ACPD article:

# Influence of Organic Compound Functionality on Aerosol Hygroscopicity: Dicarboxylic Acids, Alkyl-Substituents, Sugars and Amino Acids

*Article by Aleksandra Marsh et al.*

Review of the revised manuscript

The authors have revised their manuscript with consideration of the comments by the two referees. Most of my initial comments have been answered and changes implemented accordingly. The manuscript has been improved in clarity and presentation of results. There are only a few minor issues remaining (see below), which I suggest should be addressed in preparation of the final revised manuscript for publication.

## Specific comments

- P5, Eq. (5): correct the symbol for saturation vapour pressure (currently $\rho°$ *"rho"*) to $p°$. This would be a more typical choice, would be in agreement with the expression given by Rovelli et al (2016) and avoids use of rho which stands for density in Eq. (2). Also, on line 15, correct spelling of "Fuchs-Sutugin" (only one t).
- P5, line 5. (Related to the response to my initial comment P 7, l. 2):
  *When referring to gradient in the text, we are referring to the gradient in water partial pressure and we believe this is correct. We do not refer to a gradient formed from (RH-aw). To be consistent with our previous publications, we have removed the subscript i entirely from the equation but not replaced it with w.*

  The revised sentence reads: "In this equation, the gradient in water partial pressure is the difference between the RH and $a_w$, the instantaneous water activity at the droplet surface."

  This remains a confusing description of what the equation actually states (and a more fitting description is given in Rovelli et al). First, "the difference between the RH and $a_w$*"* (i.e. RH - $a_w$) is simply not a (mathematical) gradient; rather it is a difference. A gradient is for example a difference per unit distance or its equivalent in partial differential from, but it is not simply a difference as implied in the statement. Second, "the difference between the RH and $a_w$" is not the gradient in water (vapour) partial pressure and does not directly represent it, even though there exist similar mass flux expressions with differences in partial pressures or differences in vapour densities as part of the formula. Both gradients as well as differences in water vapour partial pressures carry units different from RH - $a_w$. Third, from the given statement it is unclear to what "the instantaneous water activity at the droplet surface" refers to: should it refer to RH or to $a_w$? This needs to be clarified in the text as well as pointing out that RH in this equation refers to $RH_\infty$, the RH in the surrounding gas phase sufficiently far away from the droplet surface ($S_\infty$ in Rovelli et al.).

- P10, line 29: I suggest to modify the new sentence to read: "Hence thermodynamic model predictions for amino acids were generated using E-AIM, Model III (Clegg et al., 1998), using the standard UNIFAC model including certain modified main group interaction parameters introduced by Peng et al. (2001)." This modification is more clear in that it does not imply that Peng et al. parameterized the whole UNIFAC model (they only modified a small subset of main group interaction parameters).

- P12, line 15 *(related to Referee Comment: P12, l. 27: "Molecular structures presented in Fig. 10 are the open chain form, which must be used during modelling using UNIFAC."; Why "must"? AIOMFAC also allows you to use the cyclic structure of sugars in aqueous solution, e.g. glucopyranose instead of glucose, if desired.*
  *Response: Cyclic sugar structures do not appear to be available on AIOMFAC-web. Amended P11 L27 to read 'Molecular structures presented in Fig. 10 are the open chain form, which must be used during modelling using AIOMFAC-web.'*

  I do not understand how the authors come to that "which must be used" conclusion about the availability of cyclic sugar structures in AIOMFAC-web. AIOMFAC-web allows you to select from a wide range of organic subgroups and there is no problem in choosing those subgroups referring to cyclic sugar structures to define an organic compound (using the optin "Define Subgroups" on the input form for organic compounds). There are even examples given in the "Predefined List" input option, e.g. for D-mannopyranose, $(CH_2^{[OH]})(CH^{[OH]})_4(CHO[ether])(OH)_5$, the cyclic structure equivalent of the open-chain form of mannose. The manuscript text should be corrected and the authors may want to check whether replacing the open chain forms in Fig. 10 by equivalent cyclic sugar structures would lead to significantly different model curves.