

An evaporation flux of pure vapor in the method of lattice Boltzmann equations

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Abstract. The regularities of the evaporation flux of pure vapor in the method of lattice Boltzmann equations (LBE) are investigated. The simulations show that the mass flux during the evaporation of a flat surface is proportional to the difference in the densities of the saturated vapor at the surface temperature and surrounding vapor, which is in good agreement with the Hertz–Knudsen law. A simple method is proposed for setting the vapor flow at the flat boundary of the computational domain for the LBE method.

1. Introduction

Today, the Lattice Boltzmann Equation Method (LBE, LBM) is widely used to model fluids with liquid-vapor interfaces, e.g., in the problems of evaporation of liquid droplets and films [1,2], boiling liquid [3], coalescence and fragmentation of liquid droplets [4,5], levitation of liquid droplets over solid and liquid surfaces [6,7], etc.

In all cases, there is surface tension at the interfaces, as well as liquid evaporation. The value of surface tension is easily determined from the pressure drop for spherical droplets using Laplace's law. At the same time, the regularities of the evaporation flux of pure vapor in the LBM have not been previously studied. The Hertz–Knudsen law of evaporation for pure vapor is well known [8]. In this case, the mass flux from the surface is proportional to the difference between the pressure of saturated vapor at the surface temperature and the pressure of surrounding vapor at the same temperature.

2. Method of lattice Boltzmann equations

In this method, a continuous medium is considered as an ensemble of pseudo-particles flying in a time step Δt from one node of space grid to the adjacent nodes with fixed velocity vectors \mathbf{c}_k . For a one-dimensional model D1Q3 $\mathbf{c}_0 = 0$, $|\mathbf{c}_{1,2}| = h/\Delta t$, where h is the lattice spacing. For a three-dimensional nineteen velocity model D3Q19 three values of speed modulus are allowed $|\mathbf{c}_k| = 0$, $h/\Delta t$ and $\sqrt{2}h/\Delta t$ on a cubic lattice.

Evolution equation for one-particle distribution functions f_k includes the transfer of values along characteristics, the collision operator in the form of BGK $\Omega_k = (f_k^{eq}(\rho, \mathbf{u}) - f_k(\mathbf{x}, t))/\tau$ [9], as well as the change in distribution functions Δf_k due to body forces (internal and external):



$$f_k(\mathbf{x} + \mathbf{c}_k \Delta t, t + \Delta t) = f_k(\mathbf{x}, t) + \Omega_k(f) + \Delta f_k. \quad (1)$$

Equilibrium distribution functions f_k^{eq} are usually determined by the known formula [10]

$$f_k^{eq}(\rho, \mathbf{u}) = \rho w_k \left(1 + \frac{\mathbf{c}_k \mathbf{u}}{\theta} + \frac{(\mathbf{c}_k \mathbf{u})^2}{2\theta^2} - \frac{\mathbf{u}^2}{2\theta} \right). \quad (2)$$

Here θ is the normalized kinetic temperature of LBM pseudoparticles. The value of θ can be varied in a certain range determined by the stability of the method [11]. It is usually chosen equal to $\theta = (h/\Delta t)^2/3$. In dimensionless variables, this value is $\theta = 1/3$. Dimensionless relaxation time τ determines the value of the kinematic viscosity of the fluid $\nu = (\tau - 1/2)/3$.

In this paper, we investigate the regularities of the liquid evaporation process in LBE models with phase transitions. These models are detailed in [11–13]. One-dimensional model with three velocities D1Q3, for which the weighting coefficients are $w_0 = 2/3$ and $w_{1,2} = 1/6$, and three-dimensional model D3Q19, for which $w_0 = 1/3$, $w_{1-6} = 1/18$ and $w_{7-18} = 1/36$ [14], are used. Accounting for the action of body forces was described in detail in the works [13,15,16].

3. Modeling phase transitions

To describe the presence of different phases (liquid and vapor), the LBE method introduces internal forces between matter at adjacent lattice nodes [17]. Works [18,19] propose to introduce the concept of pseudopotential $U = P(\rho, T) - \rho\theta$, which is calculated according to the equation of state of the fluid. The force acting on the substance at the lattice node is equal to the gradient of the pseudopotential $\mathbf{F} = -\nabla U$.

