A towards the particle, A could be stuck at the interface and not transferred to the particle core. But how does that happen at the same time when A is evaporating and the particle thereby shrinking?

Technical comments:

Table 1, row BiA0D, last column: A typo: “qaueous”.

Table 1: Units missing for Kp.

P8, L15: Text refers to “SOAP-basic” although such simulations is not presented in the fig. 2.

P10, L18: “concentrations” twice.

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