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Study of evaporation–condensation problems: From liquid through interface surface to vapor

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ABSTRACT

This paper presents a conjugate approximate method for solving transfer problems in a two-phase (condensate–vapor) system that accounts for the peculiarities of atom–interface interactions and obtains a distribution function for the evaporated and reflected atoms. In this method, the Boltzmann kinetic equation is numerically solved for the vapor phase. The condensate matter and liquid–vapor transition layer are investigated through molecular kinetics and dense medium statistical mechanics. Finally, the proposed approach is validated by solving equilibrium saturation vapor–liquid lines of different substances as well as a nonsteady evaporation–condensation problem and by comparing the results with experimental data.

1. Introduction

Evaporation–condensation processes are common to natural phenomena and industrial techniques such as drying, chemical vapor deposition, vacuum distillation, cryo-vacuum pumping, and epitaxial vacuum growth. A characteristic feature of evapora tion–condensation processes is joint heat and mass transfer from the evaporation surface to the condensation surface. Generally, the liquid and vapor phases should be considered as a single combined system. In simple cases, heat transfer through the liquid layer can be determined using the stationary heat transfer equation. Vapor flow in a compressible, viscous, and thermally conductive medium can be described using mass, momentum, and energy conservation equations (continuum mechanics – CM). However, to apply these equations, the boundary conditions must be known. The temperature and gas velocity used as boundary conditions in these equations would not be equal to the temperature and velocity of the condensate–vapor interface. One approach for deriving the boundary conditions is to apply the stationary molecular-kinetic relationships. These correlation can be obtained for a specific class of problems by solving the main equation of molecular kinetic theory (MKT), i.e. the Boltzmann kinetic equation (BKE). An alternative method is to jointly solve the BKE and CM equations [1].

When solving such problems through kinetic theory–based methods, the velocity distribution of the vapor molecules flying off the interface surface (f_+) of the condensed phase must be known. f_+ generally comprises two components: f_e, which concerns the evaporated molecules, and f_r, which concerns the molecules reflected by the interface [2–4]:

$$f_+ = f_e + f_r$$

These components can be determined through molecular dynamics (MD) methods, as is well-documented in the literature [4–10], wherein the consensus is that the evaporation distribution function is rather similar to the Maxwell distribution function with zero mean velocity and temperature equaling that of the evaporation surface.

The distribution function of the reflected molecules is characterized by the reflection coefficient, which is the difference between the unit and the condensation coefficient (β). In [11], only those gas molecules falling on the surface of a liquid as determined by β condensed on the surface, whereas the others were reflected.

The evaporation coefficient is usually assumed to be equal to the condensation coefficient. This assumption is postulated in [12], where evaporation and condensation coefficients were determined through MD methods. However, [13] proved that this assumption is true only in the equilibrium state. Similarly, in [9], the coefficients of evaporation and condensation of helium II were reported to be close to unity in the case of low-intensity evaporation. In this case, this closeness has an approximate character.

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Notations

E_k	kinetic energy of a molecule, J
$f = f(\mathbf{r}, t, \xi)$	velocity distribution function of molecules
J	collision integral
j_e	density of the mass flux of molecules evaporating from an interface, kg/(s·m^2)
j_c	density of the mass flux of molecules condensed on interface, kg/(s·m^2)
m	mass of molecule, kg
r	distance between particles, m
$\mathbf{r}(x, y, z)$	Cartesian coordinates, m
t	time, s
T_s	interface temperature, K
T_0	base temperature, K
T_v	initial vapor temperature, K
U_s	potential energy of a molecule of liquid on the surface, J
ε	depth of potential well in the Lennard-Jones potential, J
$\xi(\xi_x, \xi_y, \xi_z)$	vector of molecular velocity, m/s
ρ_s	vapor density corresponding to temperature Ts along the saturation line, kg/m^3
ρ_0	base density, kg/m^3
ρ_v	vapor density at the initial instant of time, kg/m^3
σ	parameter of the Lennard-Jones potential, m

