Simulation of wetting tendency of fluids with high density ratios using RK Lattice Boltzmann method

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ABSTRACT

Several lattice Boltzmann models for multi-phase flow have been developed, but few of them are capable of modeling fluid flows with high density ratio in the order of 1000. Therefore, an advanced chromodynamics, Rothmann-Keller (RK) type model is employed in current study, which can handle liquid-gas density ratio in the order of 1000 and viscosity ratio in the order of 100. Other distinctive characteristics of the proposed model are high stability, and capability of setting parameters such as surface tension independently. In spite of these benefits, the original RK model fails to model wetting tendency of the fluids. As a result, it is impossible to correctly simulate two-fluid phase flow in porous media. To cope with this limitation, a wall-density approach is proposed here and validated against several case studies, including various contact angles near the solid phase. This methodology is implemented in our newly developed software in C++. The simulation results show that the new software can be effectively used to study wetting front shape at the pore scale near the solid phase for two immiscible fluid flows with fluid characteristics similar to water and air.

Keywords: Lattice Boltzmann method; Rothmann-Keller model; Two-phase flow; Wetting tendency; Contact angle

1 INTRODUCTION

Two-phase fluid flows in porous media is one of the most common phenomena such as water flow in vadose zone, transport of pollution in soil, oil recovery engineering, etc. The knowledge about spatial and temporal distribution of pressure of each phase is hence required for reliable analysis of multi-phase flows in porous media (Sadeghi et al. 2018). The problem becomes even more complicated if the interactions between fluids and solid phases have to be analytically considered in numerical simulations. The interaction between phases comprises physical phenomena such as wetting tendency of fluids, intrinsic permeability of the porous media, tortuosity of the flow's path and so forth. One possible solution for overcoming this limitation is to employ Lattice Boltzmann Method (LBM) which can handle most of the complexities mentioned above even in pore-scale flows.

Three popular lattice Boltzmann models for simulation of immiscible multiphase flows are chromodynamics (RK) model of (Rothman and Keller 1988; Gunstensen et al. 1991), pseudopotential (SC) model of Shan and Chen (1993), and free-energy (FE) method of Swift et al. (1996). In recent years, researchers tried to improve stability and window of parameters for these three algorithms. Among them, the improved D2Q9, RK model, developed by Leclaire et al. (2011) is adopted in the current study. The model has the advantage of handling high density ratios of order 1000, and can provide an independent window of parameters simultaneously. Furthermore, it can independently set parameters such as density and viscosity of fluids and surface tension. On the other hand, SC model cannot take into consideration surface tension independent of density and viscosity of fluids. In contrast to the SC model used by Ghassemi and Pak (2011), the RK model does not have an intrinsic way of simulating the wetting tendency of fluids near the solid phase. Since the original RK model of Leclaire et al. (2011) cannot simulate wetting tendency of fluids, it cannot also simulate flow of two fluids in porous media reliably. In order to cope with this deficiency, the wall density approach of Latva-Koko and Rothman (2005), is employed and applied to the improved RK model in current study.

2 LATTICE BOLTZMANN METHOD

The RK LBM algorithm implemented in this study consists of six main parts in each time step. The first part is streaming operator, which is a single-phase operator responsible for streaming distribution functions of each fluid in a D2Q9 lattice with the velocity vectors $\boldsymbol{c}_i$. The discretized form of Boltzmann equation is given in Eq. (1) where $N_i^k(\boldsymbol{x}, t)$ represents distribution function for a fluid of color k in i direction, $\boldsymbol{x}$ is the node position, t is time step, and Ω_i^k is the collision operator, which consists of three sub-operators.

$$N_i^k(\boldsymbol{x} + \boldsymbol{c}_i, t + 1) = N_i^k(\boldsymbol{x}, t) + \Omega_i^k(\boldsymbol{x}, t) \quad (1)$$

Velocity vectors $\boldsymbol{c}_i$ for all values of i are given in Eq. (2). And $\theta_i = (4 - i)\,(\pi / 4)$.

$$\boldsymbol{c}_i = \begin{cases} (0,0), & i = 1 \\ [\sin(\theta_i), \cos(\theta_i)], & i = 2,4,6,8 \\ [\sin(\theta_i), \cos(\theta_i)]\sqrt{2}, & i = 3,5,7,9 \end{cases} \quad (2)$$

