

Simulation of Substrate Cooling during Evaporation of Pure Vapor from the Surface of a Thin Liquid Film and Droplets

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Abstract—A numerical study of the process of cooling a substrate under the conditions of evaporation of pure vapor from the surface of a liquid film and droplets was carried out. The lattice Boltzmann method was used for modeling such a two-phase system taking into account the thermal conductivity of the substance and the evaporation. We used the van der Waals equation of state describing the liquid–vapor phase transition. A new method is proposed for setting the boundary conditions on a flat surface for modeling the contact wetting angles in the lattice Boltzmann method. The latent heat of phase transition is taken into account. It is shown that the process depends on the film thickness and the rate of vapor removal from the film surface. The cases of forced outflow of vapor, as well as the method of vapor condensation on a cooled condenser are considered. It is shown that the heat flux from the substrate increases sharply in the vicinity of the droplet contact lines. A comparison is made of the heat fluxes during the evaporation of the film and droplets on substrates with different wettabilities.

Keywords: lattice Boltzmann method, phase transition, dynamics of multiphase media, evaporation, heat flux, mesoscopic method, computer simulation

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INTRODUCTION

Liquid films and droplets are widely used to cool heated surfaces. The effectiveness of such methods is due to the fact that during evaporation the surface of the liquid cools due to the absorption of the latent heat of evaporation. At the same time, the evaporation process is associated with the parameters of the vapor near the evaporating surface, i.e., how much lower its density is than that of saturated vapor at a given surface temperature (the Hertz–Knudsen law) [1–3].

In real engineering structures, the outflow of vapor from the evaporating surface is carried out in several ways. In the simplest case, liquid vapors are carried away by diffusion in the surrounding gas. In the so-called heat pipes, the vapor condenses when enters a special section with a low temperature. The effect of enhancing heat transfer by contact lines created by breaking the film is well known, since in the vicinity of a contact line the thickness of the liquid decreases, the temperature gradient locally increases, and the heat flux intensifies [4–8]. Another method uses a flow of cold gas along the surface of a flowing film, which carries away the resulting vapor.

1. MATHEMATICAL MODEL

1.1. Lattice Boltzmann Method

The lattice Boltzmann method (LBE) [9–13] is successfully used to simulate two-phase liquid–vapor systems. In the LBE method, fluid flow is modeled by an ensemble of pseudoparticles, which, over a time step Δt , are transferred along the characteristics between neighboring nodes of the spatial

lattice. The system is described by a set of single-particle distribution functions f_k , $k = 0, \dots, m$, the evolution of which over the time step Δt is described by the equations

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

where \mathbf{c}_k are the velocity vectors of pseudoparticles. The hydrodynamic variables (density ρ and velocity \mathbf{u}) are calculated using the formulas

$$\rho = \sum_{k=0}^m f_k \quad \text{and} \quad \rho \mathbf{u} = \sum_{k=1}^m \mathbf{c}_k f_k.$$

The collision operator $\Omega_k\{f_k\}$ has the form of relaxation of distribution functions to local equilibrium [14],

$$\Omega_k\{f_k\} = (f_k^{\text{eq}}(\rho, \mathbf{u}) - f_k(\mathbf{x}, t)) / \tau,$$

where τ is the dimensionless relaxation time. The equilibrium distribution functions $f_k^{\text{eq}}(\rho, \mathbf{u})$ are written as an expansion of the Maxwell–Boltzmann distribution function for discrete velocities \mathbf{c}_k of particles

$$f_k^{\text{eq}}(\rho, \mathbf{u}) \sim \rho \exp\left(-\frac{(\mathbf{c}_k - \mathbf{u})^2}{2\theta}\right)$$

in a series in velocity \mathbf{u} up to the second order [15],

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

here θ is the normalized kinetic temperature of pseudoparticles, which is usually chosen equal to $\theta = (h/\Delta t)^2/3$, where h is the step of the computational grid.

The exact difference method (EDM) [16, 17] was used to take into account changes in the distribution functions Δf_k under the influence of internal and external forces,

$$\Delta f_k = f_k^{\text{eq}}(\rho, \mathbf{u} + \Delta \mathbf{u}) - f_k^{\text{eq}}(\rho, \mathbf{u}),$$

where the change in velocity per time step $\Delta \mathbf{u}$ is determined by the total force \mathbf{F} acting on the substance at the node, $\Delta \mathbf{u} = \mathbf{F} \Delta t / \rho$.

