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LATTICE- BOLTZMANN METHOD FOR SIMULATING TWO-COMPONENT FLUID FLOWS

Abstract. In this work, a model of binary fluids with different densities and viscosities based on the solution of the Navier-Stokes equations, the continuity and the Cahn-Hilliard equation is developed. The process of influence of surface tension and interface thickness on the phase fields of fluids is investigated. The numerical results of the study are obtained on the basis of a phase field model using the lattice Boltzmann method (LBM). The LME uses two sets of distribution functions for incompressible flow: one for tracking the pressure and velocity fields and the other for the phase field. The use of the pressure distribution function can significantly reduce the effect of numerical errors in calculating the interfacial force. A several 2D tests are carried out to demonstrate the validation, which included droplet problem and the Raleigh- Taylor instability. It is shown that the proposed method allows tracking the interface with high accuracy and stability.

Key words: phase field, binary fluid, surface tension, chemical potential, lattice Boltzmann method.

Introduction

Numerical modeling of multiphase fluid flows plays an important role in solving many applied scientific and engineering problems, including, for example, oil and gas production, chemical processing of raw materials, and steam-water mixture flows in boilers and condensers. In recent years, more and more attention has been paid to such problems due to their importance for the development of digital microfluid and the development of the laboratory of liquid crystals, gels, suspensions, and also some other technologies. Thus, the study of multiphase fluid flows is an urgent task today.

Interface tracking is widely used in two-phase flow models, which can be divided into two categories: sharp interface methods such as volume-of-fluid methods, level-sets and front-tracking methods, diffuse interface methods. The diffuse interface approach [1] has some advantages over the others in terms of maintaining mass conservation and in the ability of resolving interface curvature with higher accuracy. The main idea of diffuse interface models is to replace sharp interfaces with transition regions of a thin but nonzero layer of thickness, where density, viscosity and other physical quantities smoothly change from the values of one fluid to the values of another.

Among diffuse interface methods, the phase field method [4-5] has become a widely used method in traditional computational fluid dynamics (CFD) and lattice Boltzmann equations (LBM) methods for numerical investigation of complex interphase dynamics. In the phase field method, the thermodynamic behavior of liquids is expressed using the free energy functional of the continuous order parameter [2], which acts as a phase field to distinguish between two-phase fluids. The phase separation equation is formulated for the order parameter that defines the Cahn-Hilliard equation [13].

The concept of a diffuse interface was first proposed by [7], but it has gained popularity only in recent years as a tool for the numerical simulation of two-phase flows. There are many works on the study of multiphase models using various numerical methods [9-12]. The motion of a two-dimensional droplet using a stepwise wettability gradient (WG) was studied in [3]. Also, the diffuse boundary method for simulating the phase separation of complex viscoelastic fluids was investigated in [6] and a model of a binary fluid with free energy for the three-dimensional Bretherton problem (flow between parallel plates) performed in [8]. All of these works have a different modeling approach for boundary tracking and phase separation of liquids with different densities and viscosities. The main difference between these works is the choice of methods for numerical implementation.

In this paper, we introduce multiphase flow model for incompressible binary fluids, when interface between the different phases is tracked by LBE. To simulate phase interface, we derive free-energy based phase field method. To distinguish transition between different phases we set order of parameter ϕ. Also we obtain the numerical implementation of influence surface tension force (σ) and interface thickness (W) on the phase field.

Statement of the problem

To check the numerical algorithm, the results obtained within the framework of solving this problem were compared with the results obtained experimentally, which showed good agreement.

A mixture of two immiscible incompressible fluid in a rectangular region Ω with densities ρ_A,ρ_B and dynamic viscosity η_A,η_B is considered (Figure 1). For the computational domain, a two-dimensional rectangle with the corresponding dimensional parameters was taken: $x \in [0,1]$, $y \in [0,1]$. In the center of the area $x \in [0.2, 0.8]$, $y \in [0.4, 0.6]$ is situated a liquid drop with density ρ_A and viscosity η_A.

To distinguish the two different fluids, the order of parameter (phase field function) is introduced

$$\phi = \begin{cases} \phi_A, & fluid \text{ A} \\ \phi_B, & fluid \text{ B} \end{cases}$$

For a system of binary fluids, the Landau free energy function F can be defined on the basis of ϕ as:

$$F(\phi, \nabla\phi) = \int_V [\Psi(\phi) + \frac{k}{2}|\nabla\phi|^2] dV$$

where $\Psi(\phi)$ –the bulk free energy density, for an isothermal system the following form can be used $\Psi(\phi) = \beta(\phi - \phi_A)^2(\phi - \phi_B)^2$, k – is the coefficient of surface tension, β – is the coefficient depending on the interface thickness and the surface tension force.

