Interactive comment on "Henry's law constants of polyols" *by* S. Compernolle and J.-F. Müller

Anonymous Referee #1

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Compernolle and Müller present a new compilation of Henry's law constants of polyols. The authors apply thermodynamic relations and fitted binary interaction models to derive Henry's law constants based on a range of experimentally determined and/or estimated thermodynamic properties from various data sources. In regard to the atmosphere, Henry's law constants of organic compounds, including polyols, are of interest to predict the partitioning of volatile and semi-volatile organic trace gases to cloud droplets and dilute aqueous aerosols.

While more complex vapour pressure and thermodynamic activity coefficient models can be used to describe the gas-droplet equilibrium of organic compounds over a large range of aqueous solution concentrations, the simplicity of Henry's law is of practical use for parametrising the partitioning of water-soluble compounds to cloud droplets in large-scale atmospheric models. This work is therefore of interest to better quantify

Henry's constants for a class of chemical compounds and includes values for diols, triols, and higher polyols with chain-lengths of more than 4 carbon atoms, for which literature data is scarce.

The article is concise, well structured and well written. The methods used are described appropriately, related literature is discussed and sources of uncertainties are mentioned. Aside from a few typos and corrections to some subscripts in the mathematical expressions, I have only a few, minor comments. I recommend this work for publication in ACP after minor revisions.

General comments

- One point worth clarification concerns the sensitivity test calculations with aqueous ammonium sulphate aerosol solutions described in Section 5 and implications of this discussed in Section 6. I suggest to mention that the gas-liquid partitioning described with Henry's law actually applies to the limiting case of an organic compound being present in tiny amounts (both in gas and liquid phases) only, as defined by Eq. (1). This may therefore not apply to all situations found in the lower atmosphere. In addition, as soon as not only an aqueous ammonium sulphate phase is present in an aerosol, but, e.g., also a hydrophobic organic phase, the partitioning of the considered polyols may be quite different from the simple examples given in the calculations and shown in Figure 2; see, e.g., Zuend et al. (2010). In such a case, less hydrophilic compounds may still partition substantially to the particles, despite the simple Henry's law calculation (and activity coefficient values in the aqueous phase) suggesting otherwise.

Specific comments

- p. 13530, line 23: "enthalpy of gas phase dissolution", perhaps better: enthalpy

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of dissolution of a gas phase species. Check also the subscripts in the formula given there.

- p. 13532, line 6: "its liquid vapour pressure"; better: its pure liquid-state vapour pressure.

- p. 13532, line 7: "corresponding enthalpy change"; unclear: state what process is meant.

- p. 13532, line 15: "liquid, at infinite dilution"; change to: liquid solute at infinite dilution.

- p. 13532, 13533., Eq. (5) vs. Eq. (10): Check the equations regarding factor R.

- p. 13535, line 21: "due to the crystal contribution"; this is vague, please clarify what is meant.

- p. 13535, line 22: I suggest to write there "liquid state vapour pressure".

- p. 13536, Eq. (17): Check the subscripts "g" of $C_{p,\mathrm{g}}$ in the integrals related to the entropy/enthalpy changes of the fusion phase transition. Shouldn't it be $C_{p,\mathrm{L}} - C_{p,\mathrm{Cr}}$?

- p. 13536, line 17: Replace "solid state pressures" by "solid state vapour pressures" (for clarity, since the vapour pressure is meant, not the pressure of/in a solid).

- p. 13542, line 11: "Note that AS has a deliquescence RH (DRH) of 79.5% and an efflorescence RH (ERH) of $\sim 35\%$ (Martin, 2000)." For clarity, write: "Note that pure AS particles have a ...", since this is not necessarily true when other components are present (besides AS and water). Following sentence: "Below the ERH, only solid AS is present in the particulate phase." could be misunderstood, since also below the DRH only solid AS may be present or otherwise a

liquid, supersaturated solution, depending on the RH history of a particle (i.e., if previously dried below ERH or not). DRH is the stable equilibrium point (referring to the solubility limit of solute).

- p. 13543, Eq. (25): As done in Eq. (2), Eq. (25) refers to the limiting case of pressure and mole fraction $\rightarrow 0$. Therefore, state the limes in the expression.

- p. 13546, line 6: "diols will be partially or completely in the aqueous phase in clouds,"; should it read "gas phase" instead of "aqueous phase" here?

- Table 2: The pressure unit of `atm` is used, which is an obsolete unit. Atmos. Chem. Phys. asks authors to use SI units whenever possible, thus, use `Pa` (or `kPa`) for tabulated data. The same applies to Table 4.

- Table 4: State the temperature for which the quantities are listed.

Technical corrections

- p. 13534, line 17: delete "(see Eq. 13)".

- p. 13540, Eq. (20): RT should be math mode (RT).

References

- Zuend, A., Marcolli, C., Peter, T., and Seinfeld, J. H.: Computation of liquid-liquid equilibria and phase stabilities: implications for RH-dependent gas/particle partitioning of organic-inorganic aerosols, Atmos. Chem. Phys., 10, 7795–7820, 2010.

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