

Interactive comment on “Maxwell-Stefan diffusion: a framework for predicting condensed phase diffusion and phase separation in atmospheric aerosol” by Kathryn Fowler et al.

Anonymous Referee #1

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This study presents the Maxwell-Stefan diffusion framework that explicitly treats non-ideal interactions of components by the use of activity coefficients. by relaxing the Fickian law of diffusion. The authors demonstrate a complex interplay between the viscous and solubility effects on chemical composition. Currently it is urgent to resolve effects of phase state and phase separation on various gas-particle interactions and this paper represents an important contribution to the community. The manuscript is well written and their methods and results seem reasonable. I support publication of this manuscript in ACP after below a few points are addressed.

- Introduction is written very well. Just one point: it is claimed that there is currently

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no models that treat solubility and diffusion explicitly and separately. However, kinetic multi-layer models based on the PRA framework (Poschl et al., 2007) such as KM-GAP (Shiraiwa et al., 2012) do treat diffusion and solubility by constraining transport from surface to bulk using solubility, and also considers non-ideality by using activity coefficients (Shiraiwa et al., 2013). This could be acknowledged.

- The model assumes that the particle outer shell equilibrates instantaneously with ambient conditions. How good is this assumption? I suspect this assumption might be invalid for glassy particles under low temperatures when water diffusivity drops substantially. This is also related to adsorptive vs. absorptive water uptake. I appreciate if you extend discussions on this issue.

- This study presents simulation results for a binary system of water and one organic component. I wonder if this method also works well for complex multi-component mixtures as expected in ambient organic particles. I guess it should work in theory, but would you expect any practical challenges such as difficulty in finding converged solutions or computational time?

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