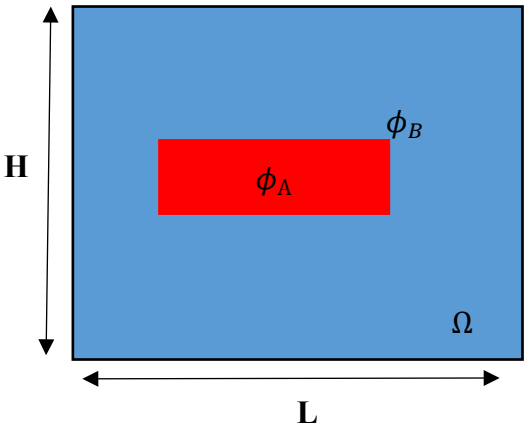


Figure 1 – Computational domain of bubble immersed in liquid

The basic equations for the phase field consist of the continuity equation, the momentum equation for the mixture and the covective Cahn-Hillart equation:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$

$$\rho\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right) = -\frac{\partial P}{\partial x} - \phi\frac{\partial \mu}{\partial x} + \eta\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$

$$\rho\left(\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y}\right) = -\frac{\partial P}{\partial y} - \phi\frac{\partial \mu}{\partial y} + \rho g + \eta\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right)$$

$$\frac{\partial \phi}{\partial t}+\frac{\partial(\phi u)}{\partial x}+\frac{\partial(\phi v)}{\partial y}=M(\frac{\partial^2 \mu}{\partial x^2}+\frac{\partial^2 \mu}{\partial y^2})$$

where u,v – are the velocity components, p – is the pressure, $\rho=\frac{\phi-\phi_B}{\phi_A-\phi_B}\rho_A+\frac{\phi_A-\phi}{\phi_A-\phi_B}\rho_B$ – is the density, here ρ_A,ρ_B – are the density of fluids, $\eta=\frac{\eta_A\eta_B(\phi_A-\phi_B)}{(\phi-\phi_B)\eta_B+(\phi_A-\phi)\eta_A}$, here $\eta_A=\rho_A\vartheta_A,\eta_B=\rho_B\vartheta_B$ – are the dynamic viscosity, ϑ_A,ϑ_B – are the kinematic viscosity, ϕ – is the phase field function , g – is the acceleration of gravity, M – is the mobility coefficient, μ- is the chemical potential, $F_x=-\phi\frac{\partial \mu}{\partial x}$, $F_y=-\phi\frac{\partial \mu}{\partial y}$ are the surface tension force, $F_b=\rho g$ is the acceleration force.

The variation of the free- energy function F with respect to the function ϕ is solving chemical potential μ as :

$$\mu=\frac{\delta F}{\delta \phi}=\frac{d\Psi}{d\phi}-k\nabla^2\phi=$$
$$=4\beta(\phi-\phi_A)(\phi-\phi_B)(\phi-\frac{\phi_A+\phi_B}{2})-k\nabla^2\phi\ ,$$

where $W=\frac{1}{|\phi_A-\phi_B|}\sqrt{\frac{8k}{\beta}}$- is the interface thickness, $\sigma=\frac{|\phi_A-\phi_B|^3}{6}\sqrt{2k\beta}$ – is the surface tension force.

The system of equations has the following initial and boundary conditions:

$$u=0,v=0,\phi=$$
$$=\begin{cases}\phi_A, & x,y\notin\Omega\\ \phi_B, & x,y\in\Omega\end{cases}\ at\ t=0,0\le x\le L,0\le y\le H$$

$$u=0,v=0,\frac{\partial\phi}{\partial x}=$$
$$=0\ \ at\ x=0\ и\ x=L\ ,0\le y\le H$$

$$u=0,v=0,\frac{\partial\phi}{\partial y}=0\ at\ y=0$$
$$и\ y=H,0\le x\le L$$

Numerical method

We use the lattice Boltzmann equation (LBE) to describe the motion of binary fluids. For this case, the collision term LBM in a two-dimensional square lattice with nine velocities (D2Q9) was used. The lattice Boltzmann equation in the Batnagar-Gross-Krook (BGK) [15] approximation is as follows:

