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UManSysProp: an online facility for molecular property prediction and atmospheric aerosol calculations

D. Topping^{1,2}, M. H. Barley², M. Bane³, N. Higham⁴, B. Aumont⁵, and G. McFiggans²

¹National Centre for Atmospheric Science, Manchester, UK

²Centre for Atmospheric Science, University of Manchester, Manchester, UK

³Research IT, IT Services, The University of Manchester, Manchester UK

⁴School of Mathematics, University of Manchester, Manchester, UK

⁵LISA, UMR CNRS 7583, Université Paris Est Creteil et Université Paris Diderot, Creteil, France

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Correspondence to: D. Topping (david.topping@manchester.ac.uk)

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GMDD

8, 9669–9706, 2015

UManSysProp

D. Topping et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Abstract

In this paper we describe the development and application of a new web based facility, UManSysProp (<http://umansysprop.seaes.manchester.ac.uk>), for automating predic-
5 tions of molecular and atmospheric aerosol properties. Current facilities include: pure component vapour pressures, critical properties and sub-cooled densities of organic molecules; activity coefficient predictions for mixed inorganic–organic liquid systems; hygroscopic growth factors and CCN activation potential of mixed inorganic/organic aerosol particles; absorptive partitioning calculations with/without a treatment of non-
10 ideality. The aim of this new facility is to provide a single point of reference for all properties relevant to atmospheric aerosol that have been checked for applicability to atmospheric compounds where possible. The group contribution approach allows users to upload molecular information in the form of SMILES strings and UManSysProp will automatically extract the relevant information for calculations. Built using open source chemical informatics, and hosted at the University of Manchester, the facilities are pro-
15 vided via a browser and device-friendly web-interface, or can be accessed using the user's own code via a JSON API. In this paper we demonstrate its use with specific examples that can be simulated using the web-browser interface.

1 Introduction

The many thousands of individual aerosol components ensure that explicit manual cal-
20 culation of properties that influence their environmental impacts is laborious and time-consuming. The emergence of explicit automatic mechanism generation techniques (Aumont et al., 2005; Jenkin et al., 2012), including up to many millions of individual gas phase products as aerosol precursors, renders manual calculations impossible and automation is necessary. For example, both inorganic and organic material can transfer
25 between the gas and particle phase. Inorganic electrolytes are restricted to a few well-understood compounds. However, organic material can comprise many thousands of

GMDD

8, 9669–9706, 2015

UManSysProp

D. Topping et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



compounds with potentially a vast range of properties (Hallquist et al., 2009). Predicting the evolution of aerosol requires calculating the distribution of all components between the gas and aerosol phase according to equilibrium partitioning or disequilibrium mass transfer. Either treatment requires knowledge of all component vapour pressures and other thermodynamic properties. In the moist atmosphere, the most abundant material that can readily interact with aerosol particles is water vapour. The formation of atmospheric liquid water has a profound influence on the aerosol life cycle and climate. Predicting the hygroscopic response of complex inorganic–organic mixtures requires treatment of solution non-ideality, for example.

It can be difficult to establish what factors are responsible for the outcome of a model prediction. This is particularly true when the number of components might be high in, for example, SOA mass partitioning simulations. It then becomes difficult for others in the community to assess the results presented. This might be complicated by the need to include pure component vapour pressures or activity coefficient predictions for a wide range of highly multifunctional compounds. For example, predictions of aerosol hygroscopicity have either been based on simplified Kohler theory at one extreme (Kreidenweis et al., 2005) or thermodynamic equilibrium models at the other (Topping et al., 2005). It isn't clear to what extent replication of results is ever achieved for a range of aerosol simulations. Whilst this might also be an issue with results from instrumentation, the development of community driven software at least enables modellers to tackle this problem directly.

In this paper we describe the development and application of a new web based facility, UManSysProp, to tackle such issues. Current facilities include: pure component vapour pressures, critical properties and sub-cooled densities of organic molecules; activity coefficient predictions for mixed inorganic–organic liquid systems; hygroscopic growth factors and CCN activation potential of mixed inorganic/organic aerosol particles with associated Kappa-Kohler values (Kreidenweis et al., 2005); absorptive partitioning calculations with/without a treatment of non-ideality. UManSysProp automatically extracts the relevant information for calculations. Built using open-source chemical

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

informatics, described in Sect. 2, the facilities are provided via a browser and device-friendly web-interface. In Sect. 3, examples of each prediction are given along with reference to our existing publications that use these tools. Providing a wide range of comparisons between predictions and measurements of each property is outside of the scope of this paper given all of the potential subtleties associated with measurement data (e.g. Topping and McFiggans, 2012). Nonetheless, by providing a minimum set of examples for each case, the ability to perform such comparisons and act as the community's point of reference is demonstrated. Relevant inputs to replicate these examples are given in the text, with larger files to upload provided in the Appendix. If you want to access UManSysProp without using a web-browser we also provide a programmer friendly JSON API that enables you to call our suite of tools from your own code. This is described in detail on our ReadTheDocs.org webpage (<https://umansysprop.readthedocs.org/>) with an example provided in the Appendix.

2 Chemo-informatics base of UManSysProp

The discipline of chemo-informatics typically concerns the use of both software and computational hardware techniques applied to a range of problems in chemistry. The emergence of the open-source movement has led to a wealth of chemo-informatics software made available, including OpenBabel, which acts as the molecular parsing software behind the service described here. OpenBabel (O'Boyle et al., 2008) is a cross-platform suite of tools. Features include the ability to interchange chemical file formats and sub-structure searching, the latter particularly relevant. For more information, the reader is referred to the OpenBabel wiki (<http://openbabel.org/>).

OpenBabel comes with wrappers for numerous languages including Perl, Ruby, Java and Python. Here we use the Python extensions of OpenBabel, Pybel, with the Flask (<http://flask.pocoo.org/>) python web-application framework to provide a user friendly and device compatible interface. Figure 1 displays a basic schematic of user interaction

with the site to perform specific calculations for a compound represented as a SMILES string.

All calculations rely on a representation of individual compounds, be it inorganic ions or neutral organic molecules. Raw model or measurement molecular information needs to be converted into an appropriate format for use in property predictions. Common molecular file formats include Wiswesser Line Notation (WLN), ROSDAL and SYBL. In addition, IUPAC and NIST recently developed the IUPAC International Chemical Identifier (InChI). Another linear notation using short ASCII strings is the SMILES format (Simplified Molecular Input Line Entry System), a simplified chemical notation that allows a user to represent a two dimensional chemical structure in linear textual form. For example, the SMILES notation for carbon dioxide is O=C=O, whereas cyclohexane is represented as C1CCCCC1. UManSysProp uses SMILES for several reasons. The notation is commonly employed in commercial and public software for prediction of chemical properties. It can be imported by most molecule editors for conversion into 2-D/3-D models and has a wide base of software support and extensive theoretical backing (www.daylight.com). Common database searches for organic molecules include NIST (<http://webbook.nist.gov/chemistry/>) and the National Chemical Database service (<http://cds.rsc.org/>). From these, the SMILES representation of individual molecules can be found. In Table 1, SMILES for common inorganic ions are provided along with a selection of organic compounds used by O'Meara et al. (2014) in their saturation vapour pressure review paper. The CAS registry number, a unique identifier assigned to every chemical substance described in the open scientific literature, is also given. SMILES and CAS numbers can often be used interchangeably for searching specific compounds on the internet.

