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Atmospheric Chemistry and Physics Discussions

# *Interactive comment on* "Molecular corridors and parameterizations of volatility in the evolution of organic aerosols" *by* Y. Li et al.

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I enjoyed very much reading the interesting paper. However, I am missing a paragraph discussing and referring the readers to the problem that our knowledge of saturation pressures of low-volatility compounds are limited because of measurement challenges, e.g. Bilde et al. (2015). All estimation methods rely on training sets of well-established vapor pressures. Those are typically biased toward compounds with saturation vapor pressures in the range of $10^3$ to $10^5$ Pa. For partitioning we are however, mostly interested in compounds with saturation vapor pressures in the range of about $10^{-7}$ Pa to 1 Pa (O'Meara et al. 2014). Those with larger saturation pressure are entirely in the gas phase whereas those with lower saturation pressures will partition entirely into the aerosol. The authors state that the EPI Suite software is "...accepted as



a good estimation method of volatility of organic compounds...". In panel (a) of the Fig. 1 I plot the estimated vapor pressures of the EPI Suite versus the experimental values taken from the PHYSPROP database that is part of the EPI Suite for the pressure range mentioned above. (Please also note, that these data are often just extrapolations from high temperature measurements.) In panel (b) the estimation error histogram is plotted. Clearly, there is a significant bias of the EPI estimation towards higher pressures even when comparing it with the training data set. Again, that is because for atmospheric applications we are interested in pressures below the majority of the pressures used in the training data set for the EPI suite. Hence, I recommend to the authors to use in Fig. 4 of their paper not (only) a comparison of their parametrization to another estimation method but (additional) also to the data available.

References:
Bilde et al., Chem. Rev., 115, 4115-4156 (2015).
O'Meara et al., Phys. Chem. Chem. Phys., 16, 19453-19469 (2014).

Interactive comment on Atmos. Chem. Phys. Discuss., 15, 27877, 2015.

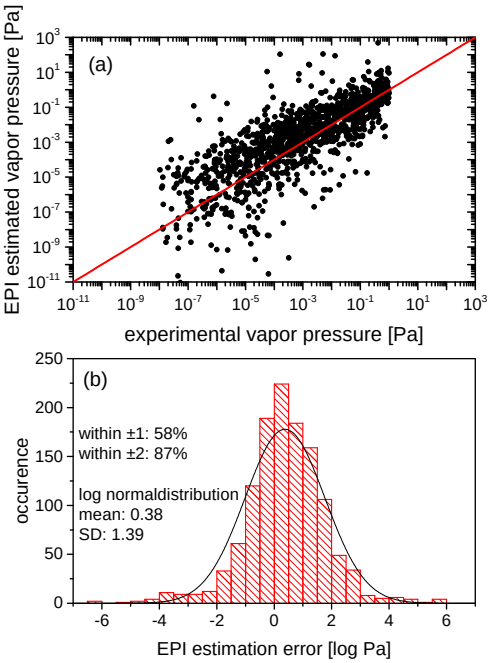


**Fig. 1.** (a) EPI estimated saturation vapor pressure versus experimental; (b) estimation error histogram