Simulation of Atmospheric Cr Chemistry and Physics

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The two chromium oxidation states found in ambient atmospheric particulate matter are trivalent [Cr(III)] and hexavalent [Cr(VI)] chromium. Cr(III) is a trace element essential for the proper function of living organisms. However, Cr(VI) is toxic and exposure to Cr(VI) may lead to cancer, asthma and bronchitis. Therefore, it is important to accurately discriminate between these two species in atmospheric particulate matter (PM). Little is known regarding atmospheric Cr chemistry and physics. It was found that atmospheric Cr(III) is oxidized to Cr(VI) in the presence of dissolved ozone in liquid coated particles or droplets or even at dry conditions, while Cr(VI) is reduced to Cr(III) in the presence of organic carbons and metal ions such as Fe(II), As (III) and V(II) (Seigneur and Constantino, 1995) at high humidity (Huang et al., 2013). This inter-conversion between Cr(III) and Cr(VI) results in some biases in measuring atmospheric Cr concentrations (Amouei Torkmahalleh et al. 2013). Therefore, it is critical to estimate the interconversion rate of Cr(III) and Cr(VI) to be able to quantify C(VI) concentrations in the ambient air. This study focuses on the simulation of interconversion of atmospheric chromium in the presence of PM matrix and dissolved gases such SO_2,O_3 and NO_2 , at different temperatures and pH conditions. In particular Cr(VI) chemistry on sampling filters is simulated. Recent field measurements of atmospheric Cr is used for model validations (Amouei Torkmahalleh et al., 2013).

The physical properties of Cr containing atmospheric particles have not been yet investigated. It is critical to understand the interactions between Cr and dissolved molecules in atmospheric droplets or deliquesced particles on sampling filters.

In the present study, radial pair density distribution of Cr(III) ions and ozone molecules, kinetic potential, and diffusivity of these molecules in the aerosol droplets at 0°C are investigated using molecular dynamics simulation. It was found that the presence of chromium molecules in the cluster influences the interaction between water and dissolved ozone including solubility and diffusivity of ozone molecules in the atmospheric droplets (Figures 1 and 2).

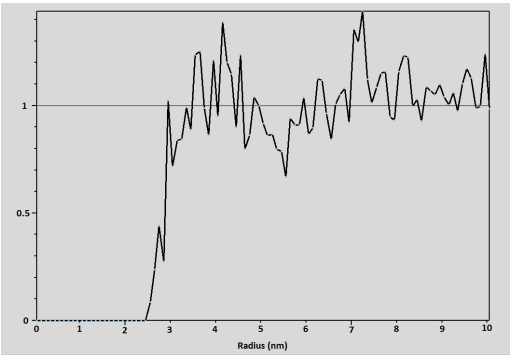

Figure 1. Pair radial distribution between molecules of water and ozone in the absence of Cr molecules

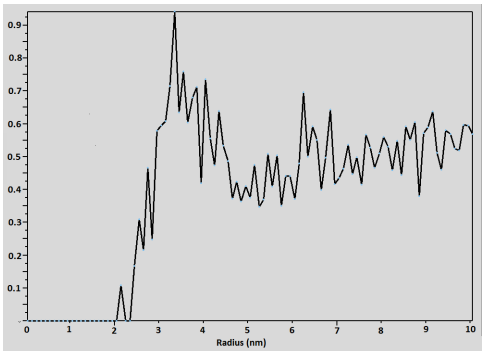

Figure 2. Pair radial distribution between molecules of water and ozone in aerosol cluster in presence of chromium molecules

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