

Simplifying the water-affinity and CCN activation of complex organic aerosols: A model study

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Introduction

The solubility in water is one of the key properties governing the water-absorption and CCN activation behaviour of aerosol particles.

Organics contribute a large fraction (20-90%, depending on the environment) of atmospheric submicron particulate mass, which is the part of the aerosol size distribution that typically dominates the CCN numbers. Atmospheric organic compounds have a wide range of solubilities, spanning from practically insoluble material to highly water soluble compounds (e.g. Raymond and Pandis 2003). To accurately predict the water content and CCN activation of atmospheric OA information on the dissolution behaviour and aqueous phase interactions of these complex mixtures is needed.

We introduce a theoretical framework (Solubility Basis Set, SBS) representing the mixture components with a continuous distribution of solubilities, similar to the VBS (Donahue et al., 2006). Using this framework, we investigate the dissolution behaviour of complex organic mixtures and furthermore their CCN activity. Particularly, we investigate the response of the CCN-activation to varying solubility ranges, distributions, and numbers of components in the mixture. We also present a simple relationship between the dissolved fraction and the apparent κ value. Furthermore, we provide recommendations for reasonable simplifications of the dissolution behaviour of organic mixtures, specifically in relation to interpretation of experimental CCN studies and activation predictions of SOA.

Methods

We consider a monodisperse population of spherical aerosol particles consisting of an internal mixture of organic compounds. When exposed to water vapour, these particles grow reaching a thermodynamic equilibrium between the water vapour and the particle phase according to the Köhler theory. The wet particle is allowed to consist of maximum two phases: the insoluble organic phase and the aqueous phase. The compositions of the organic and aqueous phases are determined by the equilibrium between the aqueous phase and the water vapour, and the equilibrium of the aqueous phase with the organic insoluble phase assuming an ideal mixture of the organics. Critical supersaturations and the dissolution behaviour at the point of CCN activation were calculated from the Köhler theory predictions.

We investigated the dissolution behaviour and CCN of 68 different organic mixtures with varying solubility distributions. We varied the range of pure component water solubilities present in the mixture, the shape of the solubility distribution, and the number of components n in the distribution.

Results

Figure 1 displays an example of the model results, namely the relationship between the apparent hygroscopicity parameter κ (as derived from fits to the model output) and the dissolved organic fraction ε at the point of activation. The dependence of κ on ε follows a simple linear relationship, and in fact could explain some of the apparent discrepancy between the κ values derived from hygroscopicity vs. CCN activation measurements. Furthermore, we present a criterion for complete solubility at the point of activation, considerably simplifying the theoretical predictions of the CCN activation of complex organic mixtures.

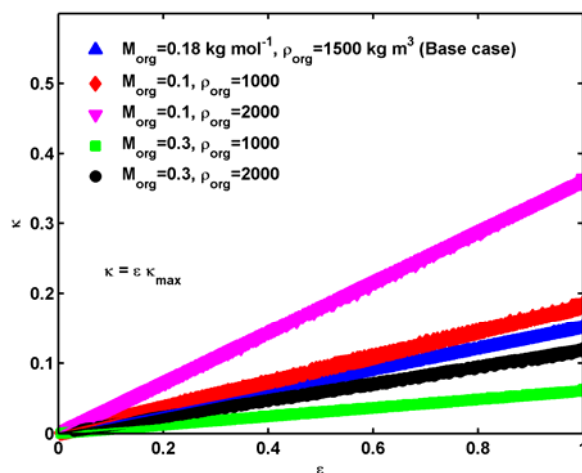


Figure 1. The hygroscopicity parameter κ vs. the dissolved fraction at the point of CCN activation.

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