

## ***Interactive comment on “UManSysProp: an online facility for molecular property prediction and atmospheric aerosol calculations” by D. Topping et al.***

### **Anonymous Referee #3**

Received and published: 17 December 2015

The manuscript by Topping et al. presents a new web-based facility for prediction of a suite of molecular, bulk-phase, and aerosol properties relevant for atmospheric and thermodynamic process-level aerosol studies. The web interface is already very user friendly and will certainly be a highly valuable contribution to the aerosol community for easy access to central properties, which are otherwise difficult to obtain for the required set of conditions. Variables such as vapor pressures, activity coefficients, absorptive phase partitioning and water uptake are readily calculated from entering compound identifiers in the form of SMILES strings. The manuscript is very well-written, and I recommend publication after addressing the following points:

C3391

#### General comments

1) My main concern is that neither the manuscript nor the website clearly describes the basic conditions and assumptions of the models used for calculating the different properties, which puts the otherwise great tool in danger of becoming a completely black box. I appreciate that the authors refer to previous papers describing model development and validation and that validation against data and other predictive tools is outside the scope of the present paper. But I would as a minimum prefer to have a short list of the most fundamental assumptions behind each model and a brief mentioning of cases where other existing models yield significantly different predictions for the same properties. For example, how is ideality defined, what does it cover? Are all components always assumed either ideal or non-ideal (to whatever degree that may be)? What are the dimensions of output variables? Are there any limits on applicability ranges of mixtures? Which components are assumed to interact and what are the assumptions regarding these interactions? For example, are some components in the mixtures always ideal or always inert? What is assumed regarding the gas-phase ideality? What are the most basic assumptions behind calculations of pure component vapor pressures? Exactly what type of vapor pressures are yielded for e.g. organics over aqueous mixtures, e.g. are they equilibrium partial pressures? This would allow the user to more readily gauge the applicability of the present predictions for their own purposes. It would also prevent obscuring the great complexity and many remaining unresolved aspects and mutual model inconsistencies behind the smooth delivery of variables with the present online tool, in particular for new users who do not have extensive experience with aerosol and liquid phase thermodynamic calculations.

2) It would be helpful to specify very clearly when a “liquid phase” is an organic mixture or an aqueous phase comprising organics, e.g. p. 9676 l. 7. Or if both options are possible in all cases. In general, the conditions for how water is accounted for would be crucial to specify explicitly, see above.

3) On a minor note, I was a bit puzzled by the use of the term “Kappa Kohler” values,

C3392

e.g. p. 9681. Is this convention replacing the use of symbol  $K(\kappa)$  and the term Köhler theory?

4) The website requires very different input variable formats, e.g. concentrations scales are requested as molecules, grams, or micromoles per some volume. It could be helpful if it would be possible for the user to give these in a number of different preselected dimensions and then the online tool would make the appropriate conversions for the models.

Specific comments

- p. 9676 l. 10: XX species?
- In Sect. 3, it is unclear what it means that properties are limited to 5000 or 1000 compounds. Are these the total number of compounds possible to handle, or at a given time?
- In Sect. 3.1, and Figs. 5 and 7, it is unclear what the dimension of vapor pressure is.
- In Fig. 5, activity coefficients are given as unitless with no reference to concentration scale or reference state. The dimension is specified on the website, but this information should be clearly stated in the documentation.
- In Fig. 7, the dimension of mass increase is not specified.
- In Fig. 4, I suggest using units of  $[g\ cm^{-3}]$  instead of  $[g/cc]$ .
- In Table 6, specify that "dry size" is diameter (if that is the case).

---

Interactive comment on Geosci. Model Dev. Discuss., 8, 9669, 2015.