Two versions of the LBE method were used: one-dimensional D1Q3 with three pseudoparticle velocities and two-dimensional D2Q9 with nine velocities [18]. The coefficients in Eq. (1) for the one-dimensional D1Q3 version are equal to $w_0 = 2/3$, $w_{1,2} = 1/6$, and for the two-dimensional D2Q9 one, we have $w_0 = 4/9$, $w_{1-4} = 1/9$ and $w_{5-8} = 1/36$.

Computer simulation of phase transitions using the LBE method is an interface capturing method for calculating phase boundaries. Instead of a density discontinuity, a thin liquid–vapor transition layer is modeled in which the density changes smoothly on the scale of several lattice nodes (similar to the shock-capturing methods for shock waves in gas dynamics). In this case, the liquid and gaseous phases are described uniformly. To do this, forces acting between matter at neighboring lattice nodes are introduced (pseudopotential method). The total force acting on a node has the form $\mathbf{F} = -\nabla U$, where the pseudopotential $U = P(\rho, T) - \rho\theta$ is expressed via the equation of state [19]. These forces provide surface tension in a thin transition layer between phases where the density of the substance changes abruptly.

The paper [20] proposed a version of the LBE method to describe heat and mass transfer in a medium with phase transitions. This version takes into account evaporation and condensation in accordance with the equation of state of the fluid, the thermal conductivity of the substance, the work of pressure forces, and the heat of phase transition. To describe convective energy transfer, the passive scalar method (an additional set of distribution functions g_k) is used. The equations for the evolution of distribution functions are

$$g_k(\mathbf{x} + \mathbf{c}_k \Delta t, t + \Delta t) = g_k(\mathbf{x}, t) + \frac{g_k^{\text{eq}}(\rho, \mathbf{u}(\mathbf{x}, t)) - g_k(\mathbf{x}, t)}{\tau_E} + \Delta g_k(\mathbf{x}, t).$$

In this case, the internal energy per unit volume has the form $E = \sum_{k=0}^m g_k$. The equilibrium distribution functions $g_k^{\text{eq}}(\rho, \mathbf{u})$ are written similarly to Eq. (1). The work of pressure forces and heat transfer due to thermal conductivity are taken into account by the usual finite-difference method. In the one-dimensional case it has the form

$$\frac{\Delta E_i}{\Delta t} = -p_i \frac{u_{i+1}^* - u_{i-1}^*}{2h} + \lambda \frac{T_{i+1} - 2T_i + T_{i-1}}{h^2},$$

here the physical velocity \mathbf{u}^* is calculated using the formula [21]

$$\rho \mathbf{u}^* = \sum_{k=1}^m \mathbf{c}_k f_k + \mathbf{F} \Delta t / 2,$$

and λ is the coefficient of thermal conductivity. In this case, the changes in the distribution functions are equal to

$$\Delta g_k(\mathbf{x}, t) = g_k(\mathbf{x}, t) \frac{\Delta E_i}{E_i}.$$

The van der Waals equation of state was chosen as the equation of state. Reduced variables are used for density, pressure, and temperature, and lattice units are used for time and linear scales.

1.2. Heat of Phase Transition for van der Waals Gas

The internal energy of one mole of gas having the van der Waals equation of state

$$P = \frac{RT}{V-b} - \frac{a}{V^2},$$

is expressed by the formula $E_{\text{mol}} = E_{\text{ideal}} - a/V$ (see [22]).

For a unit mass of the substance, this can be written in the form $\varepsilon = C_V T - a\rho$ (specific internal energy), where C_V is the specific heat capacity at a constant volume. The heat of phase transition represents the change in the internal energy of the substance in the process of decreasing the density from liquid ρ_L to vapor ρ_V at a constant temperature. From the expression for internal energy we obtain

$$Q = \varepsilon_V - \varepsilon_L = a(\rho_L - \rho_V); \quad (2)$$

here ρ_L and ρ_V are the equilibrium densities of liquid and vapor. The dependence of the specific heat of phase transition on temperature $Q(T)$ is taken into account implicitly due to the dependences of ρ_L and ρ_V on temperature. The heat of phase transition decreases to zero as the temperature approaches a critical value.