In the second part, all the boundary conditions including one-directional and fully periodic boundaries, simple bounceback boundary conditions implemented similar to the work of Sukop and Thorne (2006). The third part is a single-phase collision operator $\Omega_i^{k(1)}$. This operator is calculated by a single-relaxation-time (SRT) approximation from Eq. (3). However, according to Sheikh and Pak (2015), the SRT has some inherent deficiencies which can be eliminated by using a multi-relaxation-time (MRT) approximation for the collision operator.

$$(\Omega_i^k)^{(1)} N_i^k = N_i^k - \omega_k (N_i^k - N_i^{k(e)}) \quad (3)$$

The equilibrium distribution functions $N_i^{k(e)}$ expanded in Eq. (4) are chosen to respect the principles of mass and momentum conservation. Where ρ_k is the density of fluid k, which is calculated from Eq. (5). In addition, the macroscopic velocity $\boldsymbol{u}$ is obtained from Eq. (6).

$$N_i^{k(e)} = \rho_k (\phi_i^k + W_i [3\boldsymbol{c}_i \cdot \boldsymbol{u} + \tfrac{9}{2}(\boldsymbol{c}_i \cdot \boldsymbol{u})^2 - \tfrac{3}{2}\boldsymbol{u}^2]) \quad (4)$$

$$\rho_k = \textstyle\sum_i N_i^k = \sum_i N_i^{k(e)} \quad (5)$$

$$\boldsymbol{u} = \left(\textstyle\sum_i \sum_k N_i^k \boldsymbol{c}_i\right) / \sum_k \rho_k \quad (6)$$

The weights W_i are those of a standard D2Q9 lattice. ϕ_i values are given in Table 1. The arbitrary parameters of α_k are chosen to satisfy $\rho_r / \rho_b = (1 - \alpha_b) / (1 - \alpha_r)$.

Table 1. D2Q9 parameters: W_i, ϕ_i, B_i, used in Eq. (4) & Eq. (8).

i	W_i	ϕ_i	B_i
1	4 / 9	α_k	-4 / 27
2,4,6,8	1 / 9	$(1 - \alpha_k) / 5$	+2 / 27
3,5,7,9	1 / 36	$(1 - \alpha_k) / 20$	+5 / 108

The relaxation parameter ω_k is a function of fluid viscosity ν_k, given by $\omega_k = 1/(3\nu_k + 0.5)$. Similar to the work of Leclaire et al. (2011), when the viscosities of the fluids are different, a type of interpolation is applied to define the parameter ω at the interface.

The forth part is calculation of color gradient $\boldsymbol{F}$, which is an approximation of the perpendicular to the interface between fluids. The usual color gradient in the RK model is defined by Eq. (7). But, in this work a sixth order isotropic approximation of the color gradient, similar to the work of Leclaire et al. (2011) was used.

$$\boldsymbol{F}(\boldsymbol{x}) = \textstyle\sum_i \boldsymbol{c}_i \left(\rho_r(\boldsymbol{x} + \boldsymbol{c}_i) - \rho_b(\boldsymbol{x} + \boldsymbol{c}_i)\right) \quad (7)$$

To calculate $\boldsymbol{F}$ for each node of the lattice, the two outer layer nodes (24 nodes) are needed. In case of calculating color gradient for fluid nodes near the solid nodes, some fake densities of either red or blue fluids were assigned to solid nodes.

The contribution of this work is to define a red percentage parameter (P_{red}) so that the P_{red} portion of the initial red fluid density is assigned to solid nodes. As a color convention, the denser fluid is always represented in red. P_{red} varies from -1 to 1, where P_{red} being equal to one means that red fluid is completely wetting. The minus values of P_{red} are numerically implemented by assigning the absolute value ($|P_{\text{red}}|$) of the blue fluid to solid nodes, i.e. $|P_{\text{red}}| = P_{\text{blue}}$ for $P_{\text{red}} < 0$. For instance, $P_{\text{red}} = -0.7$ means that 70 percent of the initial value of blue fluid density, and a null density of red fluid. There is also no need to mention that setting one fluid (e.g. red) wetting, would automatically make the other one (e.g. blue) non-wetting. A completely wetting fluid should make a contact angle of 0° near walls (solid phase). On the other hand, a completely non-wetting fluid should make a contact angle of 180° near walls (solid phase). Therefore, the wetting tendency of fluids is adjustable through the red percentage parameter ($-1 < P_{\text{red}} < +1$).

