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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Water activity in polyol/water systems: new UNIFAC parameterization" *by* C. Marcolli and Th. Peter

Anonymous Referee #1

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This paper reports the water activities of a series of polyol/water systems at 298K. The experimental results are compared with those predicted with the UNIFAC model. The authors have demonstrated that the conventional UNIFAC model cannot account for the difference in water activities between the isomers. By minimizing the difference between the results and model predictions, new UNIFAC parameterizations and group interaction parameters are provided to improve the performance of the UNIFAC model for these polyol/water systems, especially for isomers. The authors have given a clear presentation and discussion of experimental data. This paper provides new experimental data for the polyol/water systems and new model parameters, which are of great help in modeling the properties of organic compounds in atmospheric particles.

We recommend accepting this paper after clarifying the issues listed below.

Specific Comments

1) Page 1506, line 13 “The water activity, aw of the different polyols before the addition of water varied between 0 and 0.125. Based on these values, the water content was estimated to be between 0 and 1.5wt% for the different liquids”

How was the amount of water content in the liquids determined? Some type of reference data seem to be needed. Are they literature data or UNIFAC predictions? If the latter, were the original or revised parameters used?

2) For the glycerol/water system, a smooth curve is observed in Figure 1. There is no scatter in the data, which obtained from different studies performed at a range of temperature (25-290oC).

Page 1507, line 5, “Figure 1a shows the datasets that were judged to be most reliable for the glycerol/water system.” How was the dataset of glycerol/water system presented in Figure 1a selected? I am a bit surprised to know such a weak dependence of the water activity of the glycerol/water system on the temperature.

3) Page 1508, line 21, “Figure 4 also shows the water activities for the UNIFAC parameterization by Ming and Russell (2002) with parameters specifically developed for monosaccharides as listed in Table 2.”

Elaborate on the choice of the UNIFAC parameters specifically developed for monosaccharides for comparison with data shown in Figure 4.

4) For the new UNIFAC parameterization for the isomers, different literature data are given in Table 4. The authors found that the water activities show considerable differences between the isomers for diols with four or more carbon atoms.

In Table 4, 1-propanol and 2-propanol data are included. Do the data of these two C3 isomers show different water activities in the literature? Also the ethanol is included in

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the dataset. Please elaborate on the inclusion of these compounds in the parameterization of the new parameters.

5) Page 1510, line 5, “In order achieve this, water-alkyl and water-hydroxyl groups interaction parameters were varied while keeping other parameters constant.”

Why was the alkyl-hydroxyl group kept constant?

Interactive comment on Atmos. Chem. Phys. Discuss., 5, 1501, 2005.