The following formula was proposed in [20] for the change in the internal energy of a unit volume in a transition layer cell due to a phase transition:

$$\frac{dE}{dt} = \frac{\rho_L Q(T)}{\rho_L - \rho_V} \frac{d\rho}{dt}.$$

It is assumed that the heat of phase transition Q is released in the density variation range $[\rho_V, \rho_L]$; then taking into account Eq. (2) we obtain the expression

$$\frac{dE}{dt} = a\rho_L \frac{d\rho}{dt} = -a\rho_L \rho \operatorname{div}(\mathbf{u}^*).$$

2. RESULTS OF MATHEMATICAL MODELING

Several problems with combined (conductive and convective) heat transfer are considered that take into account liquid–vapor phase transitions and are solved by the lattice Boltzmann method. In one-dimensional settings, numerical calculations using models D1Q3 and D2Q9 have shown identical results.

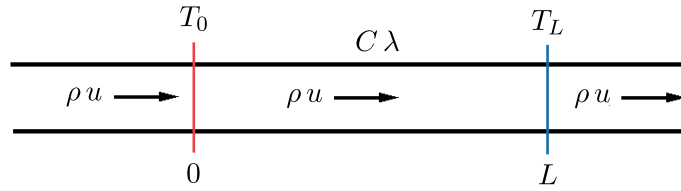


Fig. 1. Statement of the problem with a homogeneous flow of matter.

2.1. Test Problem with a Uniform Flow of Matter

A steady-state problem with a uniform flow of matter through a domain with a given temperature difference is considered (Fig. 1). The density of matter ρ and velocity u are constant. The temperature distribution in such a flow is described by the equation of conservation of the total heat flux

$$-\lambda \frac{dT}{dx} + \rho C u T = \text{const},$$

where C is the specific heat capacity of the substance. An analytic solution has been obtained for this problem,

$$T(x) = T_0 - \Delta T \frac{\exp(\alpha x) - 1}{\exp(\alpha L) - 1},$$

where L is the domain length, $\Delta T = T_0 - T_L$ is the temperature drop, and the coefficient $\alpha = \rho C u / \lambda$. The dimensionless parameter is the Péclet number $\text{Pe} = \alpha L$.

The heat flux due to thermal conductivity (conductive flux) is equal to

$$q_{\text{cond}} = -\lambda \frac{dT}{dx} = \rho C u \frac{\Delta T \exp(\alpha x)}{\exp(\alpha L) - 1},$$

and the flux due to energy transfer by moving matter (convective flux) is

$$q_{\text{conv}} = \rho C u \left(T_0 - \frac{\Delta T (\exp(\alpha x) - 1)}{\exp(\alpha L) - 1} \right).$$

Indeed, in this case the total flux along the coordinate x is constant,

$$q_{\text{total}} = \rho C u \left(T_0 + \frac{\Delta T}{\exp(\alpha L) - 1} \right).$$

Figure 2 shows a comparison of the analytical and numerical solutions by the LBE method for various values of the thermal conductivity coefficient $\lambda = 2$ ($\text{Pe} = 1.12$) and $\lambda = 20$ ($\text{Pe} = 0.112$). In this case, the colored curves (LBE calculations) are superimposed on the theoretical curves (black dotted line) and coincide up to the thickness of the lines. As thermal conductivity increases, the temperature and flux distributions tend to linear dependences.

It should be noted that for the internal energy in the LBE method there is diffusion associated with the relaxation time τ_E . In the general case, the effective thermal conductivity coefficient is the sum $\lambda_{\text{eff}} = \lambda + \rho C (\tau_E - 0.5) / 3$. With the values $\tau_E \rightarrow 0.5$, such diffusion can be neglected.

2.2. Steady-State Problem with a Phase Transition on the Liquid Boundary

The formulation differs from the previous problem in that the liquid evaporates. The problem is considered in the reference frame of the liquid–vapor interface. Liquid with temperature T_0 flows into the computational domain on the left. The thermal conductivity coefficient λ is specified for the liquid phase. The value of the thermal conductivity coefficient of vapor is assumed to be 20 times lower. An outflow of vapor at a given speed u_0 is ensured on the right boundary of the domain $x = L$.

