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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Inferring thermodynamic properties from CCN activation experiments: a) single-component and binary aerosols" *by* L. T. Padró et al.

Anonymous Referee #2

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Padró et al. report on a new method to estimate molar volume and solubility that relies on measurements of surface tension, chemical composition, and CCN activity coupled with Köhler Theory. While difficult to determine for ambient aerosols, molar volume and solubility are required for predicting the impacts of aerosols on clouds. Therefore an appropriate estimation method for these thermodynamic properties is desirable. The authors conclude that the newly developed method predicts molar volume to within 18% for single-component and binary mixtures when the organic mass fractions are between 50 and 100%, and is thus best applied to ambient aerosols with high organic mass fractions.

The paper is generally well written and relevant for ACP. There are no fundamental reasons to preclude its publication. Comments are made below regarding references and units to improve readability and traceability in the Köhler Theory Analysis (KTA) section; comments also are made regarding the applicability of KTA to ambient aerosols. Upon those comments being addressed, it is recommended that this paper be published in ACP.

Specific comments:

pp. 3808-3809: Seinfeld and Pandis (1997) is cited in reference to Eqs. (2) and (3), which describe Köhler theory for the single component case; the equivalent expression for the Raoult's term (Eq (3)) in the multi-component case, Eq (5), has no citation. It is suggested that the appropriate citation be added in order that details related to the modifications required for the multi-component case can be easily referenced. The use of appropriate units would help further describe the added terms (e.g., volume fraction), which are relevant to the derivation and application of KTA. The use of appropriate units throughout sections 2.1-2.4 would improve the readability and traceability of the derivation of KTA and the assumptions relevant to its application.

p. 3810: The parameter omega (Eqs. (7) and (8)) is not defined (i.e., named).

Abstract and Conclusions: The authors state that this method is "a powerful and ideal method for determining the CCN characteristic of ambient water soluble organic carbon" and "is a powerful tool for characterizing the droplet formation potential of ambient water soluble organic carbon". This conclusion seems a bit overstated based on the results and analysis presented. The KTA method is an important step forward in estimating the described thermodynamic properties; however its applicability to ambient aerosols remains to be determined. While the uncertainty in estimated molar volume was evaluated for uncertainty in the parameters solute surface tension (sigma), omega, and effective van't Hoff factor (upsilon), the uncertainty in those parameters has not been evaluated for uncertainty in required chemical and physical properties (which

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are largely unknown for ambient aerosols). For example, it was determined that the estimated molar volume has a greater sensitivity to uncertainties in omega and effective van't Hoff factor than to uncertainties in solute surface tension. It is unclear how that conclusion would change if uncertainty in density of the aerosol particle, required for determination of solute surface tension, is considered. In addition, the parameter omega depends on the volume fraction of each constituent in the mixture, which in turn depends on the mass fraction and density of each constituent in the mixture. For ambient aerosols, identification and quantification of constituents remains difficult and incomplete. Thus assumptions must be made as to the density of aerosol particles, as well as to the chemical characterization of particles. The effects of such assumptions on estimated parameters, and therefore estimated molar volumes, are undefined.

Interactive comment on Atmos. Chem. Phys. Discuss., 7, 3805, 2007.