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Numerical Simulation of Three-Dimensional Motion of Droplets by Using Lattice Boltzmann Method

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Key Words : *Lattice Boltzmann Method, Free-Energy Model, Cross-Junction micro channel, Droplet Formation*

Abstract

This study describes the numerical simulation of three-dimensional droplet formation and the following motion in a cross-junction microchannel by using the Lattice Boltzmann Method (LBM). Our aim is to develop the three-dimensional binary fluids model, consisting of two sets of distribution functions to represent the total fluid density and the density difference, which introduces the repulsive interaction consistent with a free-energy function between two fluids. We validated the LBM code with the velocity profile in a 3-dimensional rectangular channel. Then, we applied our code to the numerical simulation of a binary fluid flow in a cross-junction channel focusing on the investigation of the droplet formulation. Due to the pressure and interfacial-tension effect, one component of the fluids which is injected from one inlet is cut off into many droplets periodically by the other component which is injected from the other inlets. We considered the effect of the boundary conditions for density difference (order parameter) on the wetting of the droplet to the side walls.

1.Introduction

Most of the numerical works for fluid flow simulations in microchannel are based on solving the continuum Navier–Stokes (N–S) equations. The alternative technique, which has gained popularity in recent years, is to use the lattice Boltzmann method (LBM) [1, 2]. It solves the lattice Boltzmann equation (LBE) kinetically on a regular lattice where a number of fictitious particles evolve according to the laws representing the physical principles of mass, momentum and energy conservation. The LBM solver is based on a simple Bhatnagar-Gross-Krook (BGK) collision approximation [3], and so we are free from solving complicated equations needed for the full BE. Furthermore, simulating multiphase/multicomponent flows has always been a challenge to conventional CFD because of the moving and deformable interfaces. In LB scheme phase separations are generated automatically from the particle dynamics and no special treatment is needed to manipulate the interfaces as in traditional CFD methods.

In this present work, LBM is used as the 3D numerical tool to study the droplet formation and its motion in a cross-junction microchannel. In this paper, we first discuss the theoretical background of the lattice Boltzmann method, including the implementation of the multiphase model. Then, benchmark of the LBM code is done by comparing the results with those obtained with the analytical treatment for single-phase flow through a channel with the same geometry. In the next section, simulations of droplet formation in a cross-junction are presented, and the results are shown for different cases of wetting boundary conditions.

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2. Lattice Boltzmann Simulation

In the LBE approach, one solves the kinetic equation for the particle velocity distribution function (PVDF), $f(x,t)$ in which x is the spatial position vector and t is the time. In this paper we presented 3D lattice Boltzmann BGK Model based on D3Q19 (3 dimensional and 19 velocities) lattice. Several models are known in the literature to describe multiphase systems with the lattice Boltzmann approach. The model using interparticle potentials to model multiphase flows in lattice Boltzmann was first proposed by Shan and Chen [4]. The model based on a Ginzburg-Landau free-energy approach for phase transition was developed by Swift and co-workers [5, 6].

3. Numerical Simulation Method

Our simulations are based on the lattice Boltzmann scheme developed by Swift et al. [6]. This scheme is based on a free-energy functional.

3.1 Lattice Boltzmann Scheme

In this method, the dynamics is defined by the velocity distribution functions $f_i(x,t)$ used to model the total density, $\rho = \rho_A + \rho_B$, and $g_i(x,t)$ used to model the order parameter or density difference $\phi = \rho_A - \rho_B$, defined at each lattice site x at each time t. The distribution functions evolve during a time step Δt according to the lattice-Boltzmann equations.

$$f_i(x + c_i\Delta t) - f_i(x,t) = -\frac{1}{\tau}[f_i(x,t) - f_i^{eq}(x,t)], \quad (1)$$

$$g_i(x + c_i\Delta t) - g_i(x,t) = -\frac{1}{\tau_\phi}[g_i(x,t) - g_i^{eq}(x,t)]. \quad (2)$$

where $f_i^{eq}(r,t)$ and $g_i^{eq}(r,t)$ are local equilibrium distributions, τ and τ_ϕ are independent relaxation parameters, and i represents the link number of lattice velocity vector. The distribution functions are related to the total density ρ, to the mean fluid velocity u, and to the order parameter ϕ through

$$\rho = \sum_i f_i, \qquad \rho u = \sum_i f_i c_i, \qquad \phi = \sum_i g_i. \quad (3)$$

These quantities are locally conserved in any collision process. In order to obtain the continuum equations to a binary fluid mixture, we need to derive the higher order moments of local equilibrium distribution functions as follows.