$$f_i(x+e_i\Delta t,t+\Delta t)-f_i(x,t)=$$
$$=-\left(\frac{f_i(x,t)-f_i^{eq}(x,t)}{\tau_f}\right)+(1-\frac{\Delta t}{2\tau_f})F_i(x,t)\Delta t$$

$$g_i(x+e_i\Delta t,t+\Delta t)-g_i(x,t)=$$
$$=-\left(\frac{g_i(x,t)-g_i^{eq}(x,t)}{\tau_\phi}\right)+$$
$$+\Gamma[g_i^{eq}(x+e_i\Delta t,t)-g_i^{eq}(x,t)]$$

where f_i,g_i – are the velocity and phase field distribution function respectively, e_i- is a discrete lattice velocity, τ_f,τ_ϕ- are the relaxation time for the velocity and phase field respectively, F_i- is a force term, $\Gamma=2\tau_\phi-1$ constant controlling the mobility, Δt - is a time step, f_i^{eq},g_i^{eq} – are the equilibrium distribution function for the velocity and phase field respectively.

The equilibrium distribution functions are introduced as following:

$$f_i^{eq}=$$
$$=\begin{cases}-(1-w_0)\frac{p}{c_s^2}-w_0\frac{u\cdot u}{2c_s^2}\ ,i=0\\ w_ip+c_s^2\rho w_i\left[\frac{e_i\cdot u}{c_s^2}+\frac{(e_i\cdot u)^2}{c_s^4}-\frac{u^2}{2c_s^2}\right],i\neq 0\end{cases}$$

$$g_i^{eq}=\begin{cases}\phi-\frac{(1-w_0)\Gamma\mu}{(1-\Gamma)c_s^2}\ ,i=0\\ w_i\frac{\Gamma\mu+(e_iu)\phi}{(1-\Gamma)c_s^2}\ ,i\neq 0\end{cases}$$

where $c_s^2=\frac{1}{3}$ - is a lattice sound speed, $p_b=c_s^2\rho+\beta(-\frac{1}{2}\phi^2+\frac{3}{4}\phi^4)$ - is a pressure of a mixture.

For the D2Q9 model, discrete velocities are calculated as:

$$e_{ix}=(0,1,1,0,-1,-1,-1,0,1)c$$

$$e_{iy}=(0,0,1,1,1,0,-1,-1,-1)c$$

The values of the weighting parameters are defined as:

$$w_i = \begin{cases} \frac{4}{9} & i = 0 \\ \frac{1}{9} & i = 1,2,3,4 \\ \frac{1}{36} & i = 5,6,7,8 \end{cases}$$

In this paper, the scheme proposed by Guo et al. [14] is used to approximate the external force in the LBM:

$$F_i(x,t) = \left(1 - \frac{1}{2\tau}\right) w_i \left(3\frac{c_i - u}{c_s^2} + 9\frac{c_i - u}{c_s^4} c_i\right) F$$

where, $F = (F_x + F_y + F_b)$

The evolution equation is divided into two steps, collision and propagation:

1. $f_i^*(x,t) = f_i(x,t) - \frac{\Delta t}{\tau_f}\left(f_i(x,t) - f_i^{eq}(x,t)\right) + (1 - \frac{\Delta t}{2\tau_f})F_i(x,t)\Delta t$
   $f_i(x + c_i\Delta t, t + \Delta t) = f_i^*(x,t)$
2. $g_i^*(x,t) = g_i(x,t) - \frac{t}{\tau_\phi}(g_i(x,t) - g_i^{eq}(x,t))$
3. $g_i(x + c_i\Delta t, t + \Delta t) = g_i^*(x,t)$

After the second step, we update the macroscopic parameters (density, phase field, velocity) using the following formulas:

$$\rho = \sum_i f_i, \rho u_\alpha = \sum_i f_i c_\alpha + \frac{F\Delta t}{2}, \phi = \sum_i g_i$$

The following boundary conditions were used to close the system of equations.

Zero velocity condition for all walls:

$$f_i(x_w, t + \Delta t) = f_{-i}(x_w, t + \Delta t), \quad e_i \cdot n > 0,$$

Neumann condition for phase filed on all walls:

$$g_i(x_w, t + \Delta t) = g_{-i}(x_w, t + \Delta t), \quad e_i \cdot n > 0,$$

Numerical results and discussions

First we performance, the numerical calculations of problem where, a stationary droplet immersed in another fluid. This task is used to assess the capability of the proposed model in handling the surface force. Initially, a round drop with a radius of 20 (in lattice units) is placed in the center of a square computational domain with a size of 100x100.