Parsing

To use the SMILES format requires the ability to extract substructure information from each string that is meaningful to each property predictive technique. OpenBabel has the ability to filter and search molecular files using the SMARTS format (created by

GMDD

8, 9669–9706, 2015

UManSysProp

D. Topping et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Daylight Chemical Information Systems, Inc alongside the SMILES format). One can understand the role of SMARTS in the following sequential bullet points:

- Estimation methods within UManSysProp are based on the group contribution method.
- Groups must therefore be automatically and unambiguously inferred from the SMILES strings.
- SMARTS strings are used within UManSysProp to identify all groups (or substructures) required to estimate all provided properties.
- The nomenclature for SMARTS string is described in the daylight theory webpages with many examples (www.daylight.com).
- Caution was given to identify the appropriate SMARTS string matching the groups (descriptors) included in the various predictive techniques selected within UManSysProp.

Regarding the last point, it is important to note that the SMARTS used are highly specific to the property estimation method. For example, the canonical and isomeric SMILES string for Succinic acid is C(CC(=O)O)C(=O)O. By visiting the Daylight Theory webpage, generic examples on a variety of SMARTS are given, copied into Table 2.

Caution must be used however with such generic SMARTS, depending on the expected range of molecules to be passed by the parsing routine. For techniques used in UManSysProp, an extensive manual analysis of compounds used in the MCM (Jenkin et al., 2012), and a subset of GECKO mechanism (Aumont et al., 2005), were used to validate derived SMARTS libraries. Table 3 is replicated from the Supplement of Barley et al. (2011) to illustrate the careful design of SMARTS for the vapour pressure technique by Nannoolal et al. (2008), hereafter referred to as the “Nannoolal” method. As noted in that paper, whilst it is “easy” to identify all primary alcohols (SMARTS “a” in the table), the Nannoolal method requires primary alcohols to be split between NG 35

GMDD

8, 9669–9706, 2015

UManSysProp

D. Topping et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



(carbon chain of 5 or more atoms with nomenclature defined in Nannoolal et al., 2008) and NG 36 (primary alcohols on a C4 or smaller chain) although the exact criteria for this split is not clear in the literature. For our applications, the allocation of primary alcohols is achieved using a set of five SMARTS. Each predictive technique then has an appropriate library of SMARTS (Fig. 2). What happens if a technique does not capture all features of a molecule that might be passed for parsing? For example, as noted by Barley et al. (2011), alcohol groups attached to a carbon-carbon double bond (vinyl alcohols) are not covered by the Nannoolal method. SMARTS “D” in Table 3 are used to identify vinyl alcohols which are then treated like secondary alcohols within the predictive technique. For the AIOMFAC activity coefficient model (Zuend et al., 2008), care has been taken with the use of specific CH_n-OH interaction terms. In the literature there are multiple choices for parameters representing these groups. For AIOMFAC, the distinction of the terms presented by Marcolli and Peter (2005) are only made in the case of pure alcohols and polyols, whereas in other cases the specific CH_n groups are dropped. In the case of pure alcohols/polyols the categorisation of groups is solved by assuming all alkyl CH_n are in a hydrocarbon tail unless (a) they bear an -OH group, (b) they are a methyl group attached to a CH_n bearing an -OH group; and (c) they are in a ring, aromatic, C=C or C#C group (A. Zuend, personal communication, 2010).

3 Calculations currently provided

The facilities provided on UManSysProp are split into pure component properties and predictions of bulk and single particle aerosol behaviour. Pure component properties are limited to 5000 compounds, predictions involving activity coefficients limited to 1000 compounds. Limitations on the number for species are largely down to computational cost considerations for calculations involving activity coefficients. Optimising these calculations using external computational accelerators including GPUs is the subject of ongoing work and will be reported in a future publication. These are listed below along with the associated options, as displayed on the homepage:

GMDD

8, 9669–9706, 2015

UManSysProp

D. Topping et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



- HTML (view in web browser)
- Excel file
- Python pickle file (<https://docs.python.org/2/library/pickle.html>)
- XML file (<http://en.wikipedia.org/wiki/XML>)
- 5 – Zipped CSV file
- JSON file (<http://en.wikipedia.org/wiki/JSON>)

The provision of any given property predictive technique on the portal is dictated by it having been subject to the peer review process where possible. For the pure component properties, this has included a critical review of vapour pressure (O'Meara et al., 2014) and density techniques (Barley et al., 2013). The activity coefficient methods 10 AIOMFAC (Zuend et al., 2008) and UNIFAC (Fredenslund et al., 1975) are discussed extensively in the literature. The theory behind hygroscopic growth calculations and absorptive partitioning simulations are also extensively covered in various papers (e.g. McFiggans et al., 2010), with appropriate references provided on the website.

15 3.1 Pure component properties

Figure 3 displays the range of pure component vapour pressure predictions for a random subset of 30 compounds derived from the MCM compound dataset studied by Barley et al. (2011) at 298.15 K. To generate the data, after clicking on the link to “Pure component vapour pressures of organic compounds”, a text-file with SMILES 20 string was uploaded using the “upload” facility. The graph was created separately using the IgorPro package, the predictive techniques covering the combined vapour pressure and boiling point methods of Nannoolal et al. (2008) and Nannoolal et al. (2004) (Vp(N)Tb(N)), Nannoolal et al. (2008) and Joback and Reid (1987) (Vp(N)Tb(JR)) and Myrdal and Yalkowsky (1997) with Stein and Brown (1994) (Vp(MY)Tb(SB)). The list of

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[⏪](#)[⏩](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

SMILES is provided in Table A1 for replicating the results. Simply copy and paste the SMILES provided and save as a text file to upload. The figure highlights general features discussed in the recent review by Bilde et al. (2015) in which the use of the boiling point method by Joback and Reid (1987) leads to much lower values, the discrepancy between all methods increasing as the vapour pressures decrease.

Figure 4 displays a range of pure component density predictions, for the methods reviewed by Barley et al. (2013), for the same 30 MCM compound dataset at 298.15 K. As with the vapour pressure predictions, after clicking on the link to “Sub cooled liquid density” link on the homepage, a text-file with SMILES string was uploaded using the “upload” facility.

3.2 Bulk partitioning predictions and single particle hygroscopic growth factors

For predictions of absorptive partitioning, the molar based partitioning model described by Barley et al. (2011) is used (Eqs. 1–3):

$$C_{\text{OA}} = \sum_i C_i \varepsilon_i \quad (1)$$

$$\varepsilon_i = \left(1 + \frac{C_i^*}{C_{\text{OA}}} \right) \quad (2)$$

$$C_i = \frac{10^6 \gamma_i P_i^o}{RT} \quad (3)$$

where C_i is the total loading of component i ($\mu\text{mol m}^3$), P_i^o is the saturation vapour pressure of component i (atm), R is the ideal gas constant ($8.2057 \times 10^{-5} \text{ m}^3 \text{ atm mol}^{-1} \text{ K}^{-1}$), T is the temperature (K), γ_i is the activity coefficient of component i in the liquid phase and C_i^* is the effective saturation concentration of component i ($\mu\text{mol m}^3$). To the best of our knowledge, only Schell et al. (2001) refer to using Newtons method for solving

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[⏪](#)[⏩](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

the equilibrium concentration. For the case of ideal solution thermodynamics ($\gamma_i = 1$), the root of the partitioning Eq. (1) is similarly solved here using Newton's method. This is applicable to any number of components and typically this results in 6–10 iterations to arrive at a solution for the total molar concentrations of secondary organic material. When including non-ideality, an iterative method is used where the value of C_{OA} is nudged at each iteration using a weighted average of the previous value. As before, the final solution satisfies the constraint that chemical potentials are equal for each component. On UManSysProp it is possible to include an inorganic core by specifying concentrations of the ions. The user can assume solution ideality or non-ideality by selecting the appropriate selection from the drop-down menu. In all cases it is assumed that concentrations of the ions remain fixed and there is no loss of semi-volatile components such as nitric or hydrochloric acid. These will be added in a future release, along with an account for multiple liquid phase partitioning (see Sect. 4). In addition, it is possible to specify the concentration of an unidentified water soluble or water insoluble compound with a specific molecular weight that is included in the partitioning calculations.

