

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

Anonymous Referee #2

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The study presents a parameterisation of water activity based on incremental methods. It is of great interest for model applications that consider the hygroscopic growth of aerosol particles containing organics. Due to the high number of different organic species that have been identified in aerosols, incremental methods based on functional groups are preferred rather than water activity relationships for individual compounds. While previous parameterisations have focused on individual functional groups the present study exceeds this idea by accounting for different positions of functional groups (namely OH) in isomers of polyalcohols. The comparison of the newly developed parameterisation with measurements shows an excellent agreement and, thus, it is promising for future parameterisations of other functional groups. The topic of this

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manuscript is appropriate for Atmospheric Chemistry and Physics. The paper is well written and presents clearly the experimental method and discussion of the results. I have only a few minor comments that might improve the clarity of the study.

General comments

- A (very brief) introduction of the general definition of water activity would be useful in order to clarify that in a first approximation water activity is directly related to the ratio of moles water/moles solute, and, thus, to the molecular weight/size of the solute (if different compounds are compared on a mass basis).

- In order to point out the importance of the small differences in water activity for the growth characteristics of particles an exemplary comparison of particle diameters at different relative humidities calculated based on different approaches for water activities would be useful.

Specific comments

p. 1503, l. 13: Specify the influence of organics in fog (influence on what?)

p. 1508, section 4.2: Reorder this section and discuss first the C4 alcohols (Fig. 3) and then separately C5 alcohols (Fig. 4) and refer more clearly to the figures.

p. 1511, l. 6-8: The water activity has only a minor influence on cloud drop formation since at $RH \sim 100\%$ the Kelvin term is more influential. Reword this sentence.

Figure 3: All parameterisations seem to predict water activities being greater than 1. Is this an artefact or is there any physical explanation of such values?

Technical comments

p. 1508, l. 10: ...no literature data are available (not 'is')

Figure 1: Add a legend for the blue symbols (= measurements by Ming and Russell?)

Figure 5: Examples of (not 'to')

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5, S193–S195, 2005

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