Kinetic and Molecular Dynamic Modelling of n-dodecane Droplet Heating and Evaporation

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Abstract

A recently developed approach to taking into account the effects of inelastic collisions between two molecules on the solution of the Boltzmann equation is briefly described. This approach is based on presenting the change of state of molecules after collisions as a random movement along a surface of an N-dimensional sphere, the squared radius of which is equal to the total energy of the molecules before and after the collision in the reference system of the centre of mass. The projection of a point on the surface of this sphere in each of N-directions gives the root square of the kinetic energy in one of three directions in the physical space, or the internal energy of one of the degrees of freedom, of one of two molecules. The kinetic energies of two molecules are described by the first six dimensions of the system, and the remaining $(N-6)$-dimensions describe the internal energies. Recent results of molecular dynamics simulations to study the evaporation and condensation of n-dodecane ($C_{12}H_{26}$) at liquid-vapour phase equilibrium using the modified OPLS (Optimized Potential for Liquid Simulation) model are summarised. The predicted evaporation/condensation coefficient decreased from about 0.9 to about 0.3 when temperature increased from 400 K to 600 K.

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