As an example, Table 4 displays the predicted equilibrium SOA mass loadings using the 30 most abundant compounds within a scaled biogenic simulation described by Barley et al. (2011) using the MCM. For our simulation we kept the temperature at 298.1 K, varying the relative humidity between 50 and 90 %. A $2 \mu\text{g m}^{-3}$ core, with variable inorganic composition defined in Table 3, was used to demonstrate the effect of assuming solution non-ideality with full inorganic–organic interactions, using the AIOM-FAC model (Zuend et al., 2008), or assuming ideality. For the vapour pressure predictions, the vapour pressure and boiling point techniques of Nannoolal et al. (2008) and Nannoolal et al. (2004) were used. To conduct the partitioning simulations, the input file consists of the SMILES string of each compound in the left hand column and total concentration, in molecules cc^{-1} , in the right hand column. For a given relative humidity (RH), the abundance of water vapour and saturation vapour pressures are calculated implicitly as described in Barley et al. (2011). The input file used in these simulations

can be found in Table A2. To replicate the predicted non-ideal mass at 50 % RH click on the equilibrium absorptive partitioning link. To add an $(\text{NH}_4)_2\text{SO}_4$ inorganic core, first enter the SMILES string for the ammonium ion $[\text{NH}_4^+]$ in the text entry box for “inorganic ions” with a concentration of $0.0303 \mu\text{mol m}^{-3}$. Next, click on the “Add” button to create another entry for the sulphate ion. Enter the SMILES string $[\text{O-}]\text{S}(=\text{O})(=\text{O})[\text{O-}]$ in the text entry box with a concentration of $0.0151 \mu\text{mol m}^{-3}$, consistent with a concentration of $2 \mu\text{g m}^{-3}$ $(\text{NH}_4)_2\text{SO}_4$ core. For the organic compound click on the “upload file” option and select the text file created from information provided in the Appendix. In the options for “Interaction model” select “Assume non-ideal interactions” using the AIOM-FAC model, using the default Vapour pressure method options. Click on the “Calculate” button to retrieve predictions of total mass loadings, concentration of each component in the condensed phase and its activity coefficient. Results in Table 4 demonstrate the influence of assuming ideality, or not, on calculated mass loadings as a function of RH. Whilst all cases demonstrate an increase in mass at higher humidities (Topping and McFiggans, 2012), the composition of the core has a noticeable effect on the magnitude of “salting in” relative to the inert non-ideal test case. Following Topping et al. (2013), the assumption of solution non-ideality acts to “buffer” the increase in mass relative to the ideal test case. Note that each scenario will be sensitive to the range of functionalities in compounds of interest, the relative abundance of each condensate (Topping and McFiggans, 2012) and the volatility profile (Topping et al., 2013), the example here simply acting as an example of how to use the partitioning simulations in UManSysProp. Figure 5 displays the range of predicted activity coefficients for each organic compound at equilibrium as a function of RH and predicted saturation vapour pressure for the same scenario with an NaCl core. We have plotted the range of activity coefficients as a function of predicted P_{sat} as an illustration that, for specific cases, there may be no general trend, despite attempts in the literature to generalise more complex mixtures (Donahue et al., 2011). In this case, at higher RH, the activity coefficients of each component increases, explaining the reduced predicted mass compared to the ideal case for this specific simulation.

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[⏪](#)[⏩](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

Predictions of aerosol hygroscopicity have been covered extensively in the literature, ranging from detailed explicit thermodynamic models (Topping et al., 2005) to empirically determined parameter representations of water uptake (Kreidenweis et al., 2005). Topping and McFiggans (2012) discussed the potential problems associated with co-condensation of organic semi-volatile compounds on retrieved hygroscopicity in instruments and potential effects on cloud microphysics (Topping et al., 2013). The true effect of semi-volatile partitioning can only be predicted using a dynamic framework that accounts for the amount of absorptive mass, size dependencies through the Kelvin effect and instrument configuration. Rather than provide full dynamic simulations, users are provided with a “potential” for semi-volatile loss from the assumed fixed non-aqueous composition through provision of equilibrium vapour pressures above the solution. UManSysProp hygroscopicity calculations assume water is the only compound that can re-partitioning between the gas and condensed phase, providing growth factors, Kappa Kohler values, solute mass fraction and equilibrium vapour pressures above the solution. Figure 6 displays predicted growth factors and Kappa Kohler values, using the AIOMFAC activity coefficient model, for $(\text{NH}_4)_2\text{SO}_4$, and NaCl at 3 dry diameters of 100, 50 and 20 nm assuming a surface tension of 72.224 mN m^{-1} . In each case the relative molar concentration of ions must be used to define the “dry” composition. For example, for $(\text{NH}_4)_2\text{SO}_4$, the SMARTS $[\text{NH}_4^+]$ and $[\text{O}^-]\text{S}(=\text{O})(=\text{O})[\text{O}^-]$ with relative molar concentrations of 2.0 and 1.0 are used and simulations run across a range of relative humidities from 50 to 95 %.

Solute mass fractions are often compared to measurements derived from an Electrodynamic Balance, or EDB. Figure 7 compares the predicted mass increase with the measured data presented by Choi and Chan (2002) for an equimolar $(\text{NH}_4)_2\text{SO}_4$ –Glutaric acid solutions. For more complex systems, Table 5 displays the variable growth factor, with and without solution non-ideality, between 50 to 90 %RH, of a mixed aerosol comprised of $(\text{NH}_4)_2\text{SO}_4$ and the 90 organic compounds, assuming an equimolar mixture, presented by O’Meara et al. (2014) for their vapour pressure predictive technique evaluation study. The inputs used for these simulations can be found in Table A3.

[Title Page](#)
[Abstract](#)
[Introduction](#)
[Conclusions](#)
[References](#)
[Tables](#)
[Figures](#)

[Back](#)
[Close](#)
[Full Screen / Esc](#)
[Printer-friendly Version](#)
[Interactive Discussion](#)


Predictions of CCN activation potential are also provided. In these calculations, the maximum point of the Kohler curve is calculated using the secant method since the Kohler curve function is continuous and has only one maximum when water is the only semi-volatile allowed to re-equilibrate. Table 6 displays predicted Kappa Kohler values derived from the predicted critical point for an equimolar Succinic acid–(NH₄)₂SO₄ aerosol, and the two separate components, setting the surface tension to 72 mN m^{−1} as a function of dry size. Kappa Kohler values assuming solution ideality are also given, the values constant as one would expect without accounting for the effect of molecular interactions. This simply demonstrates that by using the AIOMFAC activity coefficient model, even at the point of activation there is a significant deviation from ideality, due to organic–inorganic interactions, in a system in which solutes are “forced” to remain in the condensed phase. As stated in the introduction, it is not the purpose of this paper to provide a full sensitivity analysis of such effects but rather provide researchers with the facility to do similar in specific case studies. Following Topping and McFiggans (2012), we also provide predictions of the equilibrium vapour pressure of the organic solutes, when present, to assess the potential for evaporation or condensation, similar to the predictions of sub-saturated hygroscopicity.

