Natural surfactants promote the uptake of soot-particles in aerosols

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The effects of light absorbing carbon particles (soot) are amongst the most uncertain, and they are also considered to cause climate warming on the same order of magnitude as anthropogenic carbon dioxide. This study contributes to the understanding of the potential for transformation of the surface character of soot from hydrophobic to hydrophilic. We use molecular dynamics simulations to show how natural surfactants facilitate solubilization of fluoranthene, which we use as a model compound for soot, in nano-sized water clusters.

The aim if the study is to explore whether natural surfactants can increase the water-solubility for soot or BC in airborne aerosol particles. Such surfactants can be found among the secondary organic aerosols (SOA) (Grieshop et al., 2009). Cis-pinonic acid (CPA) is a secondary organic oxidation product of α-pinene evaporated from trees (O´Dowd et al., 2002).

CPA is amphiphilic with surfactant properties (Li et al., 2010). In a previous study (Hede et al., 2011) we showed that CPA is able to form aggregates inside nanosized particles. The nanoaerosols that we have simulated here are 8.6 nm in diameter and consist of 10000 water molecules together with a number of organic molecules. Fluoranthene, which is a polycyclic aromatic hydrocarbon (PAH) abundant in soot, is like other PAHs emitted from incomplete combustion from various sources such as diesel engines (Maricq, 2007).

Fig. 1 shows how one fluoranthene molecule is solubilized in an aggregate inside the nanoaerosol (red square).

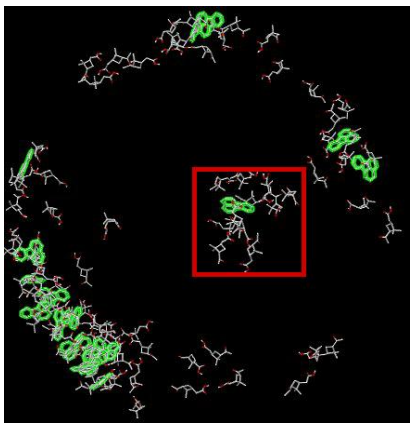

Figure 1. Fluoranthene solubilized at the surface and in an aggregate (red square). Water molecules removed for clarity

The rest of the fluoranthene molecules are solubilized at the surface. The radial number density (RND) plot for the system of 81 CPA and 27 Fluoranthene molecules is shown in Fig. 2. As we can see, the CPA and fluoranthene molecules are found at almost the same radial distance, namely in the aggregate or at the surface.

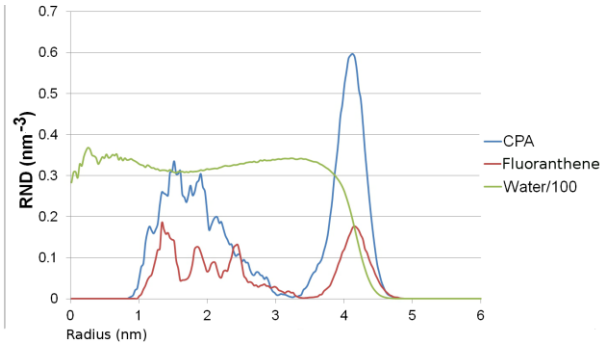

Figure 2. RND for CPA, fluoranthene and water.

The solubilization of fluoranthene in the aggregates and at the surface promoted by the natural surfactant CPA shows that the uptake of hydrophobic material such as soot is facilitated by SOA in the nanoaerosols. This may also change the light absorbing properties (Schnaiter et al., 2003).

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