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

S.A. Epstein (Referee)

sepstein@aqmd.gov

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The authors introduce a web-based facility for the prediction of a wide-range of aerosol properties. Properties can be calculated directly from SMILES strings. For each thermodynamic property prediction, the user can select an appropriate method within the web interface. The web-based facility is user- friendly and makes the prediction of complex aerosol properties efficient and straightforward. The authors also have developed a JSON API to allow users to integrate these capabilities into their own code. The manuscript describes the capabilities of the web-based facility and provides several examples. The authors do not evaluate the model performance of the various predic-

tion options, but instead, refer the user to the relevant publications that describe model performance.

This manuscript and the accompanying web-based facility are an important contribution to the aerosol community. I recommend publication after the authors address the following comments:

General Comments

1. A brief summary of other thermodynamic property prediction facilities (such as EPI Suite) would be a useful addition to the introduction.

2. In cases where physical property measurements are available, the thermodynamic calculations that rely on these physical properties would be more accurate if it was possible to use the measurements instead of the predicted values. The ability to use physical property measurement values, when available, in the aerosol calculations will significantly improve the accuracy and utility of the prediction facilities.

Specific Comments

1. Page 9673: It is unclear whether CAS numbers can be used directly in the prediction facility

2. Page 9675, lines 21-23: It is unclear what the phase "Pure component properties are limited to 5000 compounds, predictions involving activity coefficients limited to 1000 compounds" means. Are these limits on the number of molecules that can be submitted at one time?

3. Page 9676, line 21-22: It would be helpful to have the methodology options for predicting sub-cooled liquid density predictions in this bullet-point, as in the previous bullet-points

4. Page 9676, line 23-24: It would be helpful to have the methodology options for predicting pure component vapor pressures in this bullet-point, as in the previous bullet-

GMDD

8, C3319–C3321, 2015

points

5. Figure 3: A key to the axis labels should be provided in the caption

6. Figure 3: It may make more sense to combine both plots and use different marker symbols to represent each vapor pressure prediction

7. Section 3.2: The following papers should be cited when introducing predictions of absorptive partitioning.

a. Pankow, J. An absorption model of the gas/aerosol partitioning involved in the formation of secondary organic aerosol. Atmos. Environ. 1994, 28, 189.

b. Donahue, N.M., Robinson, A.L., Stanier, C.O., Pandis, S.N., 2006. Coupled partitioning, dilution, and chemical aging of semivolatile organics. Environ. Sci. Technol. 40, 2635–2643.

Technical Corrections

1. Page 9676, line 10: “xx” was never replaced with a number

2. Page 9678, line 16: the quantity in parenthesis should be raised to a power of -1

3. Page 9681, line 13: “re-partitioning” should be “re-partition”

4. Page 9705: there should be a space after “size” in the first line of the figure caption

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