

Atmos. Chem. Phys. Discuss., referee comment RC2
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Comment on acp-2021-561

Anonymous Referee #2

Referee comment on "Comparison of six approaches to predicting droplet activation of surface active aerosol – Part 1: moderately surface active organics" by Sampo Vepsäläinen et al., Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2021-561-RC2>, 2021

Vepsäläinen, Calderón, Malila, and Prisle contribute a comparison of simplified formulations for treating surface tension in droplet nucleation (manuscript #acp-2021-561). They compare six published thermodynamically consistent models of the bulk-to-surface partitioning behaviour of moderately strong surfactants and the effects this has on droplet surface tension, water uptake, and cloud droplet nucleation. For mixtures of dicarboxylic acids with ammonium sulphate, cloud droplet activation predictions were similar for lower organic fractions (organic < 50% of dry aerosol mass), but for dry organic fractions greater than 80%, differences emerge based on the partitioning calculations.

Predicting cloud droplet nucleation from aerosol chemistry is challenging and of interest to the broader atmospheric chemistry community. Though the models are all previously published, the direct comparison between the models is useful. The models ingest parameters derived from experimental data, but the present paper does not include a comparison of the model to measurements. I recommend publication if the authors can address several shortcomings of the present manuscript.

Major comments

Sensitivity analysis is provided for the compressed film model. However, for all models, various parameters are taken from measurements and could vary as a function of composition, temperature, and mixing state (among others). The manuscript presents the implementation of six published models with no additional experiments nor a comparison to published measurements. The value of the publication is in the direct comparison between formulations. The community gains nothing from this paper if the results do not include analysis of the sensitivity of each model to perturbation in the input parameters.

None of the models treat nonideal interactions of the organic with the other solution components. This is a significant simplifying assumption that should be discussed. Especially at the onset of water uptake and early droplet growth, nonideal solution activity influences the Koehler curve. In the supplement, after equation S7 the activity is expressed $a_w = x_w * \gamma_w$. The activity coefficient is not defined or used and is subsumed into the constants of equation S7. This is the only activity coefficient in the paper, and it appears not to have been used in the calculations. Prediction of activity, independent of surface partitioning, is also an active area of research, particularly for organic/inorganic mixtures. How would nonideal activity introduce error in the authors' calculations? This needs to be discussed.

It would improve the impact of the paper if a schematic illustration were introduced to describe and differentiate between the models, given that the present manuscript presents the implementation of published equations.

Technical

Line 5-6: you might rephrase to clarify and list the surface-active materials

Line 41: can you clarify "microscopic and submicron"

Line 57: you might consider citing all papers that have demonstrated this, including more recent papers and those from other groups.

59: "finite-sized" please give the size range

71-74: this seems redundant

96: before, this was called sodium. Why natrium now?

248: "for phase the bulk phase " a typo?

Please define and quantify the term, 'moderate surfactant'

Line 397 - Pure malonic acid is a powder; is this surface tension the CMC value?

394,395 – surface tension is reduced by higher concentration, or as a size-dependent effect?