Water adsorption on organic aerosols: modeling at a molecular scale

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Aerosols formed by carboxylic acids represent a significant fraction of the total organic matter in the atmosphere. These aerosols, which are often characterized by an intricate composition, generally have carboxyl groups and free hydroxyls on their surface that can form hydrogen bonds with water molecules. Organic aerosols are thus suspected to be effective condensation nuclei for the formation of clouds in the troposphere and lower stratosphere.

The importance of organic aerosols on the physico-chemistry of the atmosphere therefore requires a better understanding of their interaction with the surrounding water molecules, to which studies at the molecular level can contribute.

In the present work, we studied the interaction of organic aerosols in the presence of water molecules by means of molecular dynamics (MD) simulations. The organic aerosols considered were modeled by small aggregates of various carboxylic acid molecules (formic, acetic, propionic, valeric and butyric acids and also some mixing of them) and their interaction with a variable amount of water molecules representing different relative humidities has been simulated. Calculations have been carried out with temperature values in the range of 150–250 K (Vardanega, 2014 ; Radola, 2015).

Our results showed that both the temperature and the water content have a strong influence on the behavior of the acid–water system. Different situations have thus been evidenced for the acid–water aggregates, corresponding either to water adsorption on large acid nuclei at low temperatures (~150 K) or to the formation of droplets consisting of acid molecules adsorbed at the surface of water aggregates at higher temperatures (typically above 200 K) and high water content. At intermediate temperatures, a more intricate situation was obtained, characterized by a partial deliquescence of the acid core of the aggregates.

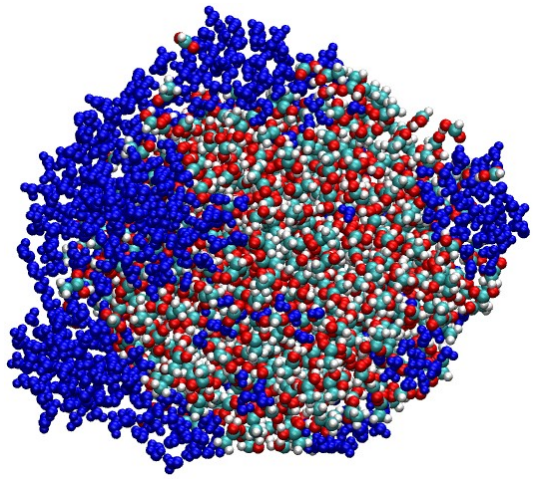

Figure 1. Water molecules adsorbed on a mixed formic and acetic acids aggregate as modeled in the MD simulations at 150 K.

Although the present results cannot be directly compared with any field measurements, they represent an additional step towards modeling of organic cloud condensation nuclei (CCN) and ice condensation nuclei (ICN).

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