Geophysical Research Abstracts
Vol. 18, EGU2016-7650, 2016
EGU General Assembly 2016

UManSysProp: An online and open-source facility for molecular property prediction and atmospheric aerosol calculations

David Topping (1,2), Mark Barley (1), Gordon McFiggans (1), and Bernard Aumont (3)

(1) University of Manchester, Centre for Atmospheric Science, Manchester, United Kingdom , (2) NCAS National Centre for Atmosopheric Science, University of Manchester, Manchester, United Kingdom , (3) LISA, UMR CNRS 7583, Universite Paris Est Creteil et Universite Paris Diderot, Creteil, France

The many thousands of individual aerosol components ensure that explicit manual calculation of properties that influence their environmental impacts is laborious and time-consuming. The emergence of explicit automatic mechanism generation techniques, including up to many millions of individual gas phase products as aerosol precursors, renders manual calculations impossible and automation is necessary. 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.

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. Here 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; absorptive partitioning calculations with/without a treatment of non-ideality.

The website can be found here: http://umansysprop.seaes.manchester.ac.uk/