Table 1 – Modeling parameters

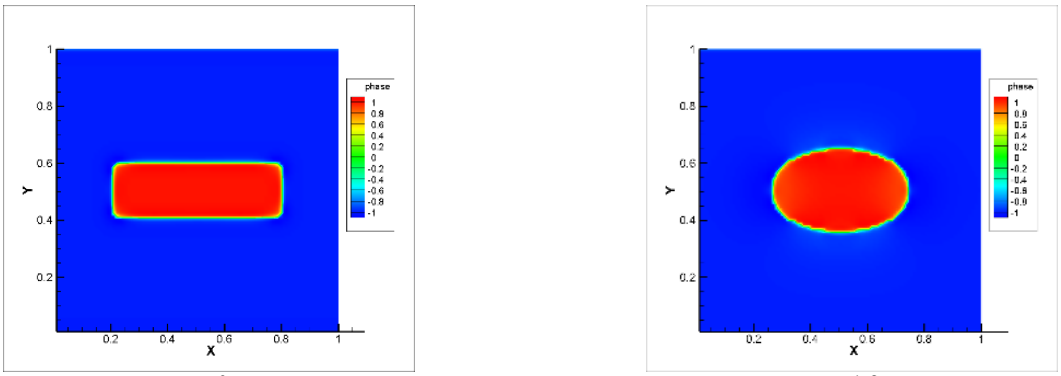
Parameters	Physical parameters	LBM parameters
Characteristic length	$L_{char} = 0.01$	
Number of points by x, y	$N_x \times N_y = 128 \times 256$	
Kinematic viscosity	$\vartheta = \frac{\eta}{\rho}$	$\vartheta = c_s^2(\tau - \frac{1}{2})\frac{\Delta x^2}{\Delta t}$
Characteristic time	$T_{char} = \sqrt{\frac{L_{char}}{g_{char} * At}}$	$\tau = c_s^2(\tau - \frac{1}{2})\frac{\Delta x^2}{\vartheta}$
Maximum velocity	$U_{char} = \sqrt{L_{char} g_{char}} = 0{,}31305$	$U_{lbm} = \frac{U_{char}}{c_u}, c_u = \frac{\Delta x}{\Delta t}$
Mixture density	$\rho_{A.char} = 800,\ \rho_{B.char} = 600$	$\rho_A = \frac{\rho_{A.char}}{\rho_{A.char}}, \rho_B = \frac{\rho_{B.char}}{\rho_{A.char}}$
Dynamic viscosities of fluids A and B	$\eta_{A.char} = 0.02,\ \eta_{B.char} = 0.01$	$\eta_A = \frac{\eta_{A.char}}{\eta_{char}}\ \eta_B = \frac{\eta_{B.char}}{\eta_{char}}$

Model parameters are set as: $\tau_f = \tau_\phi = 1, \phi_A = 1, \phi_B = -1, \rho_A = 1, \rho_B = 0.7$. The basic dimensionless parameters for the droplet problem are shown in table 1.

The time step was taken $\Delta t = 0.0001$ seconds. In numerical simulation, when interface width W and the surface tension σ are given, the coefficients k and β can be determined as follows:

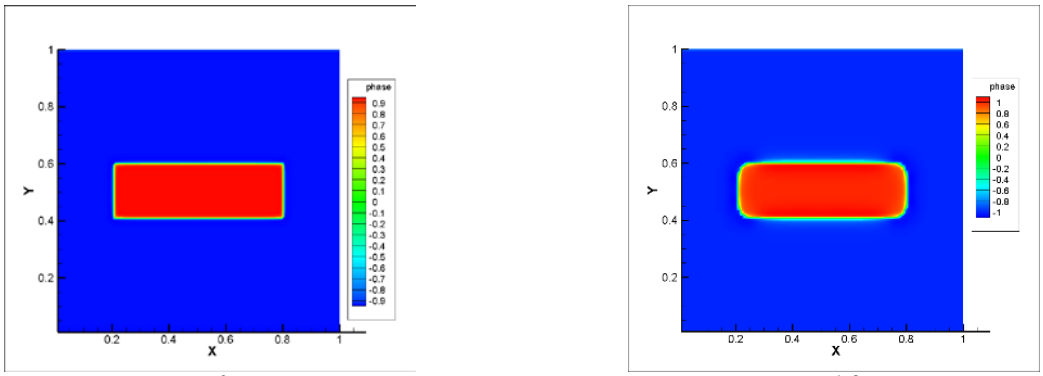
$$k = \frac{3\sigma W}{8}, \beta = \frac{3\sigma}{4W}$$

