Atmos. Chem. Phys. Discuss.,
https://doi.org/10.5194/acp-2017-424-RC1, 2017

Atmospheric Chemistry and Physics Discussions

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

Received and published: 15 September 2017

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

Printer-friendly version

Discussion paper

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 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 simulations results for 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 on finding converged solutions or computational time?

Interactive comment on Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2017-424, 2017.

Printer-friendly version

Discussion paper