In the method developed in [11-13], it was proposed to introduce the function $\Phi = \sqrt{-U}$. Then the expression for the force was written in the form $\mathbf{F} = A\nabla(\Phi^2) + (1-A)2\Phi\nabla\Phi$, where the coefficient $A = -0.152$ is for the van der Waals equation of state. When approximating this formula, good isotropy of the surface tension is achieved. Moreover, it is possible to ensure good agreement with the coexistence curve for liquid-vapor phases calculated from the equation of state. Van der Waals equation of state in reduced variables $\tilde{P} = P/P_{cr}$, $\tilde{\rho} = \rho/\rho_{cr}$ and $\tilde{T} = T/T_{cr}$ has the form

$$\tilde{P} = \frac{8\tilde{\rho}\tilde{T}}{3-\tilde{\rho}} - 3\tilde{\rho}^2. \quad (3)$$

Here P_{cr} , ρ_{cr} and T_{cr} are the pressure, density and temperature at the critical point. In these

dimensionless variables, the dimensionless parameter $k = \frac{P_{cr}}{\rho_{cr}} \left(\frac{\Delta t}{h} \right)^2$ will appear in the formula for

the pseudopotential [11,13]. This parameter determines the stability range of the LBE method.

The pseudopotential method provides an end-to-end description of the phase boundaries, that is, liquid and vapor are described uniformly. In this case, the interface is spread over several cells [12] depending on temperature and dimensionless parameter k . In this work, the value of the parameter is fixed $k = 0.01$.

4. Boundary conditions

Modeling is carried out in the computational domain, which has the shape of a parallelepiped, on a grid $(nx \times ny \times nz)$. A liquid layer is placed at the bottom in a weak gravitational field (figure 1). Boundary

conditions in x and y directions are periodic. For the distribution functions, the impermeability and no-slip conditions are set at the lower boundary, the so-called “bounce-back” rule [20].

To simulate quasi-stationary evaporation of a liquid, it is necessary to remove vapor from the computational domain. For this purpose, at the upper boundary, a uniform constant outflow of vapor along the axis z with a dimensionless velocity u_0 is set (figure 1), that is $\mathbf{u}_0 = (0,0,u_0)$.

In terms of the hydrodynamic problem, the boundary conditions are set at the upper boundary of the computational domain: the continuity of the density $\frac{\partial \rho}{\partial z} = 0$ and the desired value of the vapor flow velocity u_0 .

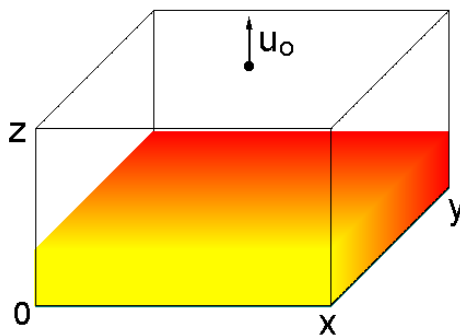


Figure 1. Evaporation of a flat liquid layer. Computational grid $400 \times 400 \times 240$.

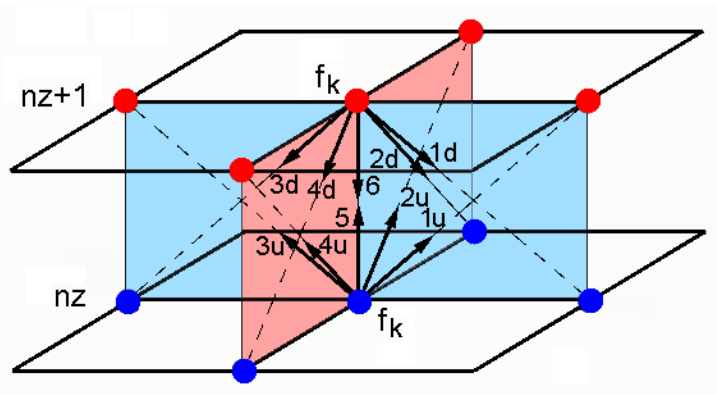


Figure 2. Boundary conditions for distribution functions f_k to provide outflow of vapor at the boundary of the computational domain.