$$\sum_i f_i^{eq} c_{i\alpha} c_{i\beta} = c^2 P_{\alpha\beta} + \rho u_\alpha u_\beta, \quad (4)$$

$$\sum_i g_i^{eq} c_{i\alpha} = \phi u_\alpha, \quad (5)$$

$$\sum_i g_i^{eq} c_{i\alpha} c_{i\beta} = c^2 \Gamma \Delta\mu \delta_{\alpha\beta} + \phi u_\alpha u_\beta. \quad (6)$$

where Γ is a coefficient related to the mobility of the fluid, $\delta_{\alpha\beta}$ is the Kronecker delta, $P_{\alpha\beta}$ is the complete pressure tensor, and $\Delta\mu$ is the chemical potential difference between the two fluids, which is responsible for phase separation. The local equilibrium distribution functions can be expressed as an expansion at the second order in the velocity u

$$f_0^{eq} = A_0 + C_0 u^2,$$
$$f_i^{eq} = A_k + B_k u_\alpha c_{i\alpha} + C_k u^2 + D_k u_\alpha u_\beta c_{i\alpha} c_{i\beta} + G_{k\alpha\beta} c_{i\alpha} c_{i\beta}, \quad (7)$$

$$g_0^{eq} = a_0 + c_0 u^2,$$
$$g_i^{eq} = a_k + b_k u_\alpha c_{i\alpha} + c_k u^2 + d_k u_\alpha u_\beta c_{i\alpha} c_{i\beta}. \quad (8)$$

The constants A, B, C, D, G, a, b, c, and d take different values for the nearest (i = 1-6 k=1) and next-nearest (i = 7-18 k=2) vectors.

3.2 Free energy model

The free-energy functional F generally used for studies on a binary system is given by [7].

$$F = \int dr[\frac{1}{3}\rho\ln(\rho) + \frac{2}{a}\phi^2 + \frac{b}{4}\phi^4 + \frac{\kappa}{2}(\nabla\phi^2)], \quad (9)$$

The thermodynamic properties of the fluids follow directly from the free energy. The functional derivative of (9) gives the chemical potential difference between the two fluids

$$\Delta\mu = \frac{\delta F}{\delta\phi} = a\phi + b\phi^3 - \kappa\nabla^2\phi, \quad (10)$$

The pressure tensor $P_{\alpha\beta}$ can be written in the form

$$P_{\alpha\beta} = p_0\delta_{\alpha\beta} + \kappa\partial_\alpha\phi\partial_\beta\phi, \quad (11)$$

The scalar part , of the pressure tensor is given by

$$p_0 = \phi\frac{\delta F}{\delta\phi} + \rho\frac{\delta F}{\delta\rho} - h(\rho,\phi) = \frac{1}{3}\rho + \frac{a}{2}\phi^2 + \frac{3b}{4}\phi^4 - \kappa\phi(\nabla^2\phi) - \frac{\kappa}{2}(\nabla\phi)^2. \quad (12)$$

In this equation, $h(\rho,\phi)$ is the free-energy density, which is the integrand of (9).

4. Validation of code

Our numerical code is verified by applying it to the single phase flow in a rectangular channel. Fully developed flow in a long channel with a flat rectangular cross section, of width $2W$ and height $2H$ (walls at $x = \pm W$ and $z = \pm H$) has a specific flow profile depending on the values of W and H. The general solution for flow in a rectangular cross section channel is given below[8]

$$v_y(x,z) = \frac{\Delta P W^2}{8\mu}\left[1 - \left(\frac{2x}{W}\right)^2 + \sum_{n=1}^{\infty}(-1)^n \frac{32}{(2n-1)^3\pi^3}\right] \times \frac{\cosh[(2n-1)\pi z/W]}{\cosh[(2n-1)\pi H/2W]}\cos[(2n-1)\pi x/W]. \quad (13)$$

where μ is the dynamic viscosity, ΔP is the pressure drop over the channel. Fig. 1 shows the comparison of Lattice boltzmann velocity profile with analytical solution give by (13).

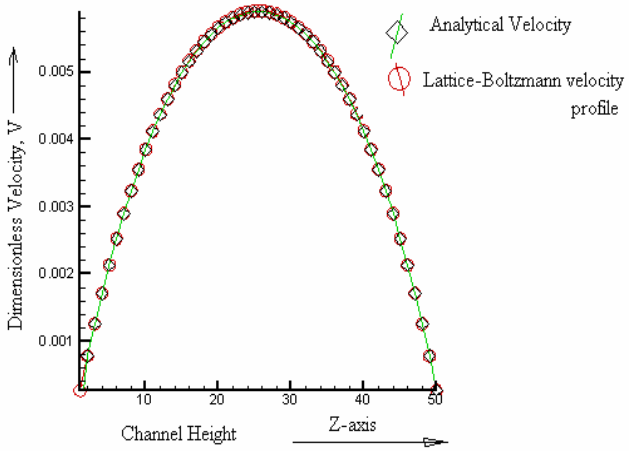


Fig. 1 Comparison of the simulation velocity profile with the analytical solution

It is seen that the agreement is almost exact indicating that our numerical code is reliable.