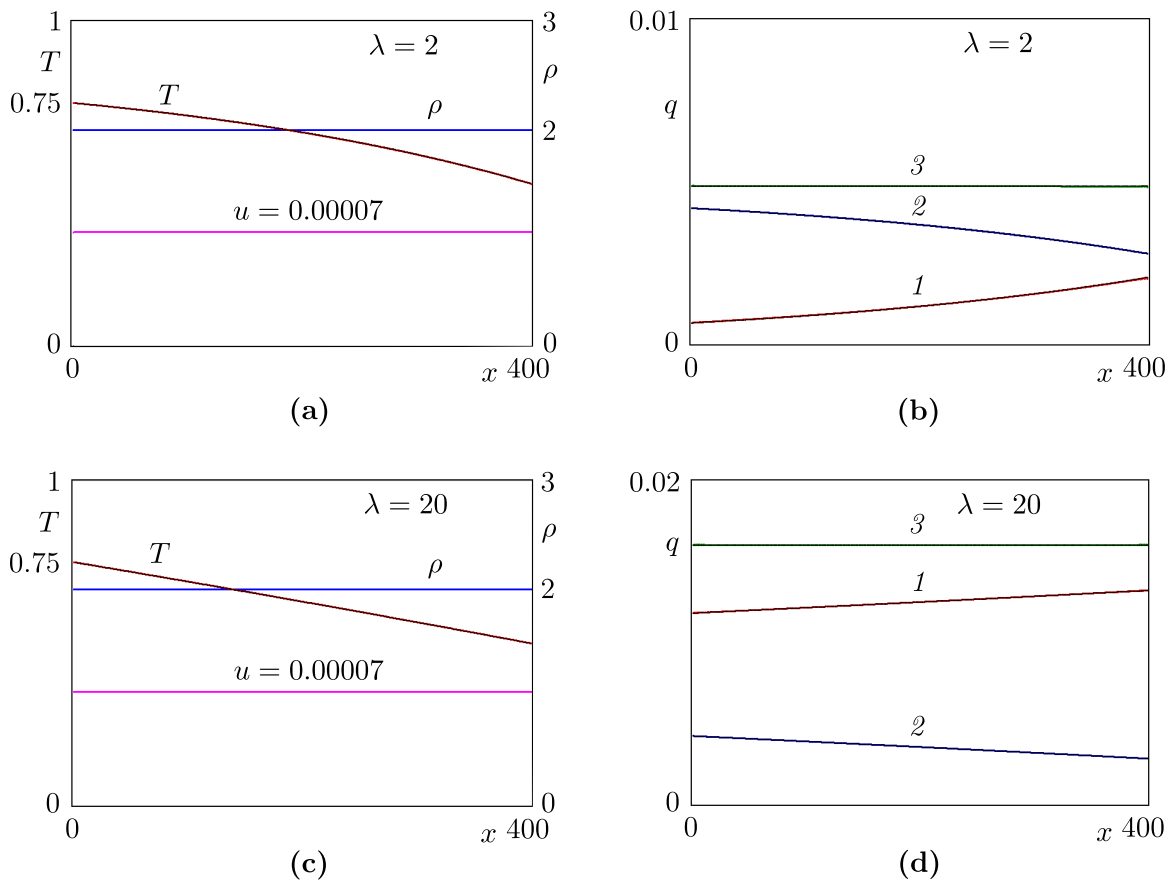


Fig. 2. Graphs of temperature, density, and velocity (a), (c). Graphs of conductive (curves 1), convective (curves 2), and total (curves 3) heat fluxes (b), (d). The density of matter is $\rho = 2$, the velocity is $u = 0.00007$, $T_0 = 0.75$, $T_L = 0.5$, $C = 40$, and $\tau_E = 0.5003$.

In this case, the mass flows of the inflowing liquid and the mass of the outflowing vapor are equal. To this end, boundary conditions for the LBE distribution functions f_k are set on the right boundary of the domain. In the one-dimensional case this corresponds to [3]

$$f_2(n_x + 1) = \beta f_1(n_x), \quad \text{where} \quad \beta = \frac{1 - 3u_0 + 3u_0^2}{1 + 3u_0 + 3u_0^2}.$$

For the evaporation process we have $u_0 > 0$ and, accordingly, $\beta < 1$. After some time, a steady-state distribution of temperature and density is established. The results are shown in Fig. 3. Heat is absorbed on the film surface due to the latent heat of evaporation at the phase boundary (curves 1 in Figs. 3a, 3c). As the coefficient of thermal conductivity increases, heat fluxes become greater despite the fact that the temperature difference decreases.

2.3. Liquid Film on the Surface of a Heated Substrate with Vapor Outflow

In the initial state, a film of the liquid phase with density ρ was set on the horizontal surface of the substrate, and saturated vapor was set above it. A small gravity field was specified with a free fall acceleration equal to $g = 10^{-7}$ in lattice units. The constant temperature T_0 and matter velocity u equal to zero were specified in the entire domain. Then the substrate temperature ($y = 0$) increased abruptly to $T = T_0 + \Delta T$. Due to the thermal conductivity of the liquid, the film begins to warm up. An outflow of vapor at a given speed u_0 is ensured at the upper boundary of the domain $y = L$. Then, in the one-dimensional case, a quasi-steady-state regime of vapor outflow is established between the film surface and the boundary of the domain after some time, i.e., a homogeneous vapor flow with constant speed, density, and temperature is created (Fig. 4a).