The numerical solution showed that with decrease the coefficient σ of surface tension, leads to decrease a chemical tension of the phases, as shown in Figure 2.



t= 0 t= 1.3

Figure 2 – The dynamics of the change in the shape of a drop in a fluid at different time for $\sigma = 0{,}01, W = 1$. The time normalized by characteristic time T_{char}



t= 0 t= 1.3

Figure 3 – The dynamics of the change in the shape of a drop in a fluid at different time for $\sigma = 0{,}001, W = 1$. The time normalized by characteristic time T_{char}

Figure 3 shows when surface tension σ is decrease , the force of surface attraction decreases and the shape of the drop does not change. In addition, with an increase interface thickness coefficient W, the surface tension β decreases, which contributes to a more rapid formation of a ball-like shape, as shown in Figure 4.

To further demonstrate the ability of this model to solve more complex flows, we simulated the Rayleigh-Taylor instability, which occurs when there is a small disturbance at the interface between a heavy (fluid A) and a light fluid (fluid B).

The basic dimensionless parameters for the Rayleigh-Taylor instability problem are shown in table 1. The initial interface between the two fluids is shown in Figure 5 (t=0). Reflection boundary conditions are applied to the lower and upper boundaries, and periodic boundary conditions are applied to the side boundaries. In our simulations, the physical parameters are fixed as:

$U_{char} = 0.04, W = 4, \sigma = 0.1,$

$$Re = \frac{\rho_{char} U_{char} L_{char}}{\eta_{char}}, At = \frac{\rho_{A.char} - \rho_{B.char}}{\rho_{A.char} + \rho_{B.char}} = 0.1$$

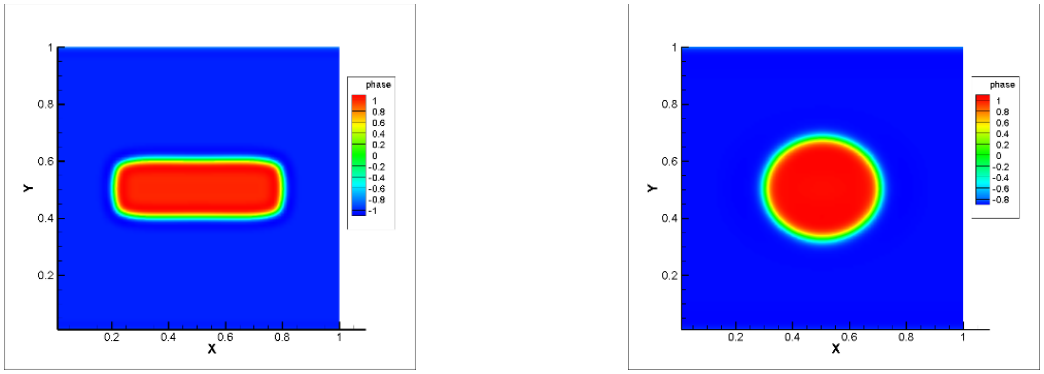


Figure 4 – The dynamics of the change in the shape of a drop in a fluid at different time for $\sigma = 0{,}01, W = 4$

