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Comment on acp-2022-698

Anonymous Referee #1

Referee comment on "Impact of phase state and non-ideal mixing on equilibration timescales of secondary organic aerosol partitioning" by Meredith Schervish and Manabu Shiraiwa, Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2022-698-RC1>, 2022

Schervish and Shiraiwa apply a multi-layer kinetic model (KM-GAP) to estimate the timescales for equilibration between the gas and particle phase when a condensable gas-phase species is present. This work expands upon previous KM-GAP studies by simulating a phase-separated, core-shell morphology and non-ideal mixing conditions in the shell. Non-ideality is explored by varying the activity coefficient of the condensing species in the shell. Other parameters are varied including the diffusion coefficient of the condensing species. The trends in the simulation outcomes are not particularly surprising and the authors do a nice job of rationalizing/ explaining the simulation results. Where these simulations are very useful is in providing some level of quantification to when diffusive limitations/ non-ideality become important for mixing timescales. This information/ data is significant in that it can help interpret experimental results and help identify the conditions that are important to account for phase separated morphologies in atmospheric chemistry models. The work is well executed and well presented, solidly within the scope of ACP, and the conclusions are well supported by the data presented. I support publication in ACP but have a few minor comments:

- Throughout the manuscript, various extrema in physical/ chemical parameters are applied to simulate a wide range of possible conditions, e.g., activity coefficients from 10^{-3} to 10^5 , diffusion coefficients from 10^{-5} to 10^{-20} cm²/s. These values indeed cover the full range of potential values that are likely to be observed. What is missing is discussion of the relevance of the extreme low/ high values. It would have been helpful to provide some specific examples to go along with these extrema. For example, is there a specific condensing molecule that is known to have an activity coefficient of 10^{-3} (or 10^5) in a organic-enriched shell? Citing specific examples would go a long way to giving the reader a sense of when these extrema could be relevant under atmospheric conditions.
- It is stated in the abstract and again in the conclusions that this work can "reconcile apparent discrepancies between experimental observations of fast particle-particle mixing and predictions of long mixing timescales...". However, it was unclear to me exactly how the work was reconciling these discrepancies. Could the authors expand

more?

- In Figure 2, I had a difficult time seeing the differences in the shade of blue in both the pdf and a printed version. More extreme shading difference could be helpful.
- Minor quibble, but from the title ("Impact of phase state...") I had anticipated more phase morphologies to be considered (e.g., a gel, partially effloresced, etc.). Since only phase separated morphologies were considered, the authors could consider a title that reflects the emphasis on phase separation.