Atmos. Chem. Phys. Discuss., 11, C4554–C4556, 2011
www.atmos-chem-phys-discuss.net/11/C4554/2011/


Atmospheric Chemistry and Physics Discussions

# *Interactive comment on* "EVAPORATION: a new vapor pressure estimation method for organic molecules including non-additivity and intramolecular interactions" *by* S. Compernolle et al.

**Anonymous Referee #2**

Received and published: 8 June 2011

The authors present development of a new vapour pressure method for use in atmospheric science. Currently available models have been designed largely for industrial engineering purposes, thus introducing a significant source of uncertainty when used for predicting SOA formation, for example.

The new method presented here covers a broad range of functionality and temperatures, accounting for intramolecular and non-additivity effects. The document is very thorough. As this model may be very useful for the research community I recommend it for publication after the authors address some minor and general points.



General questions

Do the authors believe the current implementation of EVAPORARTION would improve greatly as new data becomes available? This is a very broad question but I wonder if there is a limiting accuracy of any model framework such as the one presented here. Do we know, as a community, what an acceptable level of accuracy would be. I get the feeling that we are some way from knowing this and require sensitivity studies using the wide range of gas phase degradation mechanisms available, comparing predicted and measured composition and mass. One useful way of assessing this would be to provide bands on, for example, figure 5 for the range of vapour pressures expected to be of major importance?

Data weighting. In section 2.3 the authors specify the weighting factor given to experimental data vapour pressures. It is a little unclear whether 'one reference' refers to a specific source (e.g. Booth et al 2010) or a specific molecule (e.g. succinic acid). If it is the former, rather than the latter, how does one prescribe confidence in a specific set of estimations, such as multifunctional compounds, if there tends to be only one source? It might be my understanding but this is a little clear. I would presume the weighting factor takes into account the dominance of data from un-atmospherically representative compounds here, and this is the point the authors wish to make. Also, the choice of weighting using a factor of (1/3) seems very arbitrary. Have the authors assessed the impact of changing this factor? It is unclear at this point.

It would help if the authors would give examples of vapour pressure estimations using their new model..for simple hydrocarbons and more complex molecules.

As with most fitted group methods, the true test arises from applying the model to data not used within the fitting procedure. This is partly why we know the existing models do not perform very well. How do the authors plan on testing this new method beyond the safe confinds of the data used within the fitting procedure? Can the authors comment on if there is any advantage in refitting existing frameworks despite some of the failings

in the frameworks (such as group location).

Minor points:

Please check the reference to abbreviations throughout. It can be quite hard to remember what each refers to. I would suggest re-iterating some definitions.

Page 13235: Equation 1.. reference is missing.

Page 13244. Where has equation 22 come from?

Page 13245, line 12. I would suggest another reference other than Wikipedia is used.

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Interactive comment on Atmos. Chem. Phys. Discuss., 11, 13229, 2011.