ABSTRACT

Aluminium is favored over other metals for propulsion applications due to their high energy density, abundance and relative safety. Energy accommodation coefficient is an important parameter to accurately predict the heat transfer characteristics of nano-aluminum particle combustion. Previous studies have shown that appropriate accommodation coefficient is required to reproduce peak particle temperatures and burning times for nano-aluminium particles. The accommodation coefficient is however a poorly known parameter. Molecular dynamics simulation technique is employed to calculate accommodation coefficient for near equilibrium conditions for Al-noble gas systems. Helium, Argon and Xenon are chosen since they are unreactive and have only translational degrees of freedom. Surface temperature is taken as 300K and gas temperature is varied for a range from 320K to 450K. Using a method of two equilibrated parallel slabs with the gas sandwiched between them, the dynamics of the gas–surface interactions is studied. The calculated EACs at 20K temperature difference for He, Ar and Xe are 0.090 ± 0.01, 0.27 ± 0.02 and 0.39 ± 0.02, respectively. Results suggests that EAC obtained for Al-He system is weakly dependent on gas temperature at near equilibrium conditions. Effect of mass ratio and well depth is also investigated. It is found that EAC is a strong function of potential well depth and weak function of mass ratio. The parallel slab method is compared with the single slab method for high and low temperature differences. Data obtained using single and parallel slab methods are comparable for high temperature differences. Single slab method fails to produce reliable results for lower temperature differences. However, parallel slab method shows realistic EAC values and the method can be employed to study EAC characteristics for near equilibrium conditions effectively.