4 Future work

Alongside relevant property predictive techniques, all current aerosol particle predictions are based on equilibrium thermodynamics with single particle or bulk representations. Whilst providing useful insights into the role of composition dependent processes, capturing the evolution of an aerosol population requires dynamic ensemble frameworks (Topping et al., 2013). To meet these demands, future capabilities will include gas-particle box-model frameworks with a range of complexity with regards to the number of compounds and processes included in calculations. Regarding the latter aspect, current work involves profiling the use of external computational accelerators for mitigating the cost of accounting for solution non-ideality in future variants of

UManSysProp to increase the maximum number of compounds allowed in subsequent calculations.

Appendix: Accessing predictions outside of a web-browser

Here we provide brief details on how to call UManSysProp from your own code, without the need for a web-browser. For full details, please refer to our documentation on our ReadTheDocs.org webpage (<https://umansysprop.readthedocs.org/>). It is recommended that you use the local client installation UManSysProp from within the IPython shell. This is simply because the API is designed with documentation built in which can be queried from within the environment, and this is considerably easier from within the IPython shell. The client component of UManSysProp can be installed on any machine with Python available, provided you have Python 2.7 or greater. On Ubuntu, the waveform PPA can be used for simple installation:

```
$$ sudo add-apt-repository ppa:waveform/ppa
$$ sudo apt-get update
15 $$ sudo apt-get install python-umansysprop
```

On other platforms, the package can be installed from PyPI. Specify the client option to pull in all dependencies required by the client component:

```
$$ sudo pip install "umansysprop[client]"
```

The first step in using the UManSysProp system is creating a UManSysProp instance, as demonstrated in the Python code snippet given below. By default this requires the URL of the UManSysProp server. Currently this is <http://umansysprop.seaes.manchester.ac.uk>.

```
>>>import umansysprop.client
>>>client = umansysprop.client.UManSysProp
```

GMDD

8, 9669–9706, 2015

UManSysProp

D. Topping et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



(<http://umansysprop.seaes.manchester.ac.uk>)

Once you have a client instance, you can query it to find out what methods are available from the web API. Within the IPython shell this can be done simply by entering client. and pressing the Tab key twice. Alternatively, the following one-liner in the regular

5 Python shell can be used to query non-private methods:

```
>>>[m for m in dir(client) if not m.startswith('_')]
>>>['absorptive_partitioning', 'sub_cooled_density', 'test', 'vapour_pressure']
```

Once you have selected a method to call you can discover what parameters it takes and what it expects in those parameters by querying the method's documentation.

10 Within the IPython shell this can be viewed simply by appending ? to the method name. Alternatively, the help() function can be used in a regular Python shell:

```
>>>help(client.vapour_pressure)
Help on method vapour_pressure in module umansysprop.client:
client.vapour_pressure(self, compounds, temperatures, vp_method,
15 bp_method)...
Calculates vapour pressures for all specified *compounds*
(given as a~sequence of SMILES strings) at all given
*temperatures* (a~sequence of floating point values giving
temperatures in degrees Kelvin). The
20 *vp_method* parameter is one of the strings:

* 'nannoolal'
* 'myrdal_and_yalkowsky'
* 'evaporation'...
```

25 The documentation for each tool can viewed on the UManSysProp API documentation page. Calling any of the tools will (in the event of success, given a valid SMILES or temperature quantity, for example) return a Result instance. This is simply a list() which contains a sequence of Table instances. Each table has a name and this can be used to access the table in the owning Result list. For example:

```
30 >>>result = client.vapour_pressure(['CCCC', 'C(CC(=O)O)C(=O)O',
' C(=O)(C(=O)O)O'], [298.15, 299.15, 300.15, 310.15], 'nannoolal',
```

9684

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion




```
'nannoolal')
>>> result
[<Table name="pressures">]
>>> result.pressures
5 <Table name="pressures">
```

Table instances have a friendly string representation which can be used at the command line for quick evaluation of the contents:

```
>>> print(result.pressures)
      |          CCCC | C(CC(=O)O)C(=O)O | C(=O)(C(=O)O)O
10 ---+-----+-----+-----+
298.15 | 0.220914923012 | -6.33293991048 | -5.19636054531
299.15 | 0.235479319348 | -6.28117761855 | -5.15170377256
300.15 | 0.249933657549 | -6.22986499517 | -5.10742877511
310.15 | 0.388688301563 | -5.74023509659 | -4.68464352888
```

15 *Acknowledgements.* The authors would like to acknowledge NERC grants NE/H002588/1, NE/J009202/1 and NE/J02175X/1 for enabling Mark Barley to perform SMARTS library constructions and property prediction comparisons. Topping was similarly funded through the National Centre for Atmospheric Science (NCAS). The authors would also like to thank Andreas Zuend, of McGill University, for his discussions on automating functional group selections for the AIOMFAC method. The authors would also like to thank David Hughes, of Waveform Computing Ltd Manchester UK, for constructing the UManSysProp web framework.

20

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Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

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[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[⏪](#)[⏩](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

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[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)**Table 1.** Example SMILES of common inorganic ions and organic compounds with associated CAS numbers.

Compound name	SMILES strings SMILES string	CAS number
Hydrogen ion	[H+]	12408-02-5
Ammonium ion	[NH4+]	14798-03-9
Sodium ion	[Na+]	7440-23-5
Calcium ion	[Ca+2]	7440-70-2
Sulphate ion	[O-]S(=O)(=O)[O-]	14808-79-8
Nitrate ion	[N+](=O)([O-])[O-]	14797-55-8
Chloride ion	[Cl-]	16887-00-6
Tridecanoic acid	O=C(O)CCCCCCCCCCCC	638-53-9
Tetradecanoic acid	CCCCCCCCCCCCC(=O)O	544-63-8
Oxalic Acid	C(=O)C(=O)O	144-62-7
Malonic acid	C(C(=O)O)C(=O)O	141-82-2
2-methyl malonic acid	O=C(O)C(C(=O)O)C	516-05-2
2-hydroxy malonic acid (tartonic)	O=C(O)C(O)C(=O)O	80-69-3
2-keto succinic acid	O=C(O)C(=O)CC(=O)O	328-42-7
Glutaric acid	C(CC(=O)O)CC(=O)O	110-94-1
Adipic acid	C(CCC(=O)O)CC(=O)O	124-04-9
1,1-cyclopropane dicarboxylic acid	O=C(O)C1(C(=O)O)CC1	598-10-7
1,1-cyclobutane dicarboxylic acid	O=C(O)C1(C(=O)O)CCC1	5445-51-2
nitrocatechol	N(=O)(=O)c1cc(O)c(O)cc1	3316-09-4
levoglucosan	C1C2C(C(C(O1)O2)O)O	498-07-7
1,2-Pentanediol	OCC(O)CCC	5345-92-0
3,5-di-tert-Butylcatechol	Oc1c(cc(cc1O)C(C)C)C(C)C(C)C	1020-31-1
Ethyl vanillin	O=Cc1cc(OCC)c(O)cc1	121-32-4
Eugenol	Oc1ccc(cc1OC)CC=C	97-53-0
Glycerine carbonate	O=C1OCC(O1)CO	931-40-8
Heliotropin	c1cc2c(cc1C=O)OCO2	120-57-0
Pinonaldehyde	O=CCC1CC(C(=O)C)C1(C)C	2704-78-1
Tetraethylene glycol	OCCOCCOCCOCCO	112-60-7
Triacetin	CC(=O)OC(COC(=O)C)COC(C)=O	102-76-1

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)**Table 2.** Generic SMARTS strings taken from the Daylight information webpage.

