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The impact of organic surfactants on halide ion concentrations at the aqueous liquid/vapor interface

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Reactions of gas phase oxidants (e.g., OH, ozone, oxides of nitrogen) with sea salt aerosols have been suggested as a source of reactive halogen species in the troposphere. It has been suggested that enhanced ion concentrations at the liquid/vapor interface of aqueous sea salt aerosols may play an important role in the kinetics of such interface reactions. In previous work, we have used ambient pressure photoelectron spectroscopy to verify that halide ion concentrations are enhanced at the liquid/vapor interface of pure alkali halide aqueous solutions. However, it is widely understood that aerosols in the troposphere are likely to be coated with an organic surfactant layer. In this presentation we present the results of ambient pressure photoelectron spectroscopy measurements on alkali halide solutions that have been exposed to an organic surfactant (butanol). Our measurements show that butanol is taken up from the gas phase by the salt solution and that the butanol is surface active, as expected based on previous studies of pure butanol/water solutions. Our experiments show that in the presence of butanol at the liquid/vapor interface, the halide ion concentration is not enhanced relative to the bulk. Experimental depth profiles show that the halide ion concentration remains constant from the liquid/vapor interface into the bulk of the aqueous salt solution. We have also carried out molecular dynamics (MD) simulations of butanol/salt/water solutions. The MD simulations are in agreement with the experimental measurements. The MD simulation provide insight into the interactions between the dissolved ions and the electrophilic head group of the organic surfactant. We will discuss the implications that our results have for the rates of reactions between gas phase oxidants and the surfaces of sea salt aerosols.