However, for the method of lattice Boltzmann equations, it is necessary to specify the one-particle distribution functions f_k . In reality, there is a need only in those that transfer information from the border to the computational domain (incoming characteristics). For model D3Q19 there are five distribution functions ($f_6, f_{1d}, f_{2d}, f_{3d}$ and f_{4d}), corresponding to the velocities of pseudoparticles, for which the velocity projections on the axis z are negative (figure 2). Indexes u and d denote the directions of the projections of the pseudoparticle velocities along the axis z (up and down, respectively).

In the LBE method, the so-called “stream-in” method is convenient to use during the pseudoparticle transfer step, when the values of the distribution functions are collected in a given node from neighboring nodes before performing the “collision” step. To implement this method, fictitious nodes with a coordinate $nz+1$ are introduced outside the computational domain (fictitious interval method). In this case, in these nodes it is necessary to set the corresponding values of the distribution functions for certain boundary conditions. For a quasi-stationary vapor outflow, this must correspond to the hydrodynamic conditions

$$\rho(i, j, nz+1) = \rho(i, j, nz), \tag{4}$$

$$u_z(i, j, nz+1) = u_0.$$

In the well-known method, the equilibrium values determined by formula (2) from hydrodynamic variables are used to calculate the corresponding distribution functions in fictitious nodes. In this case, we obtain the values of the five necessary distribution functions $f_k(i, j, nz+1)$.

We propose a simpler method for setting the vapor flow at the boundary. To calculate the distribution functions in the fictitious layer $nz + 1$ (figure 2), a mirror image of the values of the distribution functions f_k in real nodes of the upper layer nz is used, but with the coefficient β :

$$\begin{aligned} f_6(i, j, nz + 1) &= \beta f_5(i, j, nz), \\ f_{1d}(i, j, nz + 1) &= \beta f_{1u}(i, j, nz), \\ f_{2d}(i, j, nz + 1) &= \beta f_{2u}(i, j, nz), \\ f_{3d}(i, j, nz + 1) &= \beta f_{3u}(i, j, nz), \\ f_{4d}(i, j, nz + 1) &= \beta f_{4u}(i, j, nz). \end{aligned} \quad (5)$$

To ensure the specified flow velocity $\mathbf{u}_0 = (0, 0, u_0)$ on the boundary, from the condition of density continuity (4) at $\theta = 1/3$ we find the correct value of the coefficient

$$\beta = \frac{1 - 3u_0 + 3u_0^2}{1 + 3u_0 + 3u_0^2}. \quad (6)$$

In the case of vapor outflow at $u_0 > 0$, the values of the coefficient $\beta < 1$. For values $\beta > 1$, the flow will be directed into the domain.

It is obvious that the calculations of the distribution functions by the new method are much faster than the calculations by formulas (2). And most importantly, the algorithm becomes much simpler. Velocity values u_0 can be changed over time and along the boundary.

5. Simulation of evaporation from a flat surface

The Hertz–Knudsen law of evaporation for pure vapor is well known [8]. The mass flux during evaporation is $J = \gamma(P_S - P_V)\sqrt{m/2\pi kT}$, where P_S is the saturated vapor pressure for a flat surface at surface temperature T , P_V is the actual vapor pressure near the surface, and the coefficient γ takes into account the deviation from the ideal equation and is called the accommodation coefficient. Using the formula for the pressure of an ideal gas $P = nkT$, we can rewrite the Hertz–Knudsen law for vapor densities $J = \gamma(\rho_S - \rho_V)\sqrt{kT/2\pi m}$, where ρ_S is the value of the density of saturated vapors over a flat surface at a given temperature according to the coexistence curve (binodal), and ρ_V is the actual density of the surrounding vapor near the surface. Note that the quantity $\langle V_x^+ \rangle = \sqrt{kT/2\pi m}$ is the average velocity of an ideal gas molecules flying toward the evaporation surface or away of it.

In numerical calculations, the evaporation of a flat liquid layer (figure 1) is investigated during the outflow of vapor from the computational domain at the upper boundary with a dimensionless velocity u_0 in the range from 0.002 to 0.02. The model of isothermal evaporation is used. This means that the required heat is supplied to the interface, for example, by laser or X-ray radiation or by a flux of neutrons (or other particles). Calculations are performed for the isothermal case for the values of reduced temperatures $\tilde{T} = 0.6, 0.7$ and 0.8 at a fixed value of $k = 0.01$. It turned out that the results depend on the reduced temperature and relaxation time τ .