SMARTS	Description
[CH2]	aliphatic carbon with two hydrogens (methylene carbon)
[!C;R]	(NOT aliphatic carbon) AND in ring
[!C;!R0]	same as above (“!R0” means not in zero rings)
[c,n&H1]	any aromatic carbon OR H-pyrrole nitrogen
[35*]	any atom of mass 35

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)**Table 3.** SMARTS for Nanoolal groups, as copied from the Supplement of Barley et al. (2011).

Functional group	Nannoolal group	SMARTS
A -COOH	NG 44	a: -[#6][CX3]=[OX1]][OX2;H1]
B -OOH	New group	a: -[#6;!\$([CX3]=[OX1]))][OX2][OX2;H1]
C -OH (primary)	NG 35 or NG 36	a: -[OX2;H1][CX4;H2,H3] b: -[OX2;H1;!\$(O[#6][#6,#7,#8][#6,#7,#8][#6])][CX4;H2,H3;!\$(O[#6][#6,#7,#8][#6,#7,#8][#6,#7,#8][#6])] c: [OX2;H1;!\$(O[#6][#6,#7,#8][#6,#7][[#6][#6])][CX4;H2,H3;!\$(O[#6][#6,#7,#8][#6,#7][[#6][#6])] d: -[OX2;H1;!\$(O[#6][#6,#7][[#6][#6])][#6,#7,#8][#6])][CX4;H2,H3;!\$(O[#6][#6,#7][[#6][#6])][#6,#7,#8][#6])] e: -[OX2;H1;!\$(O[#6][#6][[#6][#6])][#6])][CX4;H2,H3;!\$(O[#6][#6][[#6][#6])][#6])]
D -OH (vinyl)	assigned to OH (sec) NG 34	[OX2;H1;\$([OX2;H1][CX3]=[CX3])]

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[⏪](#)[⏩](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

Table 4. Predicted total organic mass loadings ($\mu\text{g m}^{-3}$) from the most abundant 30 compounds generated from a gas phase degradation mechanism including both ideal and non-ideal solution thermodynamics. The composition of the core, with an abundance of $2 \mu\text{g m}^{-3}$, along with the assumption of solution ideality/non-ideality, is given above each column. For the “inert core” a molecular weight of 200 g mol^{-1} was used, with solution thermodynamics accounting for interactions only between water and organic condensates.

RH (%)	$(\text{NH}_4)_2\text{SO}_4$ [non-ideal]	NaCl [non-ideal]	NH_4NO_3 [non-ideal]	Inert core [non-ideal]	Inert core [ideal]
50	0.1181	0.2371	0.2179	0.0045	0.1547
60	0.1164	0.2157	0.1771	0.0054	0.1965
70	0.1260	0.2354	0.1655	0.0070	0.2691
80	0.1584	0.3138	0.1867	0.0104	0.4261
90	0.2845	0.5807	0.3104	0.0206	1.0008

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

Table 5. Variable growth factor, with and without solution non-ideality, between 50 to 90 % RH, of a mixed aerosol comprised of $(\text{NH}_4)_2\text{SO}_4$ and the 90 organic compounds, assuming an equimolar mixture, presented by O'Meara et al. (2014) for their vapour pressure predictive technique evaluation study.

RH (%)	GF (non-ideal)	Kappa (non-ideal)	GF (ideal)	Kappa (ideal)
50	1.0249	0.0796	1.0379	0.1226
60	1.0323	0.0698	1.0554	0.1226
70	1.0414	0.0589	1.0829	0.1226
80	1.0534	0.0461	1.1322	0.1226
90	1.0715	0.0302	1.2496	0.1226

Table 6. Predicted Kappa Kohler values, with and without accounting for solution non-ideality, derived from the predicted critical point for an equimolar Succinic acid– $(\text{NH}_4)_2\text{SO}_4$ aerosol, and the two separate components, setting the surface tension to 72 mN m^{-1} as a function of dry size.

Dry size (nm)	Kappa		Critical saturation ratio (%)			
	Succinic– $(\text{NH}_4)_2\text{SO}_4$	$(\text{NH}_4)_2\text{SO}_4$	Succinic	$(\text{NH}_4)_2\text{SO}_4$ - 72 mN m^{-1}	$(\text{NH}_4)_2\text{SO}_4$ - 50 mN m^{-1}	
100	0.6585	0.6317	0.3443	0.1463	0.0835	
200	0.6824	0.6646	0.3473	0.0505	0.0290	
300	0.6920	0.6788	0.3481	0.0272	0.0156	
400	0.6973	0.6869	0.3485	0.0176	0.0101	
500	0.7007	0.6922	0.3486	0.0125	0.0072	
600	0.7032	0.6961	0.3487	0.0095	0.0055	
700	0.7050	0.6989	0.3488	0.0075	0.0043	
800	0.7064	0.7012	0.3489	0.0062	0.0035	
900	0.7075	0.7030	0.3489	0.0051	0.0030	
1000	0.7085	0.7045	0.3489	0.0044	0.0025	
Ideal Kappa values						
	0.4331	0.7235	0.3490			

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

I◀

▶I

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Table A1. To replicate the predicted vapour pressure and density predictions covered in Sect. 3.1, copy and paste these SMILES strings into a text file and follow the procedures outlined in the main body of text. Be sure to copy just the SMILES strings.

SMILES string
COO
CC1(C2CCC(=O)C1C2)C
C(C(=O)OON(=O)=O)C1C(C(C(=O)C)C1)(C)C
CC(=O)OO
CCO
C(=O)(OON(=O)=O)CO
C1(C(C(CG=O)C1)(C)C)C(=O)C
CC(=O)C=C
C(=O)O
C=C(C)C=C
CC(=O)CO
C12C(C(CC(C1(C)OO)O)C2)(C)C
O=C1C2CC(C(=O)C1)C2(C)C
CC(=O)O
OOC1(CCC2C(C1C2)(C)C)CO
CC1(C2CCC(CO)(C1C2)ON(=O)=O)C
OCC(=O)C(C)(C)O
CC(=O)C
C(OO)C1C(C(C(=O)C)C1)(C)C
CCCC
O=CCC(=O)OON(=O)=O
CC=O
OCC(C=C)(C)OO
CC(=O)OON(=O)=O
N(=O)(=O)OC
OCC(=O)O
C12C(C(CC=C1C)C2)(C)C
C(O)C1C(C(C(=O)C)(C1)OO)(C)C
C(O)C=O
C=O

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

Table A2. SMILES strings and molecular abundance used for the partitioning predictions presented in Sect. 3.2. To replicate the results, copy and past both SMILES and abundance information into a text file and following the procedures outlined in the main body of text. Please ensure there is space between a given SMILES string and the abundance.

SMILES string	
CC(=O)C	3.94381 E + 11
C=O	1.69175 E + 11
CC(=O)CO	79083500000
CC(=O)OON(=O)=O	77758900000
N(OC)(=O)=O	465002000
CC(=O)O	43340464110
C(O)C=O	42707600000
COO	35736100000
CC1(C2CCC(=O)C1C2)C	30157700000
CC(=O)OO	27534600000
C(OON(=O)=O)(=O)CO	24247000000
CC(=O)C=C	22076400000
C=C(C)C=C	21243400000
O=C1C2CC(C(C1)=O)C2(C)C	20484500000
OOC1(CCC2C(C1C2)(C)C)CO	16366200000
CC1(C2CCC(CO)(C1C2)ON(=O)=O)C	13559600000
OCC(=O)C(C)C(O)	12492500000
CCCC	12475100000
CC=O	12241000000
OCC(C=C)(C)OO	11486200000
C12C(C(C-C=C1-C)C2)(C)C	11410300000
C(O)C1C(C(C(C)=O)(C1)OO)(C)C	11241600000
OCC(=O)O	10444600000
C(OO)C1C(C(C(C)=O)C1)(C)C	10090900000
C(C(=O)OON(=O)=O)C1C(C(C(C)=O)C1)(C)C	9914850000
CCO	9863210000
C1(C(C(CO)C1)(C)C)C(C)=O	9654730000
C(=O)O	9612616618
C12C(C(CO)C1(C)OO)C2(C)C	9447850000
O=CCC(=O)OON(=O)=O	9287460000
CC	9233180000
CO	9195410000

Table A2. Continued.

