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Interactive Comment

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

D. Topping et al.

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We would like to thank the reviewer for comments provided which we feel has improved the submitted manuscript. In the following text we respond to all comments made and highlight where changes have been made in the next version of the manuscript.

General Comments
Referee comment:. *A brief summary of other thermodynamic property prediction facilities (such as EPI Suite) would be a useful addition to the introduction.*
Response: We agree. In the introduction, after the sentence: *'..the development of community driven software at least enables modellers to tackle this problem directly'*

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we have added the following line. *'There are a number of property predictions facilities that are available online. For example, the US EPA host predictive models and tools for assessing chemicals under the Toxic Substances Control Act (TSCA) (http://www.epa.gov/tsca-screening-tools). From this site one can access the simulation program 'Estimation Programs Interface' (EPI) Suite facility http:// www.epa.gov/ tsca-screening-tools/ download-epi-suitetm-estimation-program-interface-v411. This provides a number of facilities including estimates of physical / chemical properties (melting point, water solubility, etc.) and environmental fate properties (breakdown in water or air, etc.). The Dortmund Databank (DDB) provide a wide range of database and software products related to fundamental properties of molecules and mixtures. With varying proprietary and free educational access, their program package ARTIST was developed for the estimation of pure component properties from molecular structure. In the UK the National Chemical Database Service (CDS) provides free access to web-based services including ACD/Labs Inc Physchem and NMR predictions http:// cds.rsc.org/ . Services specifically tailored to atmospheric studies include the E-AIM community model for calculating gas/solid/liquid partitioning http:// www.aim.env.uea.ac.uk/ aim/ aim.php and the AIOMFAC portal for calculating activity coefficients in mixed inorganic/organic liquid systems http:// www.aiomfac.caltech.edu/ .'*

Referee comment: *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.*
Response: We agree. In a follow-up development we now have funds to link the existing website to a new database of measurements linked to property predictions provided. Creating a standardized database in itself can be challenging, as noted in the recent review of saturation vapour pressures by Bilde et al (2015). To allude to these developments, we have added the following sentence to the section 'Future work': *Where property measurements are available, these might prove more accurate than*

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any given estimation technique. With this in mind, in addition to extending the range of predictions provided, UManSysProp will also be linked to a standardized database of property measurements.'

Bilde et al (2015). Saturation Vapor Pressures and Transition Enthalpies of Low-Volatility Organic Molecules of Atmospheric Relevance: From Dicarboxylic Acids to Complex Mixtures. Chemical Reviews 2015 115 (10), 4115-4156 DOI: 10.1021/cr5005502

Specific Comments

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

Response: Presently they cannot. We have added the following line to the table caption:*' Please note, CAS numbers cannot be used directly in the prediction facility.'*

Referee comment:. *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?*

Response: Yes this is correct. We have limited the number of compounds for different predictions due to computational burden and delays on providing results. We have added the following text to this sentence:*'[..] at any one time via the web portal'.*

Referee comment:. *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*

Response: This has now been added.

Referee comment:. *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-points*

Response: This has now been added.

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Referee comment: *Figure 3: A key to the axis labels should be provided in the caption*
Response: This has now been added.

Referee comment: *Figure 3: It may make more sense to combine both plots and use different marker symbols to represent each vapor pressure prediction*
Response: This has been changed.

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.***Referee comment:*** *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.

Response:*This has been changed and added to the line 'Equilibrium absorptive partitioning [. . .]' in section 3.*

Technical Corrections
Referee comment: *Page 9676, line 10: "xx" was never replaced with a number*
Response: *This has now been corrected.*

Referee comment: *Page 9678, line 16: the quantity in parenthesis should be raised to a power of -1*
Response: *This has now been corrected.*

Referee comment: *Page 9681, line 13: "re-partitioning" should be "re-partition"*
Response: *This has now been corrected.*

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Referee comment: *Page 9705: there should be a space after "size" in the first line of the figure caption*
Response: *This has now been corrected.*

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

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