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Geoscientific
Model Development
Discussions

Interactive comment on "An analytical solution to calculate bulk mole fractions for any number of components in aerosol droplets after considering partitioning to a surface layer" *by* D. Topping

Anonymous Referee #3

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The authors of this paper present a model to account for the partitioning of solute to the surface layer of a droplet. The inputs require only surface tension parameters from binary systems. The approach is computationally efficient however the predictions have yet to be tested against measurements.

The paper is well written and the concept is relevant to the cloud droplet and geoscientific modeling community. However the model is in its formative stages; logical ideas are proposed, idealistic assumptions are applied, key surface tension parameters must be prescribed (Kappa_i and Gamma_i), but little conclusive evidence of the model's validity is given. The reviewer has serious concerns that the theory and application has

not been properly tested.

The author is aware of many of these shortcomings. However the reviewer believes there are additional, quick, yet effective methods to evaluate the model. The authors could compare their simulations to additional already published data points where surface layer partitioning is evident (e.g, Sorjmaa et al., 2004). Currently the author compares his model to 3 pendant drop surface tension measurements. The author could also compare his model with other partitioning models to strengthen his arguments. How do these results compare with the numerical technique of Laaksonen (2006) and Kokkola et al (2006), Li et al, 2004?

The author states the changing concentration gradients approach the surface. Are those concentrations at equilibrium? If not, can assuming chemical equilibrium in the system be valid? Would it make more sense to apply pseudo-steady state assumptions to the system?

The author assumes that the activity of the droplet can be represented by the mole fraction of material. This is true under ideal conditions, but is of greater concern for non-ideal systems where partitioning of bulk material occurs. This is an example of an assumption that will only be validated with comparison to actual measurements.

MINOR CONCERNS:

P1092. “Validated using bulk empirical data” This phrase seems to negate the importance of this study, if bulk data works well and is relevant. Can all bulk empirical data be used? That is pendant drop surface tension measurements appear to agree, how about other methods (e.g. De Nuoy ring?)

P1095, L14. LiLu? Or Li and Lu 2001 model?

Equations 18 and 19 are redundant. Equations 15 and 16 are redundant.

Figure 1. Please specify if data points are actual measurements or derived in models. If measurements (provide the source in caption or figure).

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What is the meaning of the positive solution? Is it possible to have imaginary solutions to the quadratic equation? If so, under what circumstances.

Interactive comment on Geosci. Model Dev. Discuss., 3, 1089, 2010.

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