Geophysical Research Abstracts,
Vol. 11, EGU2009-12672, 2009
EGU General Assembly 2009

A Methodology for the Prediction of the Chemical Composition of Secondary Organic Aerosol

M Barley (2), D Topping (1), G McFiggans (2), and M Jenkin (2)

(1) NCAS, SEAES, Manchester, United Kingdom (david.topping@manchester.ac.uk), (2) SEAES, Manchester, United Kingdom

Atmospheric aerosols have been identified by the Intergovernmental Panel on Climate Change in their recent reports (IPCC, 2007) as a key influence on climate change, but as also an influence about which we have minimal understanding. Atmospheric aerosols can contain a wide range of components but most are believed to be mainly composed of an inorganic part, an organic part and associated water. The inorganic component is relatively well understood and is composed of a limited number of ionic species. However, the organic component is much more complex as any of the thousands of organic compounds found in the atmosphere can potentially condense into the aerosol. A major contributor to the organic aerosol is believed to be from chemicals formed by atmospheric processes. Volatile organic compounds (VOC's) from both anthropogenic and biogenic sources (primary emissions), undergo progressive oxidation in the atmosphere and the products of these atmospheric reactions may contribute to the formation of secondary organic aerosol (SOA) particles. The oxidation process leads to increased functionalization of the VOC with a resulting increase in polarity and decrease in volatility. The less volatile components in this mixture may condense to form SOA particles by nucleation or by condensation onto particles (such as involatile primary emissions, or polymerised water soluble material) already present in the atmosphere. There is much speculation about the composition of SOA particles as complete analyses are not available. One approach is to model the formation of SOA using an explicit atmospheric chemistry scheme coupled to a condensation/absorption model. We will report on the use the Master Chemical Mechanism (MCM:- see http://mcm.leeds.ac.uk/MCM/) with a modified version of the Pankow absorption model to predict the chemical composition of SOA particles formed under a range of conditions.

The MCM provided the atmospheric abundances of 3700 non-radical atmospheric chemical species in a trajectory model of a heavily polluted air parcel that arrived at Writtle (Essex) in the south of England at 18:00 on August 6th 2003 during the TORCH campaign. A similar set of abundances were simulated for an air-parcel arriving on August 12th with high concentrations of VOC's from biological sources. These two sets of atmospheric concentrations formed the inputs for the calculation of the chemical composition of anthropogenically dominated and biogenically dominated SOA respectively.

The condensation of the oxidised VOC's were modelled using the following methodology:-
1) The model used was a modified version of the Pankow absorption model.
2) Estimated vapour pressures were used for all components and liquid phase ideality was assumed.
3) It was assumed that water condensed into the SOA alongside the organic components.
4) As liquid phase water is expected to be present the acid anhydrides predicted to be present in the atmosphere are expected to hydrolyse to their corresponding acids.
5) The presence of an involatile core onto which the organics can condense is assumed.

Formation of SOA by condensation was modelled for both the anthropogenic and biogenic case over a range of temperatures, relative humidity and target mass (=core mass+SOA mass). This provided a range of SOA masses- particularly for the anthropogenic case where it was clear that the chemical composition of the SOA was strongly affected by the mass of SOA predicted. The results showed that anthropogenic SOA contained significant dicarboxylic acids derived from the hydrolysis of cyclic anhydrides while the biogenic SOA contained pinic acid (another dicarboxylic acid) and a range of multifunctional compounds dominated by hydroxyl and hydroperoxide groups.