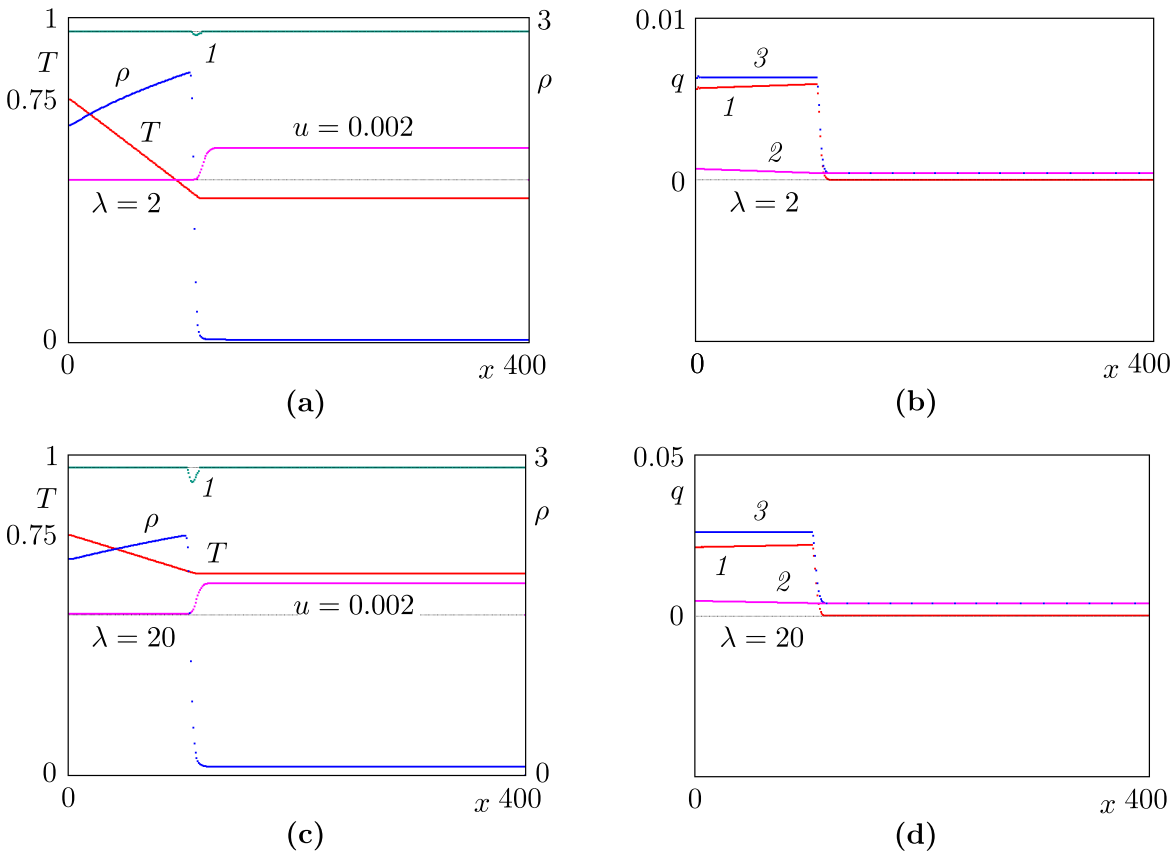


Fig. 3. Graphs of temperature, density, and velocity (a), (c). Graphs of conductive (curves 1), convective (curves 2), and total (curves 3) heat fluxes (b), (d); $C_V = 40$; $\lambda = 2$, $\tau_E = 0.505$ (a), (b); $\lambda = 20$, $\tau_E = 0.501$ (c), (d).

The heat flux from the heated substrate to the surface of the liquid film depends on its thermal conductivity, thickness, and temperature difference. For thin films and relatively high thermal conductivity of the liquid, the temperature distribution over the film thickness in the quasi-steady-state evaporation mode is close to linear (Figs. 4a, 4b). Heat is absorbed on the film surface due to the latent heat of evaporation at the phase boundary (curves 1 in Figs. 4a, 4b). The heat flux removed from the substrate depends on the rate of evaporation of the liquid on the surface, i.e., on the rate of vapor outflow from the film. As the vapor outflow rate increases, the heat flux from the substrate increases. The heat flux also depends on the film thickness d (Fig. 4c). With a constant temperature difference, the dependence on $1/d$ should be linear, $q = \lambda \Delta T / d$ (curve 2). However, the temperature drop on the film also depends on its thickness (Figs. 4a, 4b), so the dependence on $1/d$ turns out to be nonlinear (curve 1 in Fig. 4c).

