ENERGY TRANSFER AND GAS DIFFUSION

AT GAS-LIQUID INTERFACES

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ABSTRACT

The interactions of gasses and liquids play an important role in many systems in chemistry. Gas-liquid surface scattering techniques are a useful tool towards the investigation of energy transfer resulting from gas-liquid collisions. We use molecular dynamics to simulate surface scattering in order to investigate the effects of incident energy, incidence angle, and surface temperature on energy transfer of a CO_2 molecule scattering from a liquid indium surface modeled as a simple Lennard-Jones liquid. We focus our investigation on the two-channel theory of gas-liquid scattering with a primary focus on the trapping-desorption scattering channel. We use a novel technique to investigate the average trajectory of the scattering gas species to determine the effects of energy transfer on this channel. We find species scattering via this channel are unaffected by incident energy and incidence angle in agreement with experimental trends. We find our gas species scattered by the trapping desorption channel emerge with four degrees of freedom thermalized to the surface temperature, with substantial variance in the translational degree of freedom in the surface normal direction which we attribute to both the enthalpy of desorption and interactions with vapor-phase indium atoms. We observe a substantial increase in interactions with vapor-phase indium with increasing temperature.

Our second simulation uses molecular dynamics to examine the diffusion of various gas species through a room temperature ionic liquid at standard pressure conditions. We were able to replicate the bulk properties of the bmim PF_6 ionic liquid with reasonable accuracy compared

with other experimental and theoretical work. We varied the gas species mass, the gas species dipole moment, and the ionic liquid temperature to examine the effects of each variable on gas diffusivity. We find a general trend of increased diffusivity with increasing temperature; however, we are unable to discern a definite trend relating to gas species mass or dipole moment. We observe significant short-time trapping effects on our diffusing gas species, particularly at low temperatures, that make examining the diffusivity of our gases problematic.