

Interactive comment on “The critical assessment of vapour pressure estimation methods for use in modelling the formation of atmospheric organic aerosol” by M. H. Barley and G. McFiggans

Anonymous Referee #1

Received and published: 4 October 2009

The authors test some of the leading available methods of estimating vapour pressures of liquid organic compounds, based upon their structure. This is valuable and worthwhile work.

I have two main comments:

(1) The authors correctly identify a problem with the method of Moller et al., which is from the same group as that of Nannoolal et al. (which is Barley & McFiggans' ir primary recommended method). This is unfortunate, as the former method is supposed to be better optimised for the prediction of very low vapour pressures - the main requirement of atmospheric scientists.

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I contacted Moller about this, and he has implemented what is supposed to be a straightforward "fix" for the problem. I also asked him and the senior author on his paper to contribute to the ACPD discussion. (At the time of writing I have not checked to see whether they have done so.)

I suggest that the authors of this ms carry out at least some tests with the corrected Moller et al. method, rather than reject it. While this involves some extra work, it will be a valuable service to the community.

(2) Although the authors searched for measured vapour pressures that are very low, it is still the case that they are not entirely within the atmospheric range for SOA. It would be very helpful if the authors provided a plot that shows, in some way, the errors in the predictions of the various models as a function of the measured vapour pressures of the test compounds. It would be worthwhile because some trend might emerge (most likely smaller vapour pressure = larger error) that would give at least a rough impression of what kind of errors might be expected at lower vapour pressures than those of the test compounds.

Other comments:

The vapour pressure prediction methods available on the E-AIM website will, over the next several days, be revised to include both the corrected Moller et al. method, and the method of Nannoolal et al. that the authors are currently recommending. Some changes are needed in the ms to reflect this. E-AIM also needs to be cited, giving both its full name (the Extended Aerosol Inorganics Model) and the URL.

Not a major part of the paper, but I disagree with the last sentence of the first paragraph of the Introduction. I think successful models of OA formation in the atmosphere will always be semi-empirical and are unlikely to be based on accurate vapour pressures of any but a small fraction of the compounds present.