2.4. Liquid film on the Surface of a Heated Substrate with Vapor Condensation on the Upper Boundary of the Domain

In the initial state, films of the liquid phase were created on the surface of the substrate and on the upper boundary, with saturated vapor between them (Fig. 5a). A small gravity field was specified with the free fall acceleration equal to $g = 10^{-7}$ in lattice units. The constant initial temperature T_0 and velocity u equal to zero were specified in the entire domain. Then the substrate temperature increased abruptly to $T = T_0 + \Delta T$ and decreased to T_{con} at the upper boundary of the domain $y = L$ (condenser). After some time, a quasistationary regime is established, in which evaporation of the film on the substrate occurs with the absorption of latent heat of evaporation and condensation of vapor on the surface of the liquid film at the cold boundary of the domain with the release of latent heat of condensation (curve 1 in Fig. 5b). In fact, this is a model of heat pipes, widely used in technology for cooling equipment and microelectronics.

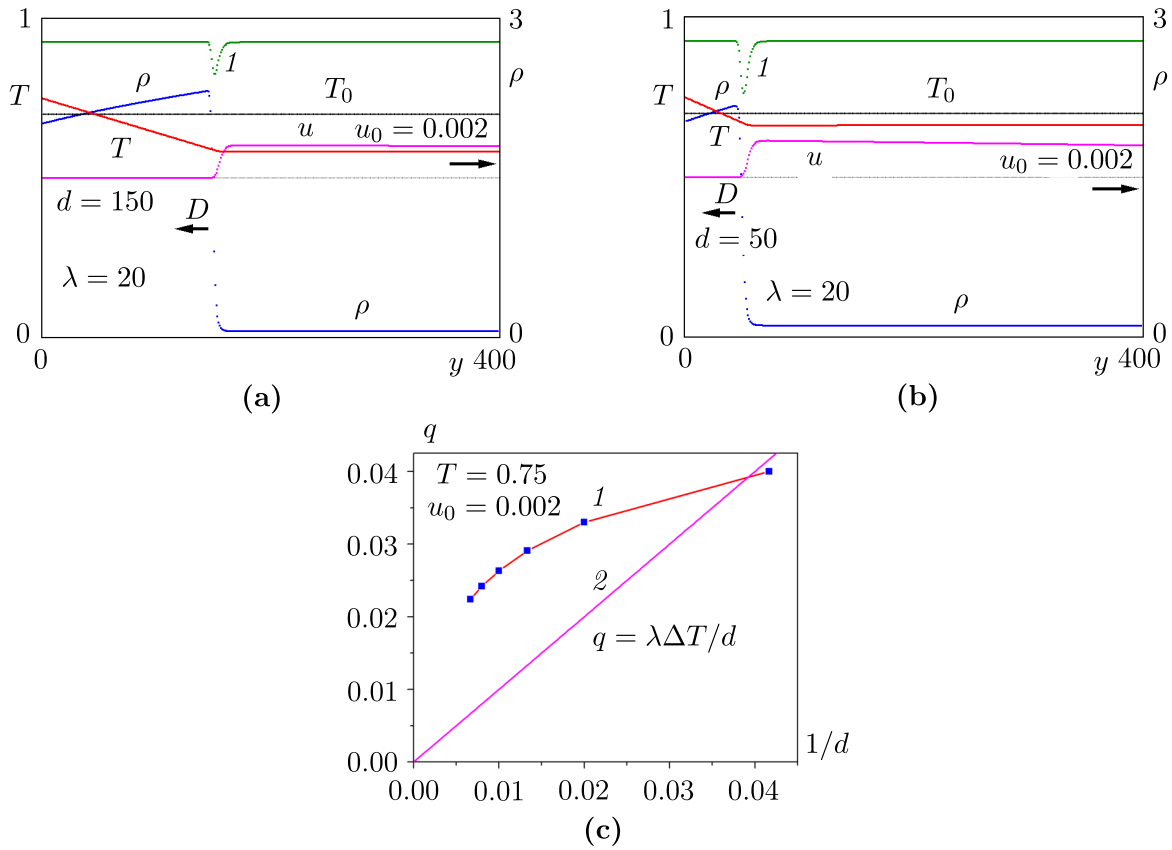


Fig. 4. Quasi-steady-state flow regime with vapor outflow at the upper boundary (a), (b); $u_0 = 0.002$. The initial state is $T_0 = 0.7$, $u = 0$. The current film thickness is 150 (a) and 50 (b). The substrate temperature is $T = 0.75$. The thermal conductivity coefficient is $\lambda = 20$. Dependence of heat flux from the substrate q on the current thickness of the evaporating liquid film d (c).

