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

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We thank the reviewer for his/her comments and remarks, which we discuss below.

To 1) We determined the water content of the purchased materials based on the experimentally determined water activity / water content relationship: When the water activity as a function of water content does not pass through the origin of the coordinate system, we know that water is present in the probe as purchased. We determine the amount of water by shifting the curve so that its extrapolation passes through the origin of the coordinate system.

To 2) We excluded some vapor-liquid equilibrium datasets for the glycerol/water system from Figure 1a because of their large scatter. These datasets did not show any tem-

perature trend. Based on the collected experimental data for all alcohol/water systems, there is again no clear temperature dependence of the water activity.

To 3) We show the Ming & Russell parameterization in the Figures 1 and 4 because their parameterization for monosaccharides was specifically developed for substances with a high number of hydroxyl groups. This parameterization is therefore suited to predict the water activity of polyol/water systems. This is confirmed by the improved agreement compared with the standard UNIFAC in Figures 1 and 4.

To 4) The comparison of different vapor-liquid equilibrium datasets of 1-propanol/water and 2-propanol/water indicates slightly higher activity coefficients for the 1-propanol/water system confirming the general trend found for all alcohol/water systems - but the differences hardly exceed the variations between various datasets. Because our new UNIFAC parameterization should be applicable to all alcohol/water systems, we also used the ones with ethanol, 1-propanol and 2-propanol for the parameterization although their water activities are well described by the standard UNIFAC.

To 5) For the new UNIFAC parameterization, we focused on alcohol-water interactions because they are not well represented by the standard UNIFAC. Alkyl-hydroxyl interactions are also present in alkane/alcohol systems in the absence of water. Since we did not want to risk a decreased performance of UNIFAC for these systems we kept the alkyl-hydroxyl interaction parameters constant. We add a corresponding sentence to the manuscript at page 1510, line 6.

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