Figure 3 shows the propagation of the evaporation wave for $u_0 = 0.01$. The vapor stream at a constant outflow velocity is uniform, i.e., quasi-stationary. The vapor flux at the upper boundary of the

region $j = \rho_V u_0$, and the velocity of the evaporation wave of the liquid phase is constant and equal to $D = \rho_V u_0 / (\rho_L - \rho_V)$. Here ρ_L is the reduced density of the liquid phase at a given temperature \tilde{T} .

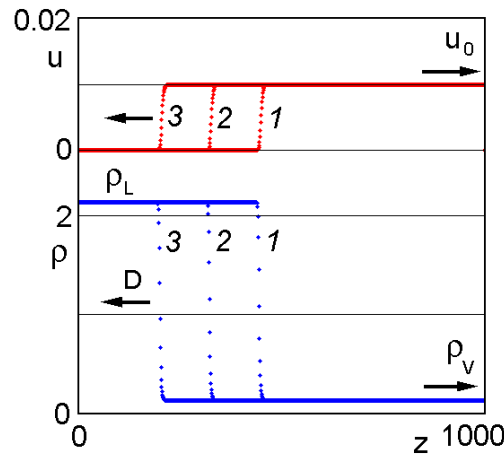


Figure 3. Simulation of the propagation of the evaporation wave for the model D1Q3. $u_0 = 0.01$, $\tilde{T} = 0.7$, $\tau = 0.8$, $k = 0.01$. $t = 500000$ (1), 700000 (2), 900000 (3).

The value of the mass flux density per unit surface of the liquid $J = \rho_L D$ for different values of relaxation time and temperature is shown in figures 4a,b,c. In numerical experiments, it turns out that the mass fluxes are proportional to the difference in the densities of the saturated and surrounding vapor $\rho_S - \rho_V$, which is in good agreement with the Hertz–Knudsen law. The dependence of the quasi-stationary evaporation flux, normalized to temperature (reduced flux), $F = J/\tilde{T}$ is shown in figure 4d for $\tau = 1$ and $k = 0.01$. The data can be also approximated well by a straight line, where the coefficient value $\alpha \approx 0.235$

$$F = \alpha(\rho_S - \rho_V). \tag{7}$$

However, in the model of lattice Boltzmann equations, the coefficient α also depends on the dimensionless relaxation time τ . The dependence of the quantity $\alpha(\tau) = F/(\rho_S - \rho_V)$ is shown in figure 5 for $k = 0.01$.

A satisfactory approximation of the calculated points is the function $\alpha \approx 0.123/(\tau - 0.5)$. In the LBM method, the dimensionless time determines the kinematic viscosity $\nu = (\tau - 1/2)/3$. As a result, the density of the evaporation flux from a flat liquid surface in the LBM method (at $k = 0.01$) can be approximately estimated by the formula