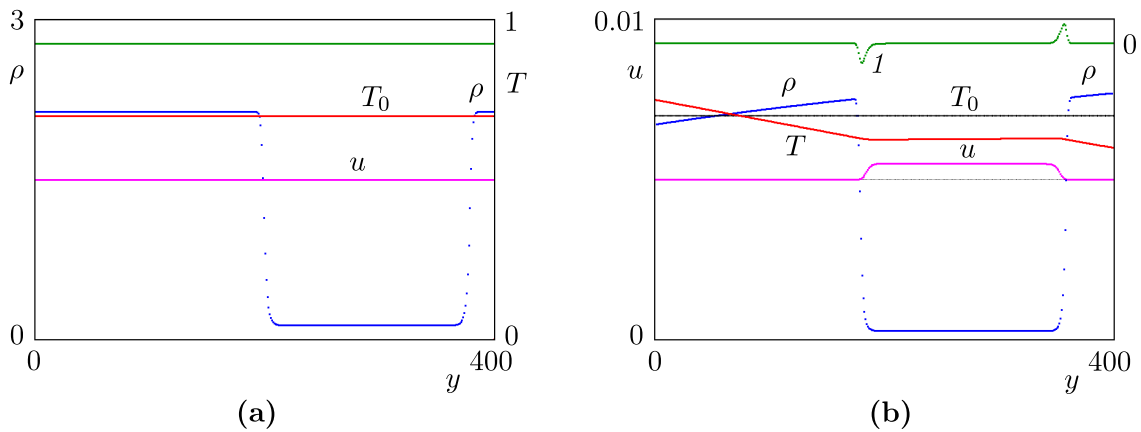


Fig. 5. Initial state: $T_0 = 0.7$, $u = 0$ (a). Quasi-steady-state flow regime (b). The state after switch on of substrate heating $T = 0.75$ and vapor condenser $T_{con} = 0.6$. The thermal conductivity $\lambda = 20$.

2.5. A Droplet of Liquid on the Surface of the Heated Substrate with Condensation of Vapor on the Upper Boundary of the Domain

A droplet of liquid of a “hemispherical” shape was placed on the surface of the substrate, a film of the liquid phase was created on the upper boundary, and “saturated” vapor was created between them (Fig. 6a). A small gravity field was specified with a free fall acceleration equal to $g = 10^{-7}$ in