SMILES string	
<chem>C(=O)C=O</chem>	8495350000
<chem>CCC</chem>	8376030000
<chem>C12C(C(CC(C1(C)O)=O)C2)(C)C</chem>	8079110000
<chem>N(OC1(C2C(C(CC1O)C2)(C)C)(=O)=O</chem>	7921030000
<chem>CC1(C2C(C1C(=O)CC2=O)=O)C</chem>	7834600000
<chem>C=C(C)C=O</chem>	7401890000
<chem>OCC(=O)OO</chem>	7293180000
<chem>C=C1CCC2C(C1C2)(C)C</chem>	7086740000
<chem>CC(=O)C=O</chem>	6778590000
<chem>C=CC(C)(C)O</chem>	6760990000
<chem>C(ON(=O)=O)C1C(C(C(C)=O)C1)(C)C</chem>	6141130000
<chem>C=CC(=O)CO</chem>	6069190000
<chem>CC=C</chem>	5991610000
<chem>OCC(OO)(C)C(=O)CO</chem>	5955210000
<chem>OC(C(O)(C)C)COO</chem>	5722410000
<chem>CC(C(CC(CO)=O)=O)=O</chem>	5708910000
<chem>C=C(C(=O)OON(=O)=O)C</chem>	5368430000
<chem>C(=O)C1C(C(C(C)=O)C1)(C)C</chem>	5305790000
<chem>O(O)C1C(C(C(C)=O)C1)(C)C</chem>	5041190000
<chem>OCC(=O)C(C)=C</chem>	4959340000
<chem>CC(=O)C(=O)CC(=O)OON(=O)=O</chem>	4389470000
<chem>C#C</chem>	4266050000
<chem>CC(=O)CC</chem>	4186060000
<chem>C12C(C(CC(C1(C)O)ON(=O)=O)C2)(C)C</chem>	4173050000
<chem>CC1(C2CC(=O)C(C1C2)=O)C</chem>	4164890000
<chem>C(C(=O)O)C1C(C(C(C)=O)C1)(C)C</chem>	4046940000
<chem>CC(C)(C(=O)OON(=O)=O)O</chem>	4036600000
<chem>CC(C)C</chem>	4015740000
<chem>CCCCC</chem>	3826030000
<chem>O=C(C)CON(=O)=O</chem>	3736020000
<chem>OC-C=C(/C)-C=O</chem>	3691840000
<chem>C=C</chem>	3681720000
<chem>C12C(C(CC(C1(C)OO)ON(=O)=O)C2)(C)C</chem>	3630020000
<chem>C(=O)CC=O</chem>	3506730000
<chem>CC(C)(O)C=O</chem>	3384520000
<chem>OC-C(=C-C=O)-C</chem>	3319200000
<chem>C(C(C(CO)OO)=O)O</chem>	3247530000
<chem>CC1(C2CCC1C2)C</chem>	3165480000

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Table A3. 90 compounds used in an equimolar mixture in Sect. 3.2 for calculating mixed inorganic/organic growth factors. Once again, to replicate those results, copy and paste these SMILES, with equal molar concentrations, into a text file and follow the procedure covered in the main body of text.

SMILES string
<chem>O=C(O)CCCCCCCCCCCC</chem>
<chem>CCCCCCCCCCCCC(=O)O</chem>
<chem>O=C(O)CCCCCCCCCCCC</chem>
<chem>CCCCCCCCCCCCC(=O)O</chem>
<chem>O=C(O)CCCCCCCCCCCC</chem>
<chem>O=C(O)CCCCCCCCCCCC</chem>
<chem>O=C(O)CCCCCCCCCCCC</chem>
<chem>O=C(O)CCCCCCCCCCCC</chem>
<chem>O=C(O)CCCCCCCCCCCC</chem>
<chem>O=C(O)CCCCCCCCCCCC</chem>
<chem>O=C(O)C(=O)O</chem>
<chem>C(C(=O)O)C(=O)O</chem>
<chem>O=C(O)C(C(=O)O)C</chem>
<chem>O=C(O)C(O)C(=O)O</chem>
<chem>C(C(=O)O)C(=O)O</chem>
<chem>O=C(O)CC(C(=O)O)C</chem>
<chem>O=C(O)C(O)C(C(=O)O)</chem>
<chem>O=C(O)CC(O)C(=O)O</chem>
<chem>O=C(O)C(O)C(O)C(=O)O</chem>
<chem>C(C(C(=O)O)N)C(=O)O</chem>
<chem>O=C(O)C(=O)CC(=O)O</chem>
<chem>C(CC(=O)O)CC(=O)O</chem>
<chem>O=C(O)CCC(C(=O)O)C</chem>
<chem>O=C(O)CC(C)CC(=O)O</chem>
<chem>C(C(=O)O)C(C(=O)O)C(=O)O</chem>
<chem>C(C(C(=O)O)C(C(=O)O)N</chem>
<chem>O=C(O)C(=O)CCC(=O)O</chem>
<chem>O=C(O)CC(=O)CC(=O)O</chem>
<chem>C(CCC(=O)O)CC(=O)O</chem>
<chem>O=C(O)CCCCC(=O)O</chem>
<chem>O=C(O)CCCCCC(=O)O</chem>
<chem>c1ccc(c(c1)C(=O)O)C(=O)O</chem>
<chem>O=C(O)c1ccc(C(=O)O)c1</chem>
<chem>c1cc(ccc1C(=O)O)C(=O)O</chem>
<chem>O=C(O)C1(C(=O)O)CC1</chem>
<chem>O=C(O)C1(C(=O)O)CCC1</chem>
<chem>O=C(O)C1CCC1C(=O)O</chem>
<chem>O=C(O)C1CC(C(=O)O)CCC1</chem>
<chem>O=C(O)CCCCC(=O)O</chem>
<chem>O=C(O)CCCCCCCC(=O)O</chem>
<chem>O=C(O)CCCCCCCCC(=O)O</chem>
<chem>O=C(O)CC1CC(C(=O)O)C1(C)C</chem>
<chem>COc1ccc(cc1)C(O)=O</chem>
<chem>COc1cc(ccc1O)C(=O)O</chem>
<chem>O=C(O)c1cc(OC)c(O)c(OC)c1</chem>

Title Page

Abstract Introduction

Conclusions References

Tables Figures

◀ ▶

◀ ▶

Back Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Table A3. Continued.

