Geophysical Research Abstracts
Vol. 12, EGU2010-3414, 2010
EGU General Assembly 2010

EVAPORISATION: a new vapor pressure model taking into account neighbour effects

Steven Compernolle, Karl Ceulemans, and Jean-Francois Muller
BIRA-IASB, TROPO, Brussel, Belgium (steven.compernolle@aeronomie.be)

Secondary organic aerosol (SOA) is a complex mixture of water and organic molecules. The vapor pressure of an organic molecule is one of the most important properties regulating its partitioning to the particulate phase, but as it is unknown for most- typically polyfunctional- organic molecules in Biogenic SOA it has to be estimated by a vapor pressure model fitted to experimental data.
While a lot of vapor pressure data is generally available for hydrocarbons and monofunctional compounds, much less data are available for bifunctional compounds. For compounds with more functional groups, data is sparse and relatively inaccurate.

We have developed a vapor pressure model, EVAPORISATION (Estimation of VApor Pressure of ORganics, Including effects Such As The Interaction of Neighbours), starting from the group-contribution principle: each functional group gives a contribution to the logarithm of the vapor pressure. On top of that, second order effects -chemically rationalized- are added due to carbon skeleton, nonadditivity of functional groups and -for neighbouring functional groups- intramolecular interactions . These effects can be very significant: eg. when two carbonyl groups are neighbouring, the vapor pressure is about 1 order of magnitude higher than when they are nonneighbouring. Due to the lack of data, some of these effects must be estimated by analogy.

The method is compared to several other vapor pressure estimation techniques, such as SIMPOL (Pankow et al. 2008), SPARC (Hilal et al. 2003), and the methods of Myrdal and Yalkowsky (1997), Capouet and Muller (2006), Nannoolal et al. (2008), Moller et al. (2008). We extended some of these methods as they are not able to treat hydroperoxides, peracids, peroxy acyl nitrates.

With our model BOREAM, outlined in a previous publication (Capouet et al. 2008), several smog chamber experiments are simulated, and the impact of vapor pressure method choice is elucidated. It turns out
that the choice of the vapor pressure method can have a major impact on aerosol yield, considerably larger than the choice of activity coefficient model (Compernolle et al. 2009).

M. Capouet and J.-F. Muller, Atm. Chem. Phys. 6, 1455-1467 (2006)
M. Capouet, J.-F. Muller, K. Ceulemans, S. Compernolle, L. Vereecken and J. Peeters, J. Geophys. Res. 113, D02308 (2008)
S. Compernolle, K. Ceulemans and J. Muller, Atm. Chem. Phys. 9, 1325-1388 (2009)
S.H. Hilal, S.W. Karickhoff and L.A. Carreira , QSAR Comb. Sci. 22, 565-574 (2003)
P.B. Myrdal and S.H. Yalkowsky, Ind. Eng. Chem. Res. 36, 2494-2499 (1997)
Y. Nannoolal, J. Rarey and D. Ramjugernath, Fluid Phase Eq. 269, 117-133 (2008)
B. Moller, J. Rarey and D. Ramjugernath, J. Mol. Liq. 143, 52-63 (2008)