ENERGY TRANSFER AT GAS-LIQUID INTERFACE: TOWARDS ENERGETIC MATERIALS

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ABSTRACT

Physicochemical surface processes have great importance in the different fields of everyday life and science. Computational characterization of collisional energy transfer at a gas-liquid interface is a helpful tool to interpret recent experimental studies and to yield insight into the energy feedback mechanism of multiphase combustion problems. As a first step, a simple Lennard-Jones system was used to investigate the dependence of the collisional energy transfer and the gas atom trapping probabilities on the temperature of the bulk liquid, on the gas/liquid particle mass ratios, on the incident angle of the impinging projectile, and on the gas-liquid interaction strength. We find in accord with the experimental results that the kinematic effects dominate the energy transfer dynamics, but the importance of the role of surface roughening as the temperature of the liquid increases is also seen.

The second system, nitromethane was chosen to extend the range of simulations. It is a molecular model system, representing nitramine-type energetic materials. Having had a good potential description for the nitromethane molecule including all internal degrees of freedom, we generated simplified molecular systems based on the original nitromethane model to isolate particular features of the dynamics. We have investigated the effect of the initial incident energy, of the inclusion of the internal degrees of freedom, of the initial incident kinetic energy and of the gas–surface interaction strength. The incorporation of internal degrees of freedom enhanced the collisional energy transfer. These calculations also point to the importance of simple
kinematics as it predicts the increase of the ratio of energy transferred with increased initial incident energy of the gas particle.