$$J \approx 0.041 \tilde{T} (\rho_S - \rho_V) / \nu. \tag{8}$$

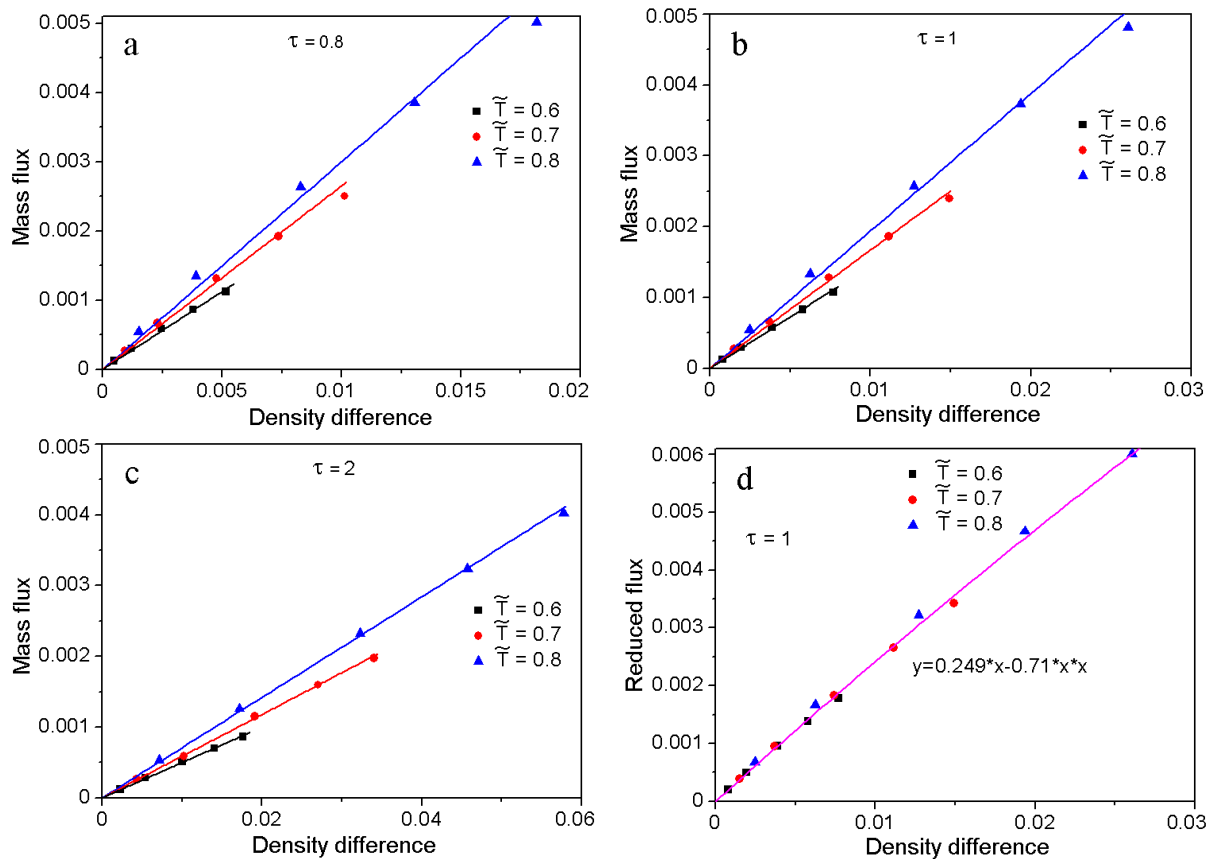


Figure 4. Dependence of the mass flux evaporating from a flat surface on the density difference. $\tau = 0.8$ (a), 1 (b), 2 (c). $\tilde{T} = 0.6, 0.7, 0.8$. Vapor outflow velocity $u_0 = 0.002, 0.005, 0.01, 0.015, 0.02$. (d) – Dependence of the reduced evaporation flux F on the density difference at $\tau = 1$.

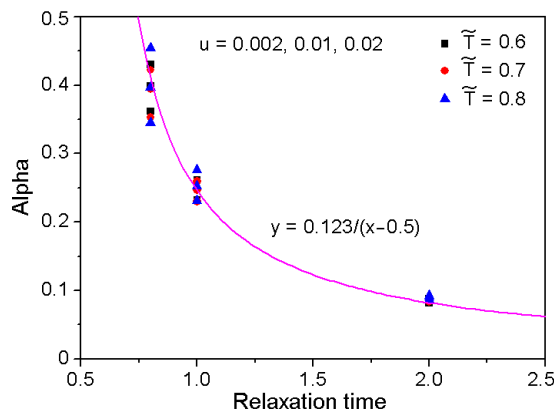


Figure 5. Dependence of the value of α on the dimensionless relaxation time τ . $k = 0.01$.

Conclusions

A simple method has been proposed for setting the vapor outflow on the flat boundary of the computational domain for the LBE method. An estimate has been obtained for the dependence of the evaporation flux from flat liquid layer for the LBE method on temperature, vapor outflow velocity, and kinematic viscosity. The stronger dependence of equation (8) on temperature, in comparison with the theoretical one, is apparently associated with a change in the thickness of the liquid-vapor

transition layer. Moreover, this is also related to the dependence on the dimensionless parameter k . For problems with evaporation of droplets, when the surface has a radius of curvature R , the saturated vapor density ρ_S must be corrected in accordance with the Laplace's law.

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