Multicomponent aerosol modelling with detailed chemical species

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A modelling study by Merikanto et al. (2009) showed that on a global average, about half of all Cloud Condensation Nuclei (CCN) originated from secondary organic aerosols. Yu and Luo (2009) claimed that secondary particles even dominate the number abundance in most parts of the troposphere (>80%). However, other studies suggest that the effect of new particle formation on CCN numbers, even with artificially enhanced SOA formation, remains modest (Pierce et al., 2008). Up to today, a complete understanding about which compounds are responsible for the formation of thermodynamic stable clusters and their growth to CCN size is not completely achieved.

The growth plays a crucial role and the mechanism widely used in regional and synoptic models is the two-dimensional volatility basis set (VBS, Donahue et al., 2011). This code employs saturation mass concentration of organic compounds and the oxygen content to describe volatility, mixing thermodynamics, and chemical evolution of organic aerosols. It has the advantage that explicit knowledge of the condensing organic species and their thermodynamic properties are not required. However, depending on the set of different reaction rates in the code it tends to over- or underestimate the simulated SOA mass.

In this study we have applied the zero-dimensional version of the model MALTE, and present the first results of simulations with measurements from the SMEAR II station in Hyytiälä, Southern Finland. We use explicit chemical species as the condensable vapours, to see if this increases our understanding of what compounds are responsible for the growth of the newly formed particles, and what effects does the use of an explicit chemistry module have on the aerosol aging in the atmosphere.

MALTE-BOX includes chemistry, emissions and aerosol dynamics. Thus it can be used to model situations that can be approximated as well mixed. Formerly all organics were classified into two classes in the aerosol module. We modified the model to use the actual chemical species as the condensing vapours. For this, the physical properties of the compounds need to be predicted. Unfortunately measurements are not available in all cases. Necessary properties were estimated based on molecular structure. There are several ways to do this (Poling et al., 2001). The method described in (Girolami, 1994) was used to predict the liquid phase density and the diffusion volume of the compounds was evaluated based on the method by Fuller et al. (1966). Saturation vapour pressures were predicted with the method presented in Nannoolal et al. (2008).

We applied MALTE-BOX to measurements made at the SMEAR II station. The measured and predicted particle compositions of the newly formed and aged particles will be presented.

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