SMILES string
<chem>N(=O)(=O)c1cc(O)c(O)cc1</chem>
<chem>C1C2C(C(C(C(O1)O2)O)O)O</chem>
<chem>O=C(O)c1ccccc1N(C)C</chem>
<chem>O=C(O)c1cc(N(C)C)ccc1</chem>
<chem>OCC(O)CCC</chem>
<chem>C(C(CO)O)O</chem>
<chem>C(CCO)CO</chem>
<chem>CNCCO</chem>
<chem>OC(C)CC(O)C</chem>
<chem>Cc1c(cccc1(N(=O)(=O)))N(=O)(=O)</chem>
<chem>C(CO)N</chem>
<chem>c1(N(=O)(=O))ccccc1N</chem>
<chem>Clc1c(cc(OC)c(O)c1OC)C=O</chem>
<chem>ClC(C(=O)O)C</chem>
<chem>c1ccc(c(c1)C(=O)O)O</chem>
<chem>COCOCOCOCc1ccccc1Br</chem>
<chem>O=C(O)CCc1ccccc1OC</chem>
<chem>COC=C(C=C(C=C1)CCC(=O)O)OC</chem>
<chem>Clc1ccc(cc1Cl)N(=O)(=O)</chem>
<chem>Clc1cc(O)c(O)cc1</chem>
<chem>Oc1e(cc(c1O)C(C)C)C(C)C</chem>
<chem>O=C(C)CCC(O)(C)C)C</chem>
<chem>COc1ccc(c(c1O)OC)Cl</chem>
<chem>Nc1cc(Cl)ccc1</chem>
<chem>N#CCCC</chem>
<chem>CCC(CC)(c1ccc(cc1)N(=O)(=O))N(=O)(=O)</chem>
<chem>O=C(O)c1ccccc1N(=O)O)c1</chem>
<chem>N(=O)(=O)c1ccccc1O)c1</chem>
<chem>O=C(O)c1ccc(N)cc1</chem>
<chem>COc1ccc(C=O)cc1</chem>
<chem>O=C(O)Cc1ccccc1)c2ccccc2O</chem>
<chem>CCCCOC(=O)c1ccccc1C(=O)OCCCC</chem>
<chem>O=Cc1cc(OCC)c(O)cc1</chem>
<chem>Oc1ccc(cc1OC)CC=C</chem>
<chem>O=C1OCC(O1)CO</chem>
<chem>c1cc2c(cc1C=O)OCO2</chem>
<chem>O=C(OCC(C)C)c1ccccc1O</chem>
<chem>O=C1C(CCC1)C2(O)CCCC2</chem>
<chem>O=C(O)Cc1ccccc1N</chem>
<chem>N(=O)(=O)c1c(c(cc(c1OC)C(C)C)C(C)N(=O)=O))C</chem>
<chem>OCCN(C)CCO</chem>
<chem>COc1ccc(cc1)C(C)=O</chem>
<chem>c1c(cc(c1O)O)O</chem>
<chem>O=CCC1CG(C(=O)C)C1(C)C</chem>
<chem>OCCOCCOCCOCCO</chem>
<chem>CC(=O)OC(COC(=O)C)COC(C)=O</chem>
<chem>N(=O)(=O)OCCOCCOCCO(N(=O)=O)</chem>

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



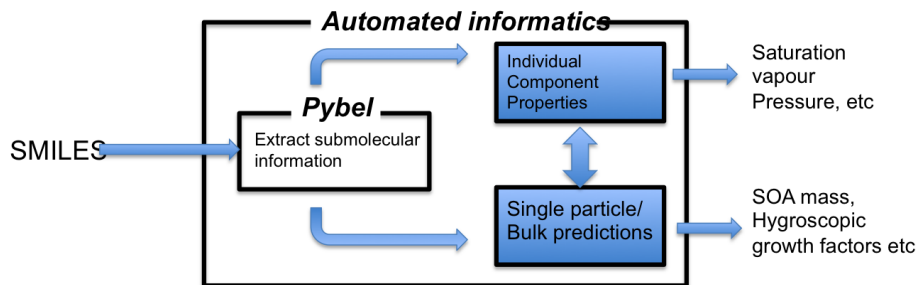


Figure 1. Workflow of calculations based on SMILES representation and the Pybel parsing module.

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

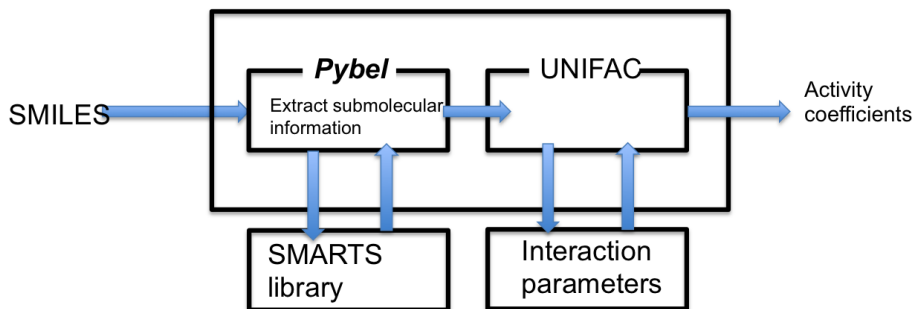


Figure 2. Workflow of activity coefficient calculations based on SMARTS libraries designed specifically for AIOMFAC (Zuend et al., 2008)/UNIFAC (Fredenslund et al., 1975).

[Title Page](#)

[Abstract](#)

[Introduction](#)

[Conclusions](#)

[References](#)

[Tables](#)

[Figures](#)

[⏪](#)

[⏩](#)

[◀](#)

[▶](#)

[Back](#)

[Close](#)

[Full Screen / Esc](#)

[Printer-friendly Version](#)

[Interactive Discussion](#)



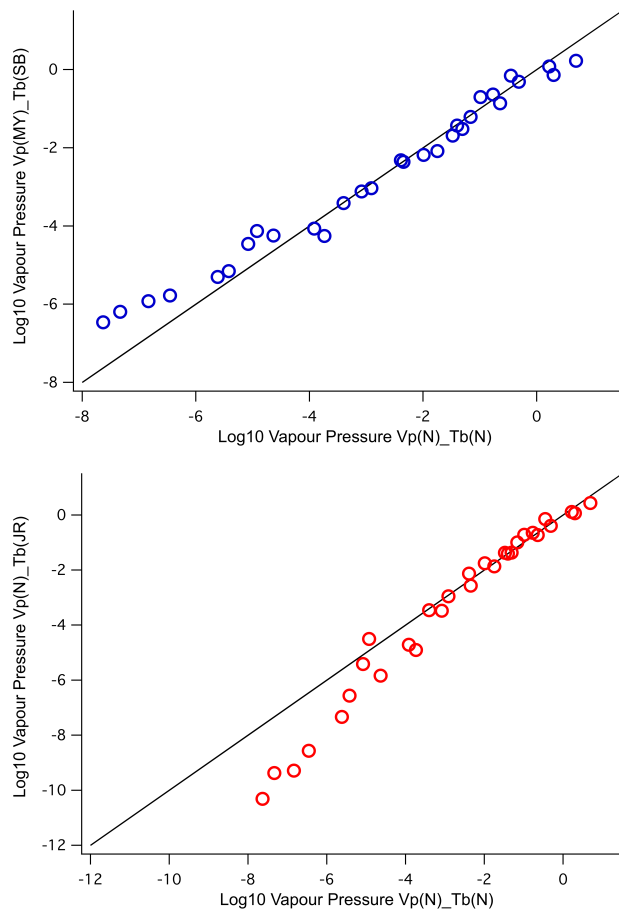


Figure 3. Predictions of pure component vapour pressures at 298.15 K using a subset of 30 compounds described by Barley et al. (2013), the list provided in the Appendix. The straight lines highlight the 1 : 1 relationship between predictions.