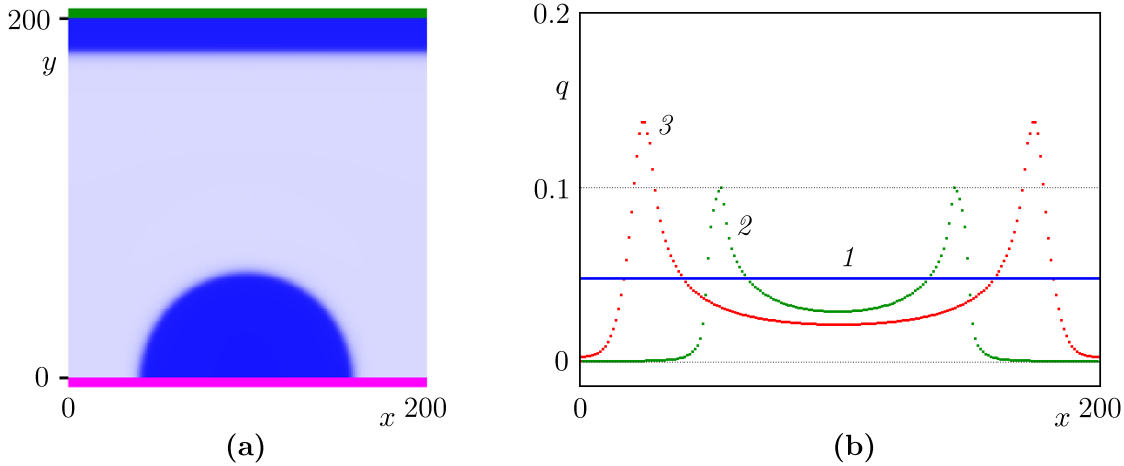


Fig. 6. Droplet on a solid substrate (a). Initial droplet radius $R = 60$, contact angle is 90° , $T_0 = 0.7$, $u = 0$; 2D calculation grid size is 200×200 . Heat flux distribution over the substrate (b): 1 flat film, 2 droplet with neutral wetting, 3 droplet on a hydrophilic surface ($\beta = -0.3$). Substrate temperature $T = 0.75$; vapor condenser temperature $T_{\text{con}} = 0.6$; thermal conductivity coefficient of liquid $\lambda = 20$.

lattice units. In the two-dimensional case, forces of interaction of the fluid with three neighboring nodes of the solid surface are introduced to ensure neutral wetting of the substrate [23, 24],

$$\mathbf{F}(\mathbf{x}) = \Phi(\mathbf{x}) \sum_{j=1}^3 w_j B \Phi_{\text{solid}}(\mathbf{x} + \mathbf{e}_j) \cdot \mathbf{e}_j.$$

Here the function Φ_{solid} at a solid surface node takes on a value equal to the value of the function $\Phi(\mathbf{x}) = \sqrt{-U}$ at the nearest node of the fluid; w_j are weighting coefficients. The parameter B determines the surface wettability and the contact angle. For neutral wettability we have $B = 1$. The disadvantage of the methods [23, 24] when wettability changes is that the liquid density changes in the adjacent thin liquid layer. In this paper, to make it possible to vary the values of contact angles, a new method that is devoid of this drawback is proposed. In this method, in addition to neutral wetting with $B = 1$, only the horizontal components of the forces acting on the fluid nodes adjacent to the substrate are additionally introduced,

$$F_x(\mathbf{x}) = \beta \Phi(\mathbf{x}) \sum_{j=1}^3 \Phi_{\text{solid}}(\mathbf{x} + \mathbf{e}_j) \cdot e_{jx}.$$

The factor $\beta = 0$ corresponds to neutral wetting, $\beta < 0$ corresponds to hydrophilic and $\beta > 0$, to hydrophobic surfaces.

In the initial state, the constant temperature T_0 and velocity u equal to zero were specified throughout the entire domain $L \times L$. Then the substrate temperature increased abruptly to $T(x, 0) = T_0 + \Delta T$, and at the upper boundary of the domain, with $y = L$, it dropped to $T_{\text{con}} < T_0$. Periodic boundary conditions $f_k(L, y) = f_k(0, y)$ and $g_k(L, y) = g_k(0, y)$ were used for the distribution functions along the x -coordinate. After this, the drop warms up and the liquid evaporates from its surface. Vapor condenses on the cooled film at the top of the domain. Figure 6a shows the initial fluid density distribution.

The heat flux q from the substrate is considerably higher in the vicinity of the droplet contact lines (Fig. 6b, curves 2 and 3); this corresponds to the experiments in [4–8]. In this case, a decrease in the contact angle increases the contribution of the contact lines (curve 3).

In the two-dimensional case, the total heat flux from the substrate is calculated as follows:

$$q_{\text{total}} = - \int_0^L \lambda_{\text{eff}}(x, 0) \left. \frac{\partial T}{\partial y} \right|_{y=0} dx.$$

For a droplet with neutral wetting it is equal to $q_{\text{total}} = 4.9$ (curve 2), and for a droplet on a hydrophilic surface, $q_{\text{total}} = 7.6$ (curve 3). These values are lower than the heat flux for a flat film of the same volume, $q_{\text{total}} = 9.8$ (curve 1). Thus, a decrease in the contact angle increases heat removal in the vicinity of the contact line.

CONCLUSIONS

A simulation of the substrate cooling process under conditions of evaporation of pure vapor from the surface of the film and liquid droplets was carried out using the lattice Boltzmann method. A new method for setting boundary conditions on a flat surface for modeling contact wetting angles in the LBE method is proposed. It is shown that the substrate cooling process depends on the thickness of the film and the rate of vapor removal from its surface. Cases of forced outflow and condensation of vapor on a cooled condenser are considered. It is shown that the heat flux from the substrate increases strongly in the vicinity of the contact lines of the droplets. A comparison was made of heat fluxes during the evaporation of the film and droplets on substrates with different wettabilities. The total heat removal from the substrate for droplets turned out to be less than for a flat film of the same volume and approximately the same surface area.

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