5. Numerical results of 3D droplet motion in a microchannel

In order to study the droplet dynamics of binary fluid model, a standard cross-junction channel is considered, which is shown in Fig. 2. Fluid *A* is injected through the horizontal channel with maximum velocity V_{in}. Fluid *B* is injected through side channels with maximum velocity W_{in}. The ratio of two velocity magnitudes, W_{in}/V_{in} is fixed as 6. Since the flow rate of fluid A is 3 times smaller than that of B, The droplet is expected to be composed of the fluid A only.

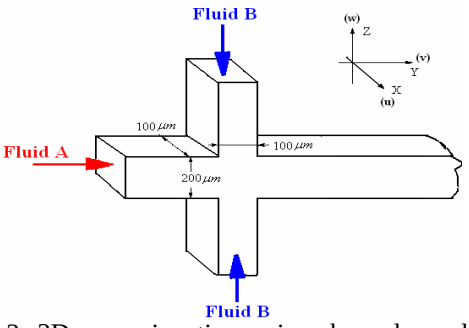
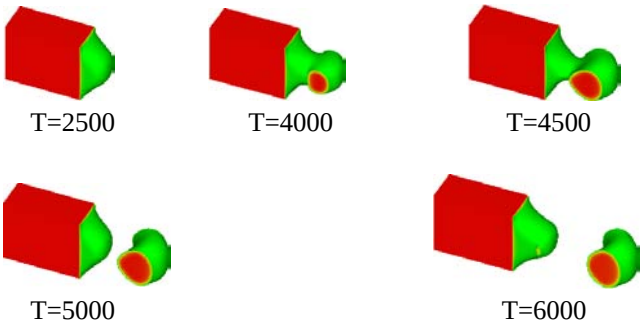


Fig. 2 3D cross-junction microchannel used in LBM simulation of droplet formation.

For the walls or other solid obstacles that have specific wetting properties, we have to assign a certain value of the order parameter (ϕ), to the solid lattice site next to the wall. However we do not have specific guides as to the right choice of the boundary condition depending on the wetting properties. We consider three cases for order parameter at walls.

5.1 Case1: Zero gradient of order parameter at walls

In this case, the gradient of order parameter normal to wall is set to be zero, i.e. $\partial\phi/\partial n|_{wall} = 0$. The results of simulation for this case at different time steps are shown in fig. 3. We plotted the results for main channel only. We observe from the results that the droplet of fluid A is formed at the junction and moving through the channel. It can also be seen that the droplet is wetting to the side walls of microchannel after it is detached from the upstream bulk of liquid A.



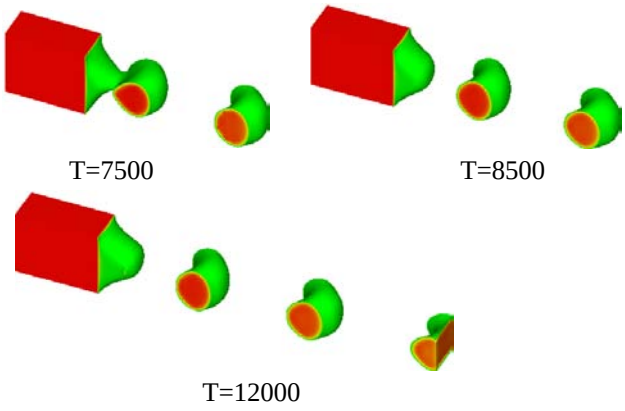


Fig.3 Droplet generation and motion in the cross-junction microchannel with zero gradient of order parameter at walls.

5.2 Case 2: Order parameter value of -1.0 at walls

In this case the value of order parameter at walls is set to be -1.0 ($\phi_{wall} = -1.0$), which is the same value of fluid B. We set this value because fluid B is injecting through side channels and the flow rate of fluid B is 3 times faster than the flow rate of fluid A. So the spreading of fluid B is expected to be more dominant at the walls than fluid A. The results of simulation for this case at different time steps are shown in fig. 4. From this results it can seen that the shape of droplet is spherical roller and no wetting of droplet is taking place.

