Geophysical Research Abstracts, Vol. 9, 10754, 2007
SRef-ID: 1607-7962/gra/EGU2007-A-10754

How organics affect the aerosol composition and hygroscopic growth – a case study with the new thermodynamic model EQSAM3 based on MINOS results

S. Metzger (1), J. Lelieveld (1), N. Mihalopoulos (2)

(1) Max Planck Institute for Chemistry, Air Chemistry Department, Mainz, Germany, (2) University of Crete, Department of Chemistry, Heraklion, Greece

(metzger@mpch-mainz.mpg.de)

We show how organics affect the aerosol composition and hygroscopic growth under Mediterranean conditions. The results are based on the MINOS (Mediterranean INtensive Oxidant Study) campaign in Crete, Greece, July and August 2001, and extend the case study of Metzger et al., 2006, which focused on the importance of mineral cations and organics in gas-aerosol partitioning of reactive nitrogen compounds. The results are obtained with a new thermodynamic model (EQSAM3) that allows to explicitly resolve the aerosol hygroscopic growth of mixed inorganic and organic salt solutions – merely based on thermodynamic principles that explain hydration and osmosis (Metzger and Lelieveld, 2007). EQSAM3 is based on a new concept, which will be presented in an accompanying presentation.

Its input is limited to the species' solubilities from which a newly introduced stoichiometric coefficient for water is derived. Analogously, we introduce effective stochiometric coefficients for the solutes to account for complete or incomplete dissociation. These coefficients can be assumed constant over the entire activity range and calculated for various inorganic, organic and nonelectrolyte compounds, including alcohols, sugars and dissolved gases. EQSAM3 calculates the aerosol composition and gas/liquid/solid partitioning of mixed inorganic/organic multicomponent solutions and the associated water uptake for almost 100 major compounds. It explicitly accounts for particle hygroscopic growth by computing aerosol properties such as single solute mo-

lalities, molal based activities, including activity coefficients for volatile compounds, and deliquescence relative humidities of single or mixed solutes.

With the application of EQSAM3, we (i) contrast its results with EQSAM2 that assumed lumped organics, and we (ii) focus on the sensitivity of the aerosol composition and hygroscopic growth to organic compounds. For instance, different organic acids such as e.g. formic acid ($HCHO_2$) or citric acid ($H_3C_6H_5O_7$) yield different organic salt compounds, if they are exposed to excess cations. Neutralization reactions with either ammonium (NH_4^+), or mineral cations such as sodium (Na^+), potassium (K^+), calcium (Ca^{2+}), magnesium (Mg^{2+}), iron(II/III) ($Fe^{2+/3+}$) yield organic salt compounds that obey a different aerosol hyrgoscopicity and therefore cause (1) a different amount of water that is associated with the aerosol particles at a given temperature (T) and relative humidity (RH), and (2) a different RH range over which the salt compounds are able to bind water. The main advantage of EQSAM3 is that it allows to explicitly compute the relative humidity of deliquescence (RHD) and the water uptake of various inorganic, organic, or mixed salt compounds.

Metzger, S., N. Mihalopoulos, and J. Lelieveld, Importance of mineral cations and organics in gas-aerosol partitioning of reactive nitrogen compounds: case study based on MINOS results, Atmos. Chem. Phys., 6, 2549–2567, 2006.

Metzger, S., and J. Lelieveld, Reformulating Atmospheric Aerosol Thermodynamics and Hygroscopic Growth into Haze and Clouds, Atmos. Chem. Phys., Discus., in press, 2007.