Indices

c	condensation
e	evaporation
k	kinetic
v	vapor
0	base values

Condensation coefficient has been defined in various ways in the literature [14–17]. The condensation coefficient used in the molecular-kinetic boundary conditions should be determined as the ratio the value of molecules flux remaining on the surface to the value of molecules flux striking with it after final collisions of molecules near the interface. An approximate method for calculating the condensation coefficient is proposed in [18]. This method enables the calculation of the condensation coefficient for various vapor molecules and interface surface temperatures through MD simulation. The authors of [18] argue that their approach among the most effective for determining kinetic boundary conditions in condensation problems.

There is an approach (Fig. 1), in which at each time step of the nonstationary evaporation and condensation problem, the MD simulation results are used as the boundary conditions for the BKE and the BKE solutions are used as the boundary conditions for CM equations.

The condensed phase is modeled using MD methods, and the nonequilibrium phase near the interface is described using the BKE. The fluid dynamics domain can be solved on the basis of CM equations. Through pairwise application of the different approaches (i.e., BKE–CM and MD – BKE), the relationship between each of the approaches can be established. An illustration of the joint application of a kinetic-equation system and fluid dynamic equations is presented in [1]. However, the joint application of MD, BKE, and CM approaches at each time step entails some difficulties [19]. A typical MD process (τ_{MD}) lasts 10^{-13} s, and its computer simulation time step usually requires approximately 10^{-14} s. Hence, information on system behavior at the kinetic scale can be obtained after 100,000 time steps at the MD scale. In the intervening time, the condensed phase does not remain stable, which contradicts the problem statement in the kinetic theory, where the vapor–liquid temperature interface is assumed constant throughout the calculation. Moreover, in contrast to the kinetic approach, no accurate geometrical interface surface exists in the MD approach. In the MD simulation, the transition layer is approximately 10–100-Å thick [16]. Consequently, the interface location is unclear.

Combining the MD and MKT approaches is rather difficult. The MD approach provides information on particle coordinates and velocities, using which the velocity distribution function can be calculated. However, the velocity distribution function cannot be used to calculate the particle coordinates and velocities. In addition, this description is too comprehensive. By contrast, a less-detailed statistical description is used in the MKT approach, wherein the system is described using a velocity distribution function defined as the ratio of the number of molecules ΔN in the defined volume element ΔV, with velocity ranging from ξ to $\xi + \Delta\xi$

$$F^{MD} = \frac{\Delta N}{\Delta \xi}$$

However, information on particle velocities and coordinates, which is essential for MD simulation, cannot be obtained through MKT calculations.

In [10,20], the boundary conditions for the kinetic equation were determined using MD and MKT solutions of evaporation–condensation problem in the same formulations. Comparing the evaporation–condensation solutions yields information on the evaporation and condensation coefficients, using which the distribution function of molecules moving out of the interface surface can be determined. Few studies [10,21–25] have investigated the evaporation–condensation processes by using unified calculation methods.

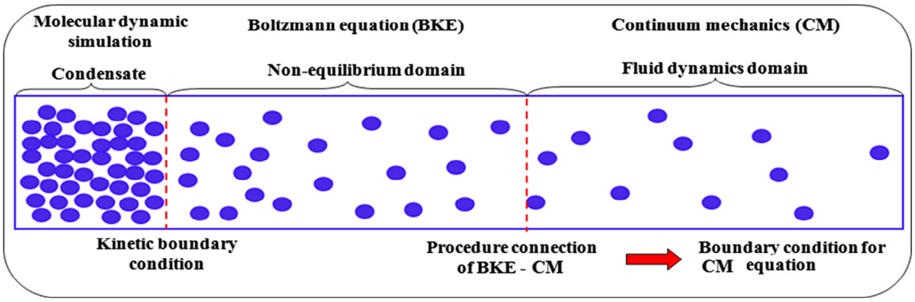

Fig. 1. Stages of vapor–liquid interface transfer.