Geophysical Research Abstracts, Vol. 9, 01893, 2007
SRef-ID: 1607-7962/gra/EGU2007-A-01893

Modelling of structure and gas phase uptake at aqueous and organic atmospheric surfaces by molecular dynamics simulations

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A large number of environmentally and technologically important processes can be traced to chemical reactions occurring at surfaces. Our primary objectives are to elucidate the molecular scale structure of aqueous and organic atmospheric surfaces and to unravel the mechanisms of interfacial bonding, diffusion, and uptake that control many atmospherically relevant reactions occurring, e.g., in or on aqueous atmospheric aerosols and cloud droplets as well as in thin water films on solid surfaces.

In this contribution, results of classical molecular dynamics simulations are presented that provide molecular level insight into the process by which gas-phase molecules such as OH and O_3 with thermal impact velocity become accommodated at the water surface and/or taken up into the bulk liquid. The mass accommodation coefficients of OH and O_3 on liquid water at 300 K, evaluated from a series of scattering trajectories, are reported. These simulations have also indicated that OH and O_3 preferentially bind to the water surface. Driving forces for the surface activity of OH and O_3 are discussed, and partitioning of OH and O_3 between the interface and bulk under tropospheric conditions is predicted.

Both OH and O_3 play an important role in oxidizing the atmospheric organic matter present, e.g., as a film on atmospheric aerosols. To explore the interactions between the gas phase OH and O_3 and the organic film in the presence of humidity, molecular dynamics simulations of several organic self-assembled monolayers in contact with water and/or OH and O_3 were carried out. This contribution will present the first results of this study.