Needless to mention that these fake densities - which exist in the solid nodes- never flow through the fluid domain and never interrupt with the standard simple bounce-back boundary condition. Indeed, they only affect color gradient in the neighboring fluid nodes, that are only one or two lattice units away from solid nodes. These fake densities also affect the two next two-phase collision operators. In the fifth and sixth part of the algorithm, the two-phase collision operators, namely perturbation $\Omega_i^{k(2)}$ and recoloring $\Omega_i^{k(3)}$, were implemented respectively based on the calculated color gradient, using Eq. (8), Eq. (9). In these equations, $\rho = \rho_r + \rho_b$, and φ_i is the angle between the color gradient $\boldsymbol{F}$ and the direction $\boldsymbol{c}_i$. The free parameter β influences the thickness of the interface. For N_i^r, Eq. (9) is used with the plus sign, otherwise with minus sign. The constant parameters B_i are given in Table 1. In addition, A_k values are chosen to set surface tension $\sigma = \rho\,(A_r + A_b) / 9\omega$.

$$(\Omega_i^k)^{(2)} N_i^k = N_i^k + \frac{A_k}{2} |\boldsymbol{F}| \left[W_i \frac{(\boldsymbol{F} \cdot \boldsymbol{c}_i)^2}{|\boldsymbol{F}|^2} - B_i\right] \quad (8)$$

$$(\Omega_i^k)^{(3)} N_i^k = \frac{\rho_k}{\rho} N_i \pm \beta \frac{\rho_r \rho_b}{\rho^2} cos\varphi_i \textstyle\sum_k N_i^{k(e)} (\rho_k, 0) \quad (9)$$

In the RK model, the perturbation operator is responsible for modeling surface tension between fluids. The recoloring operator guarantees immiscibility of fluids and simultaneously respects the principles of conservation of mass and total momentum. Comprehensive details on the mathematical implementation of D2Q9 RK model used here can be found in Leclaire et al. (2011).

3 NUMERICAL SIMULATIONS

Sadeghi (2013) indicated that the code can precisely simulate fluid flow around a circle, sudden-expansion flow, shear-driven cavity flow, Couette flow, and Poiseuille flow. In this section, the validity of the code for simulating just two-phase flow problems is examined.

Afterwards, the new approach of simulating wetting tendency is studied and discussed.

3.1 Two-phase flow problems

Bubble test is the standard verification test for all two-phase LB models. Nine squares with different sizes of the red fluid with density of 1000 kg/m^3, and kinematic viscosity of 0.01667 cm^2/s were submerged in a 200×200 domain, filled with the blue fluid with density of 1 kg/m^3, and kinematic viscosity of 0.1667 cm^2/s. Both fluids tend to have the minimum interface with each other. As a result, the surface tension changes the form of square to a stable circular bubble. Laplace's law relates the pressure difference (Δp), with radius of curvature (R), and surface tension (σ), following Eq. (10):

$$\sigma = R(p_{in} - p_{out}) \quad (10)$$

Figure 1 shows pressure difference against curvature for nine simulated bubble tests. The linear trend in the figure reveals that the surface tension which was first given to the developed RKLBM code is in accordance with the one obtained from theoretical Laplace law.

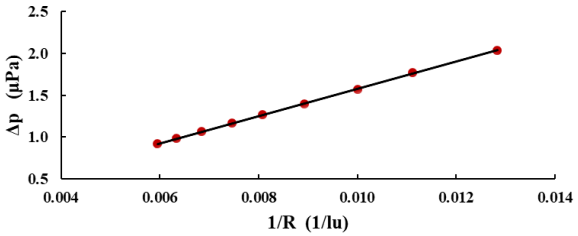

Fig. 1. Nine bubble test results compared to Laplace's law.

To further illustrate the robustness of RKLBM, a 100×100 domain was filled randomly with both fluids. Red fluid was assumed to have a density of 1000kg/m^3, and a kinematic viscosity of 0.01667cm^2/s, while the density and kinematic velocity were assumed as 1kg/m^3, and 0.1667cm^2/s for blue fluid, respectively. Fully periodic boundary condition was applied to all four boundaries. There is no unique solution to find the interface between the fluids in stable state. Joseph and Renardy (1993) predicted the formation of one giant bubble or some large bubbles of the fluid having a less viscosity compared with that of domain fluid at final stable state. This prediction is the consequence of the energy minimization principle, which subsequently leads to minimization of the area of the interface between the fluids. Figure 2(a) shows the initial condition and Figure 2(b) indicates the final stable state reached by RKLBM simulation. Results may not look like a bubble at the first glance, but as we used fully periodic boundary conditions, the domain repeats in all directions infinitely. Reconstructing the domain shows the exact formation of a large bubble of blue fluid inside red fluid in figure 2(c). It is worthy to mention that the simulation of such complex situation is extremely difficult using conventional CFD techniques, if not impossible. Our studies showed that even some two-phase LBMs, like SC LBM with SRT operator cannot solve this problem even for identical fluids (Sadeghi 2013).