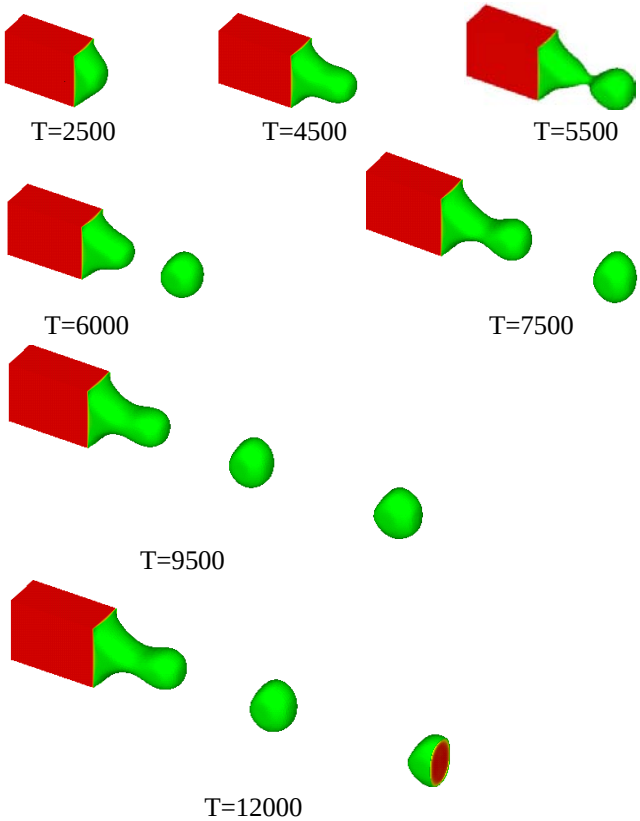


Fig.4 Droplet generation and motion with value of order parameter is -1.0 at walls.

5.3 Case 3: Zero value of order parameter at walls

In this case the value of order parameter at wall is set to be zero ($\phi_{wall}=0$).If the value of the order parameter assigned to the solid lattice sites is equal to that of fluid A($\phi_A=1.0$), then the fluid A close to these lattice sites will spread on the surface, and the fluid B phase will not spread on this surface. However, if the value of the order parameter assigned to the solid lattice sites is equal to that of fluid B ($\phi_B=-1.0$), then fluid B will spread on the surface and fluid A will not. For neutral wetting, the order parameter of the solid lattice sites should be exactly between the order parameters of the fluid A phase and the fluid B phase ($\phi_{wall}=0$). The results of simulation for this case at different time steps are shown in fig. 5.

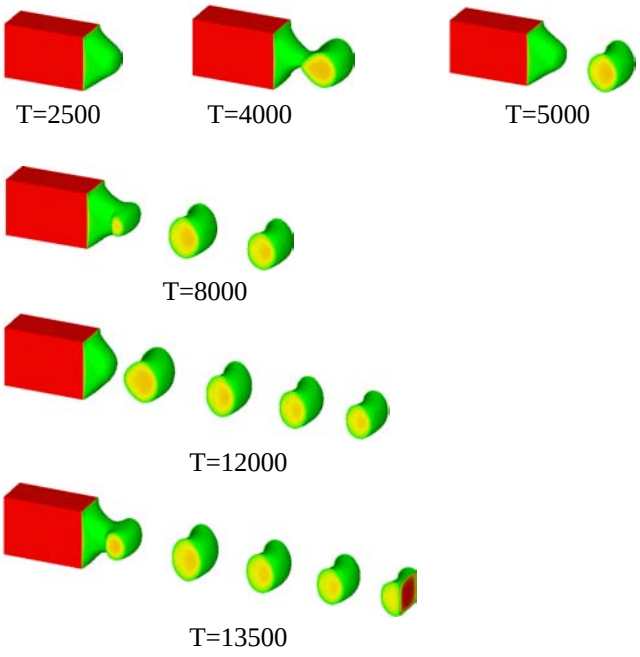


Fig.5 Droplet generation and motion with zero value of order parameter at walls.

5. Conclusion

FORTRAN code is developed for lattice-Boltzmann method to simulate the droplet formation in a microchannel. From the numerical results we can conclude that the free-energy model of the LBE method can be successfully used for the simulation of the droplet motion. The droplets are smoothly generated in the junction area of microchannel. The boundary conditions of order parameter at walls of microchannel is important, because the wetting phenomena of droplet at walls is depend on the surface properties of material which is used for microchannel. Studying on the effect of parameters such as a,b,κ and Γ on the simulation results as well as the stability is a big task. In the future, we are planning to parallelize our LBM code and conduct the stability test for different value of parameters.

6. Acknowledgment

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7. References

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