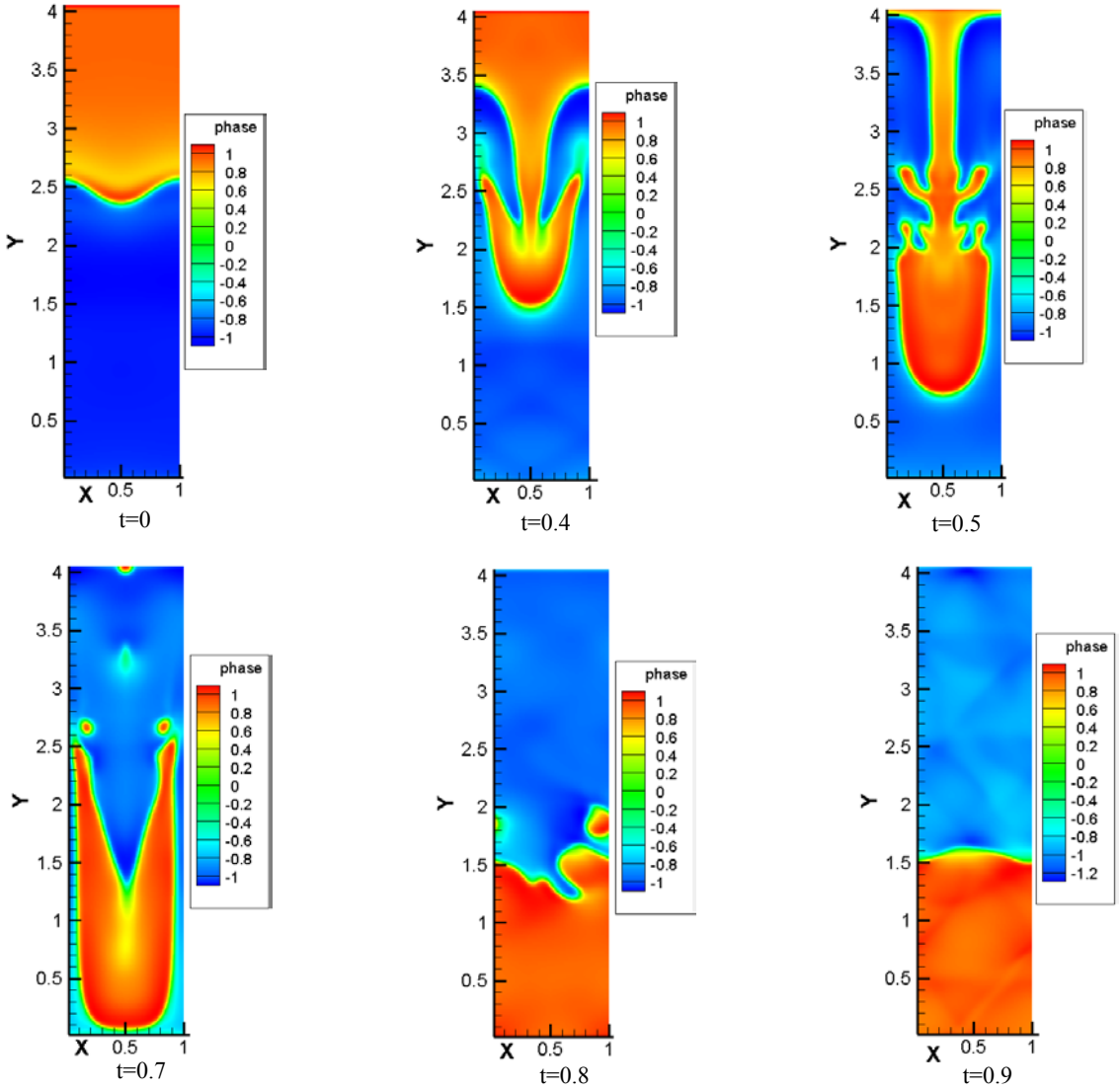


Figure 5 – Dynamics of concentration separation in the fluid phase at different times

In the early stages, the growth of the fluid interface remains symmetrical up and down. Later, the heavy liquid settles down, and the light fluid rises, forming bubbles. Starting from t = 0.4 (Fig. 5), the heavy fluid begins to curl up into two oncoming vortices. These discontinuities disappear over time, as at t = 0.7 , the Rayleigh-Taylor instability appears. At t = 0.9 , it can be seen that the heavy fluid has completely settled, and the light fluid has gone up. Thus, the problem of the Rayleigh-Taylor instability describes well the process of settling of a heavy fluid.

The problem was also solved for the case when $At = 0.1428, \tau_f = 0.8, \sigma = 0,01, W = 2$. Below in Figures 6- 8 the simulation result is shown, which illustrates the dynamics of concentration separation of a mixture of heavy and light liquids at different times: Figure 6 - for times t = 0; 0.2; 0; 32; 0.36 (from left to right, respectively); Figure 7 - t = 0.4; 0.5; 0.56; 0.6 (left to right, respectively); Figure 8 - t = 0.64; 0.72; 0.74; 0.8 (left to right, respectively). It can be seen from the figures that for the case when a more viscous liquid is considered (the separation boundary of the mixture components is thinner), a slower process of establishing equilibrium is observed - over time, first the formation of vortices occurs, then a rupture of the interface of the liquid boundaries is observed, the formation of separate structures of a fluid of higher density occurs inside a fluid of lower density, the formation of bubbles, the boundary of which breaks over time, equilibrium is established due to the chemical velocity of attraction of the phases.

