Molecular simulations of droplet evaporation processes: Adiabatic pressure jump evaporation

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Abstract

For the assessment of droplet evaporation by molecular dynamics simulations prescriptions for the calculation of the time dependent number of droplet particles and of several space and time dependent hydrodynamic quantities like density, drift velocity and temperature are given. Then two cases of adiabatic pressure jump evaporation are treated by molecular simulations using a Lennard-Jones potential. First, a droplet wrapped by its vapour, and second, a bare droplet is brought into vacuum. In both cases evaporation takes place and after a transition process a new droplet-vapour equilibrium is reached at lower temperature. Results are presented for the space and time dependent hydrodynamic quantities as well as for the number of droplet particles as function of time.
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1. Introduction

Evaporation and condensation play an important role in energy engineering, in chemical engineering as well as in environmental processes. The use of liquid fuels requires their evaporation outside or inside the combustion chamber. Other frequently used evaporation processes include most drying processes, cooling of water in cooling towers, and cooling of gases by quenching. Evaporation and condensation occur in Rankine and refrigeration cycles as well as in rectification columns. The scientifically interesting aspect of evaporation and condensation processes is that of combined heat and mass transfer and in most cases droplets are involved. Presently there is still a certain tendency in particular in drying technology to model these processes in the framework of fluid mechanics with some adjustable model parameters. We believe, however, that considerations on the molecular scale are required for a full understanding and a physically sound modelling of these processes.

A first molecular approach to describe evaporation and condensation is that by Hertz, Knudsen and Volmer [1–3], who assumed two half-sided Maxwell–Boltzmann (MB) velocity distribution functions outgoing from and incoming to the liquid–vapour interface. The outgoing MB-function has the temperature of the liquid T_1 and the density of the saturated vapour $\rho''(T_1)$ at temperature T_1. The incoming MB-function has the temperature T_g and the density of the gas ρ_g. Whilst this model captures already essential features of the physics of evaporation and condensation, details concerning the gas phase, the liquid–gas interface and the liquid phase remained open and deserve more detailed studies. Such studies were performed since about 1960 according to the available theoretical and computational possibilities.

First, the gas phase was studied by using the kinetic theory of gases [4] which allows assessing collisions between the gas molecules. Interesting findings in case of evaporation into vacuum [5] are that about 15% of the evaporated molecules are backscattered to the surface by collisions with other evaporated molecules and that the kinetic temperature in the gas is considerably lower than at the

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