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Interactive comment on “Vapor pressures of substituted polycarboxylic acids are much lower than previously reported” by A. J. Huisman et al.

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I consider these new data very valuable, as it will allow improvement of partitioning models. Given the results of this work, we have now added the option to turn on or off the empirical correction term of the web-application of our EVAPORATION vapour pressure model, available at <http://tropo.aeronomie.be/models/evaporation.htm>.

I have the following remarks:

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General remarks

Comparison with other models and other data

In this work, the experimental results are compared only with the EVAPORATION model. I suggest to compare also with other models, e.g. the model of Nannoolal et al. (2008) available at http://www.aim.env.uea.ac.uk/aim/ddbst/pcalc_main.php.

de Wit et al. (1983) have obtained a solid-state vapor pressure for tartaric acid, so I think it is appropriate to compare also with this value. Chattopadhyay et al. (2005) and Frosch et al. (2010) have also reported data on diacids with an extra functional group. Although citric acid and tartaric acid were not among them, it might be worthwhile to add the reference, and to discuss if the data are higher/lower than expected, compared to diacids without this functional group.

Correlation $\log_{10}(p^0) - \Delta H_v$

The authors point out that in their case, and opposed to the results of Booth et al. (2010), more functionalised diacids have a lower vapor pressure compared to less functionalized ones, which is more in line with chemical intuition. One could also investigate the correlation between $\log_{10}(p^0)$ and enthalpy of vaporisation (Epstein, 2010), as done in Fig. 2 of Compennolle et al. (2011). Adding the 3 $\log_{10}(p^0) - \Delta H_v$ points of the present author's data, for 2-methyl malonic, 2-methyl glutaric and 2-hydroxy malonic acid, one can see that the points are somewhat below the correlation, but closer than the data of e.g. Booth et al. (2010) or Chattopadhyay et al (2005). As the correlation is empirical, this is no proof in itself for the correctness of the data, but it is an extra element in the discussion, which the authors could use.

Specific remarks

Title. This statement is quite strong, as it implies that previous data were simply incorrect. While I agree that intuitively the current data make more sense (more functionalized species have a lower vapour pressure), I feel that more data is needed, as well as a good understanding of why the previous data would be incorrect, before this statement can be made.

Abstract, line 11-12:

'empirical correction terms in vapor pressure estimation models'. The plural suggests that such correction terms are introduced for multiple models, not only EVAPORATION. If so, which are these other models? Otherwise, use 'empirical correction term in a recent vapor pressure estimation model'.

p. 1136, line 16

'...are not able to rationalize these effects.' This is true, and we also noted that there could be problems with the measurements, and that new measurements, using the methodology of Soonsin et al. (2010) could resolve this issue. (see e.g. our section 2.5.3, and section 6)

So I would suggest adding a sentence like: 'They noted that measurements using the methodology of Soonsin et al. (2010) were needed for these compounds.'

p. 1144, line 5. The vapour pressure of 2-methyl malonic acid is presented as $1.1 \cdot 10^{-4}$ Pa, yet in Table 4 I read $1.1 \cdot 10^{-3}$ Pa. Given the context, I assume that the $1.1 \cdot 10^{-4}$ Pa value is a typo.

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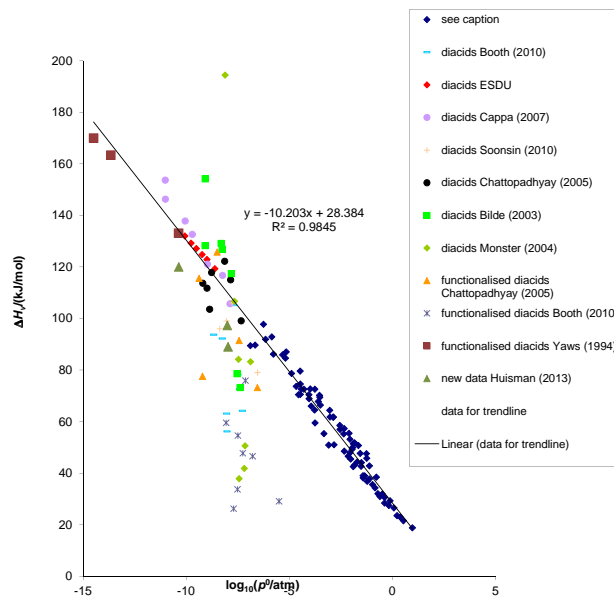
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Fig. 1.

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