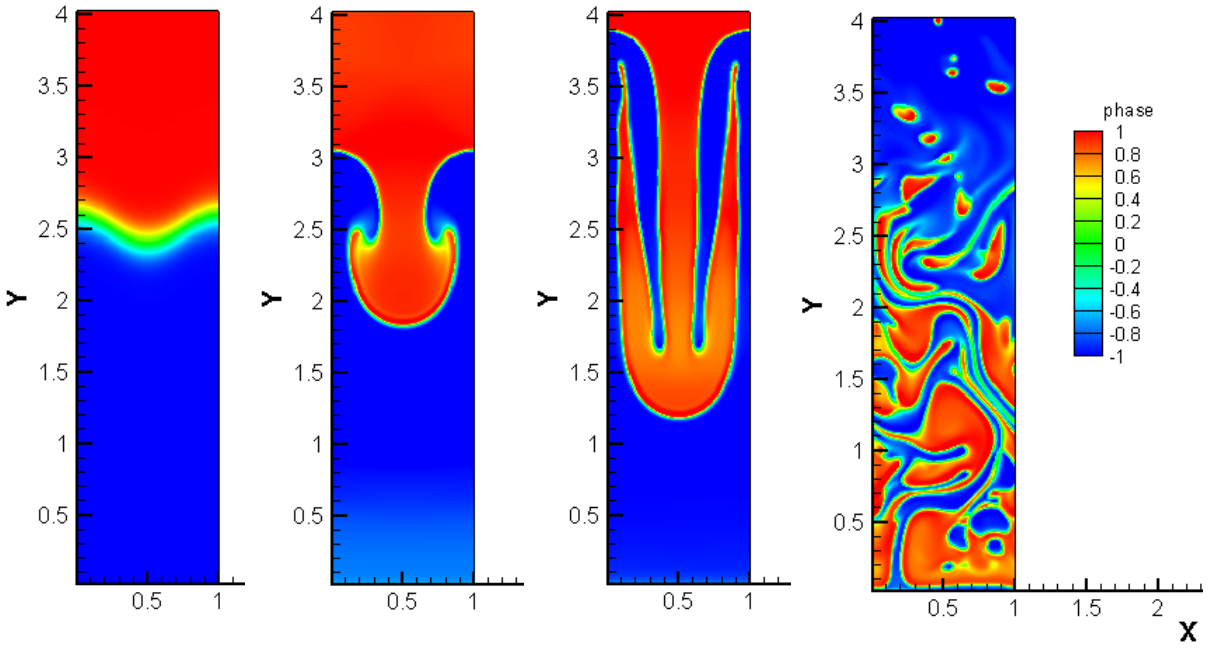


Figure 6 – Dynamics of concentration separation in the fluid phase at different times