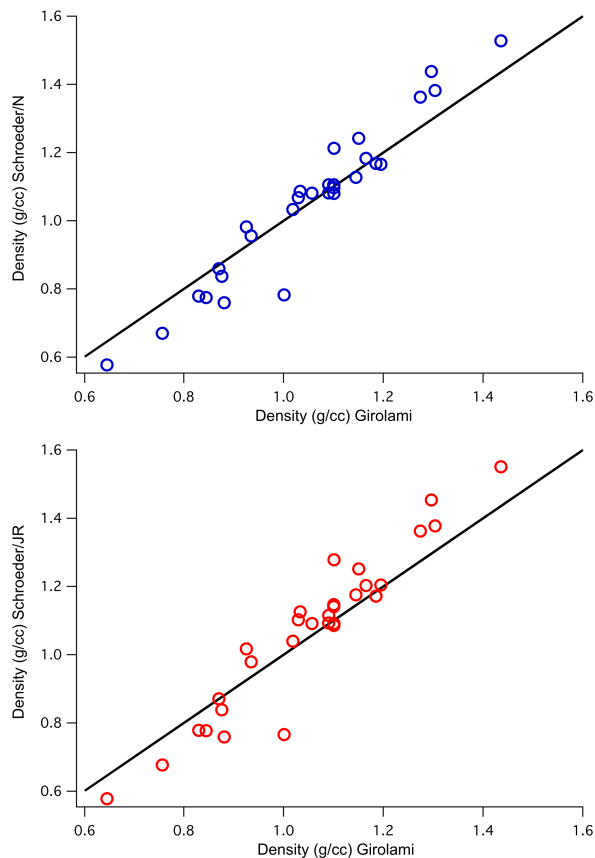


Figure 4. Predictions of pure component density at 298.15 K using the compounds described by Barley et al. (2011), the compound list provided in the Appendix. Methods used include those of Schroeder (Poling et al., 2001) combined with critical property estimation by both Joback and Reid (1987) and Nannoolal et al. (2008), compared to the method by Girolami (1994).



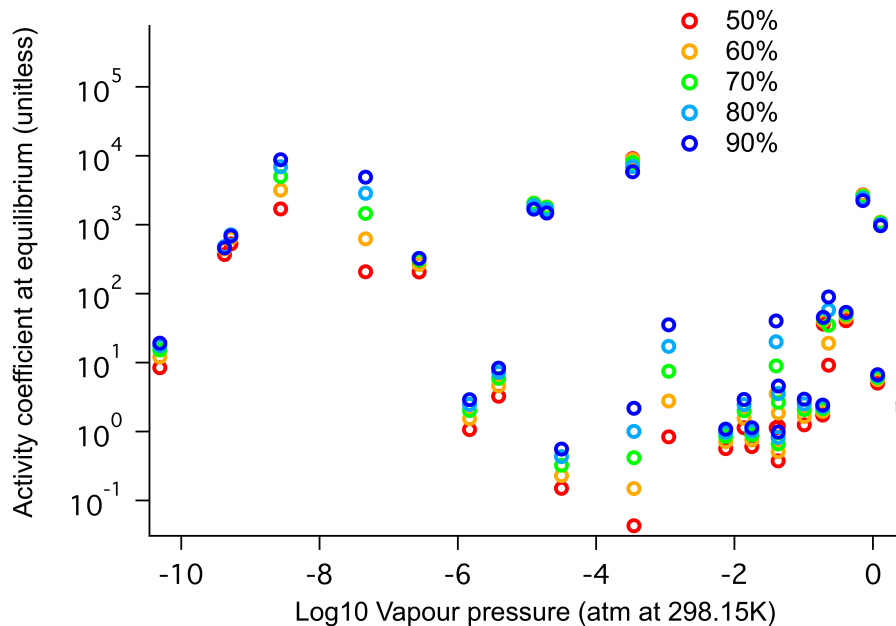


Figure 5. The range of predicted activity coefficients for each organic compound as a function of saturation vapour pressure and RH.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



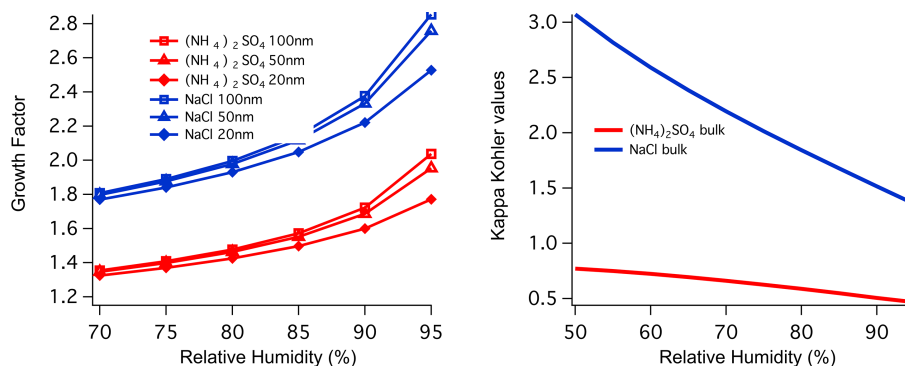


Figure 6. (left panel) Growth factor predictions for (NH₄)₂SO₄ and NaCl particles of size 100, 50 and 20 nm diameter. (right panel) Kappa Kohler value predictions for (NH₄)₂SO₄ and NaCl particles as a function of RH. All simulations use the AIOMFAC activity coefficient model.

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

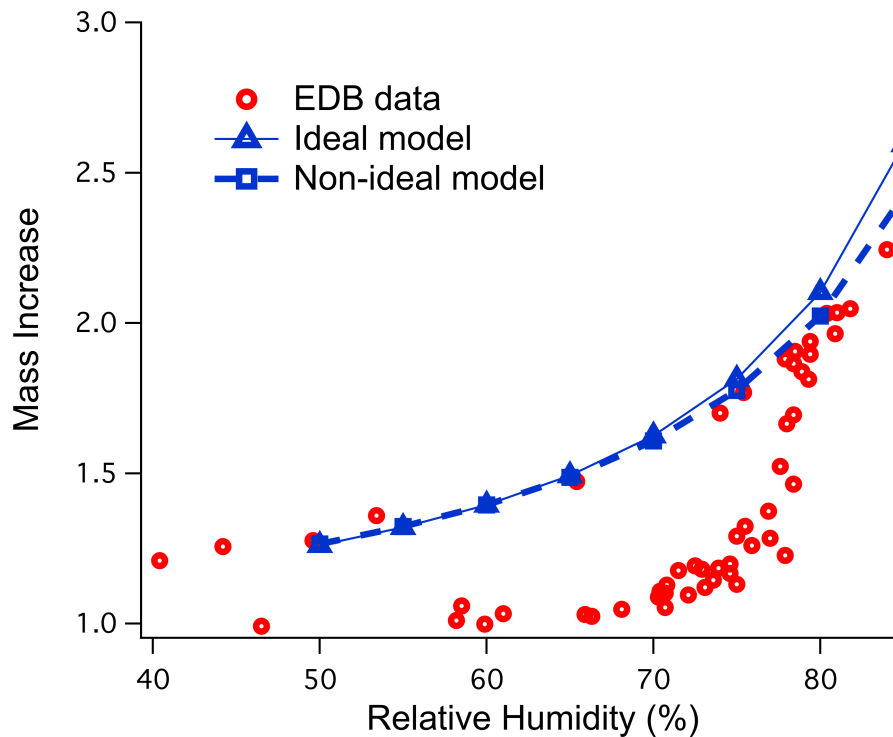


Figure 7. Comparisons of predicted water uptake, as particle mass increase, with EDB measurements on equimolar $(\text{NH}_4)_2\text{SO}_4$ -Glutaric acid systems.

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)