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Interactive comment on “Compilation of Henry’s law constants, version 3.99” by R. Sander

Anonymous Referee #1

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Henry’s law constant is essential for environmental studies involving aqueous-phase processes (e.g. cloud, aqueous aerosols). Sander ACPD presents a new compilation of Henry’s law constants of a wide range inorganic and organic compounds of atmospheric interests, as well as a detailed summary of different formulations. In general this work is constructed in a clear and concise. Meanwhile this compilation is also available online which serves as a public peer review. I have only minor comments and I recommend this work for publication in ACP after revisions.

General comments:

In Table 6 (where the Henry’s law values are summarized), the *Note* needs to include more details, e.g. whether the reported value represents physical solubility or the effective Henry’s law that includes certain equilibrium, whether the value is for pure water, salt solution, sea water, aqueous aerosol, etc. For the author’s reference, Sander et al

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Interactive Discussion

Discussion Paper



(JPL 2011) compiles pure water Henry's law constants for ~ 120 species accompanied with 93 notes, while this work summarizes >3000 species but only followed by ~ 300 notes. For example, in general I find formaldehyde is well documented in this work (e.g. sufficient details are given in notes) but glyoxal is not.

I will not be able to go through all compounds one by one but will specify a few as examples in the Specific Comments section.

Also, some compounds of great atmospheric interests are missing in the list, e.g. epoxide compounds formed from isoprene oxidation. Isoprene has large global source and potential contribution to SOA formation, and the recently identified epoxide compounds are key intermediates to the isoprene SOA formation. These compounds are expected to be highly water-soluble and Henry's law constant estimated to be on the order of $10^8 \sim 10^9$ M/atm (EPI suite by Chan et al 2010). Also epoxide formed from toluene oxidation (e.g. 2,3-epoxy-6-oxo-heptanal, $\sim 20\%$ yield) its Henry's law constant is estimated to be on the order of 10^5 M/atm (SPARC estimated by McNeill 2012). Given this work is reviewed by a journal in the field of atmospheric science, I recommend that the author include these compounds.

Specific comments:

1. Page 29616, Line 22, "... to calculate the vaporization of chemicals from rivers and during waste water treatment" citation needed. Also mass transport may be limiting for large water bodies.
2. Page 29619, Line 18, Equation (2) "...where R = gas constant" please remind the readers the R value and units associated with this formulation.
3. Page 29620, Line 11, "There are some advantages to describe... molality" the advantages are not discussed until the next page.
4. Page 29623, Line 13, Equation (16) Please specify the Henry's law constant H here follows which definition(s).

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5. Page 29624, Section 2.7. In addition to the "salting out" effect, there is also "salting in" effect. This section needs to be expanded in light of this.

6. Page 29613, Section 3.2.4. I recommend clarify which citation is for what compound, and could include this information in Table 6 for each individual compounds, or make another table. Also, a few more refs may be of atmospheric interest: Kampf et al 2013, Kurtén et al 2014.

7. Page 29726-29731, NOCl, ClNO₂, BrNO₂, HI, HOI, SO₂ sections (and perhaps others too), please include values or estimates in the table. For those commonly assumed to be with infinite effective Henry's law constant, please include an infinite symbol in the table. Note 42: if incorrect, why not just delete it?

8. Page 29927, glyoxal section: all effective Henry's law constant. Ip et al (2009) pure water, Zhou and Mopper (1990) sea water, Kroll et al (2005) aqueous aerosol (ammonium sulfate/sulfuric acid).

9. Page 30502, Line 7 "The value is probably wrong." this is rather ambiguous and lack of explanation

10. Page 30508, Line 2, Note 92 "Hedgecock et al 2005 refer to Schroeder and Munthe 1998 as the source but this value cannot be found there". Not really. In Schroeder and Munthe (1998) the authors listed Henry's law coefficients (Pa m³ mol⁻¹) for HgO (3.76e-11 at 25degC). Also what's the point of cite Hedgecock et al here? why not directly Schroeder and Munthe or the reference(s) therein?

Reference

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McNeill, V. F., Woo, J. L., Kim, D. D., Schwier, A. N., Wannell, N. J., Sumner, A. J., and Barakat, J. M.: Aqueous-Phase Secondary Organic Aerosol and Organosulfate Formation in Atmospheric Aerosols: A Modeling Study, *Environ. Sci. Technol.*, doi: 10.1021/es3002986, 2012.

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