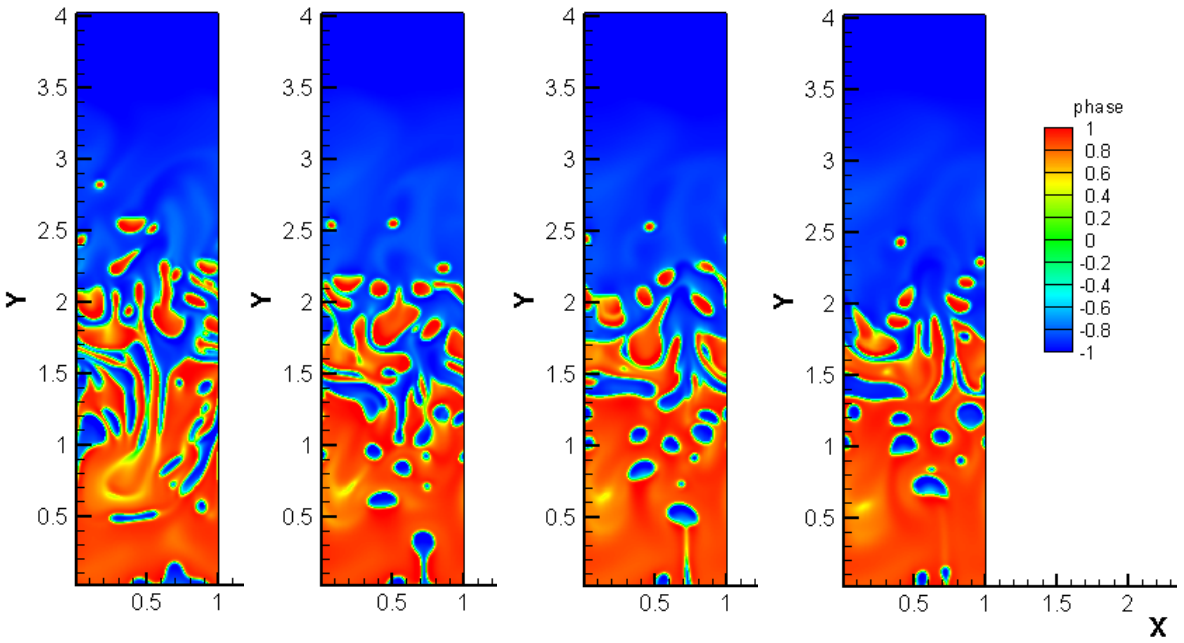


Figure 7 – Dynamics of concentration separation in the fluid phase at different times

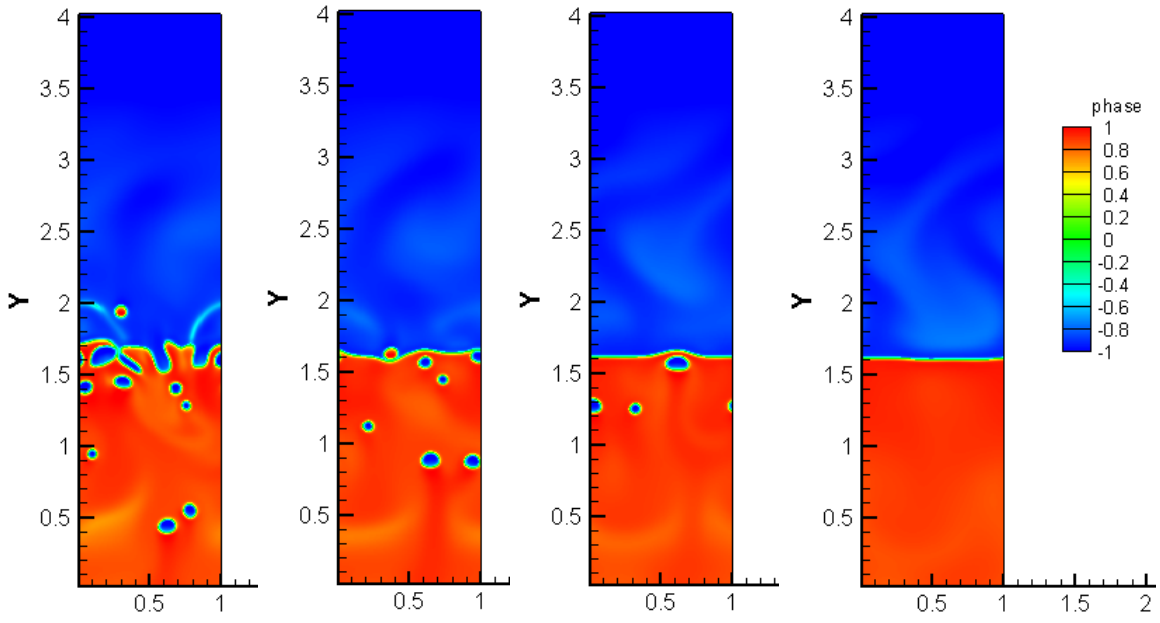


Figure 8 – Dynamics of concentration separation in the fluid phase at different times

Thus, a mathematical model has been developed for the separation of components of binary fluids with different density and viscosity. A 2D numerical algorithm based on the D2Q9 model of the lattice Boltzmann method to simulate a multiphase flow of an incompressible fluid in a bounded rectangular cavity is developed. For incompressible flow, two sets of distribution functions are used: one for tracking the pressure and velocity fields, and the other for the phase field. The use of the pressure distribution function makes it possible to significantly reduce the effect of numerical errors in calculating the interfacial force. Numerical modeling was carried out for the two-dimensional Rayleigh - Taylor instability and for the fluid droplet problem. The main conclusion of this problem can be considered the following: if the thickness interface between two immiscible fluids is large, then spherical drops appear faster than in the case when the boundary is thin. In addition, by implementation of the developed mathematical model, the process of mass transfer of two fluids of different density and viscosity in a given area is clearly shown.

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