Atmos. Chem. Phys. Discuss., 7, S1697–S1699, 2007
www.atmos-chem-phys-discuss.net/7/S1697/2007/

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 #3

Received and published: 10 May 2007

General Comments: The authors present a new method, Köhler Theory Analysis (KTA), for inferring molar volume and solubility of organic compounds in single-component and binary organic-ammonium sulfate aerosols. Application of the theory relies on measurements of droplet surface tension, chemical composition, and cloud condensation nuclei (CCN) activity, as well as knowledge or estimation of density, molar mass, and van't Hoff factor. The method is tested on single-component and binary organic-ammonium sulfate particles for six relatively high molecular weight organic compounds with known molar volume and solubility. The authors show the KTA method to predict molar volume with an average of 18% error for those solutions with organic mole fractions of 50-100%. The authors also present an analysis of uncertainty

in molar volume predictions, which shows generally large uncertainties, especially for solutions with low organic mole fractions.

This work is an important step toward characterizing the influence of organic constituents on the cloud droplet formation potential of ambient atmospheric aerosols and related climate change effects. It should be of significant interest for readers of Atmospheric Chemistry and Physics. The manuscript is well-organized and well-written, with sufficient detail of the theory, assumptions, formulas, notation, experimental methods, and calculations. However, the general conclusion that the KTA method is a "...powerful tool for characterizing the droplet formation potential of ambient water soluble organic carbon..." is an overstatement. Typical ambient atmospheric aerosols can range in chemical composition from primarily inorganic to primarily organic, and may contain numerous individual organic and inorganic components. While useful and informative, the KTA method had reasonable success for only single-component and binary organic-inorganic solutions with high organic mole fractions. Substantial errors were reported for more general aerosol mixtures having equal mole fractions of organic and inorganic components.

Specific Comments: Abstract and Conclusions: In the Abstract, the method is stated to infer molar volumes "...within 18% of their expected value for organic fractions between 90 and 100%." In fact, the 18% error value is an average, and not an upper limit. The statement should be changed to indicate this fact. In the Conclusions section, a similar statement is made, but there the range of organic fractions corresponding to the 18% error value is stated to be 50 to 100%. It is not clear why the stated ranges of organic mole fractions differ between the Abstract and Conclusions section.

Table 2: The temperature(s) corresponding to the chemical properties listed in Table 2 should be indicated.

p. 3810, line 10: It would be helpful if the authors justified the values chosen for the van't Hoff factors for the compounds studied in this work, perhaps by reference to other

ACPD

7, S1697–S1699, 2007

work.

p. 3819, line 18: It is unclear and confusing as to why van't Hoff factors equal to 1 were used for the organic compounds studied when the authors state here that the values are larger in reality.

Table 5: It would be helpful if the authors provided some interpretation of the large variation in inferred molar volume errors and uncertainties across the organic compounds studied.

Technical Comments: p. 3810, line 10: Should read "...(for which a value of..." - addition of "for"

p. 3811, line 12: Add a comma after close parenthesis.

p. 3812, line 4: Should read "...for Eq. (10) are obtained..." - substitution of "are" for "is"

p. 3817, line 11: Should read "...and organic molecules..." - not "...and organics molecules..."

p. 3817, line 19: Add a comma after close parenthesis.

p. 3818, line 8: Should read "...most compounds studied are not strong..." - addition of "studied"

p. 3820, line 12-13: The statement, "The estimated molar volume error was found to be larger than reality" is confusing. Suggest rewording for clarity.

Figure 6, Caption: Should read "Activation curves..." rather than "Activation curve..."

Figure 7: It would be helpful if the ranges of the ordinate axes in Figures 7a and 7b were equal.

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