

## ***Interactive comment on “Application of several activity coefficient models to water-organic-electrolyte aerosols of atmospheric interest” by T. Raatikainen and A. Laaksonen***

**Anonymous Referee #1**

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General comment

The present work by T. Raatikainen and A. Laaksonen compares existing and modified activity coefficient models suitable for atmospheric relevant organic-electrolyte aqueous solutions. The five selected activity coefficient models underwent several modification and new ions and organics have been added, extending so the area of applicability.

Phase equilibrium of solvent mixture containing electrolytes is poorly understood, in spite of the need for such data in the design and simulation of the processes char-

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acteristic for atmospheric sciences. Therefore I salute the initiative of the authors for gathering the information, processing it and the attempts of optimize it. The new fitted parameters make possible to calculate the activity coefficient of water and ions in organic-electrolytes aqueous solutions with an accuracy that, at least for the moment, can be considered at least satisfactory.

Specific comments:

Nevertheless, few explanations and modification are needed:

1. The original UNIFAC is common for all the models presented. I would definitely suggest the use of UNIFAC Dortmund (Gmehling at al, Ind. Eng.Chem.Res 32, 178-193, 1993), given its higher reliability; the intermolecular interactions are better reproduced and takes into account the differences in the molecular sizes. Also the temperature dependence is more accurately expressed. A very important characteristic for UNIFAC Dortmund is that the activity coefficients at infinite dilution can be predicted.

2. The work of Aznar and Teller presented in Braz. J. Chem. Eng 18. 2001 presents the prediction of electrolyte vapor-liquid equilibrium by UNIFAC-Dortmund only, by dropping the Debye-Huckel and estimating instead group interaction parameters for ions and between ions and solvent groups. The results are in fairly good agreement with the experimental data and by eliminating the DG for ion-ion interaction, the fitting and modelling work is reduced substantially. Probably the authors should consider this approach also, at least when comparing their modified predicted models with the existing ones.

3. The models behaviour at infinite dilution is not extensively presented.

4. Part of the available experimental data should be for comparison purposes only, without being included in the fitting part in order to test the reliability of the model prediction. If the authors proceeded so, they should present the result accordingly, specifying the mixture(s) and presenting the results separately.

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5. In the atmospheric science, not only the water activity is important, but also the activities for the other components, i.e. the organics. Such experimental data can be found in literature and can be compared with the UNIFAC presented here. This can be considered a test for the accuracy of the new fitting parameters.

Technical corrections

6. page 3643, lines 22-23. Add reference for the 50% of the aerosol dry

7. page 3647, line 6. Add the word 'subscript' between the brackets for c - cation and a -anion. 'a' has been used before for representing the activity.

8. page 3649, r18: there exist -> there exists

9. page 3651, lines 10-11. You should explain here, at this point, why you used the 30 mol/kg limitation and not in the appendix.

10. page 3656, line 5. The authors said that Ming and >Russel model is one the few activity coefficient models for atmospheric mixtures. In such case what other models exist and why they have not been used in this work?

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