Public Abstract

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Physicochemical surface processes have great importance in the different fields of everyday life and science; like biology (gas transfer in the lung), environment (gas transport trough water surfaces, underwater life) and industry (sulfuric acid production). For us the final goal is to be able to simulate the energy transfer at the gas-liquid interface for energetic materials. Understanding the surface processes during the combustion of energetic materials is a useful tool to control and improve performance and safety.

We used computational methods to characterize the collisional energy transfer at the gas-liquid interface. This theoretical approach is a helpful tool to interpret recent experimental studies and to yield insight into the energy feedback mechanism of multiphase combustion problems.

The first step to our goal, was to evaluate the code we modified to the purpose. A simple Lennard-Jones system (argon gas colliding with molten indium metal) 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, the incident angle of the impinging projectile, and on the gas-liquid interaction strength. We have found that the kinematic (classical mechanics) effects dominate the energy transfer dynamics, but the importance of the surface roughening cannot be ignored either.

Our second system was nitromethane a fuel additive and liquid propellant, chosen to extend the range of simulations. It is a molecular model system, representing the commonly used 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 the gas–surface interaction strength. We have found that the incorporation of internal degrees of freedom enhanced the collisional energy transfer. These calculations also point out the importance of simple kinematics as it predicts the general behavior, fro example the increase of the ratio of energy transferred with increased initial incident energy of the gas particle.