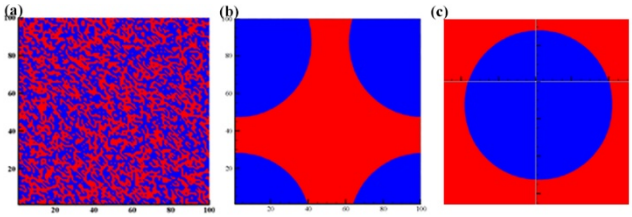

Fig. 2. Bubble formation (100×100); (a) initial condition, (b) final stable simulation result, and (c) reconstructing the domain.

3.2 Static contact angle simulation

Wettability is the inherent adhesion of one liquid to the solid surface. Wetting tendency can be mathematically defined trough the static contact angle. When the contact angle is less than 90°, the fluid is wetting; otherwise non-wetting. As explained in section 2, a new parameter (P_{red}) was introduced to the improved RKLBM to make the simulation of wetting tendency for two fluids near the solid phase or wall possible. Although a mathematical relationship between the contact angle and P_{red}, -for non-identical fluids- was not proposed, simulation results show that the introduced parameter P_{red}, enables the model to simulate wetting tendency for two fluids with density ratio of 1000. On the other hand, Latva-Koko and Rothman (2005) proved that for two identical density, and identical viscosity fluids in RKLBM, the contact angle is related to P_{red} through Eq. (12).

$$\cos\theta = P_{red} \quad (11)$$

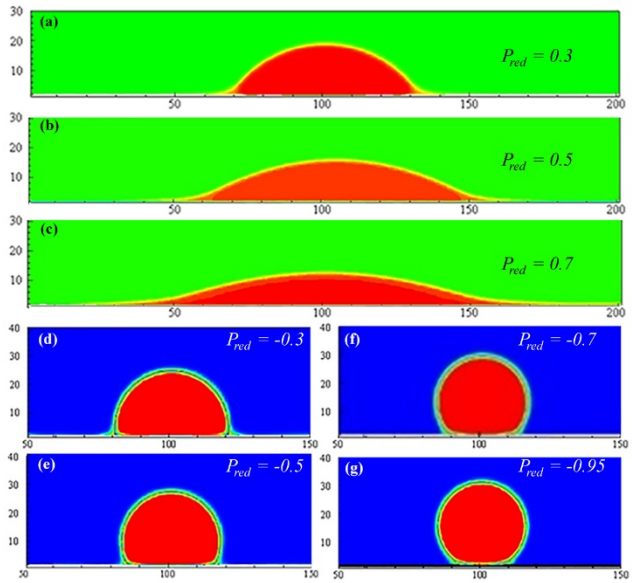

Fig. 3. Static contact angle for two fluids with density ratio of 1000 near wall at stable state for different P_{red} values including: (a) 0.3, (b) 0.5, (c) 0.7, (d) -0.3, (e) -0.5, (f) -0.7, and (g) -0.95.

A 200×100 lattice was initialized with two fluids with

density and viscosity ratios of 1000 and 0.1, respectively. All four boundaries were bounceback. The red fluid placed in a square of 40×20 on the bottom wall, and horizontally in the middle of the domain. For seven different values of P_{red}, the model was run until reaching the stable state. The simulation results for wetting red fluid with different $P_{red}>0$, are shown in figure 3(a) to 3(c). Greater values for P_{red} result in a higher wetting tendency and a lower contact angle for red fluid. Figures 3(d) to 3(g) show the results for non-wetting red fluid with different $P_{red}<0$. Also, the higher is the value of P_{blue}, the higher the contact angle and the lower the wetting tendency of red fluid will be.

3.3 Capillary rise simulation

To demonstrate the capability of proposed parameter P_{red}, another well-known problem of capillary rise was simulated for two fluids with densities and viscosities relatively similar to those of water and air.

A 25×100 domain filled half-bottom with wetting fluid (ρ = 1000 kg/m^3) and, half-top with non-wetting fluid (ρ = 1 kg/m^3) was used to simulate the capillary rise. Four bounce-back boundaries enclose the domain and a tiny downward acceleration applied only to the red fluid. At equilibrium state, capillary rise is obtained from Eq. (12):

$$h = 2\sigma \cos\theta \,/\, \rho g w \qquad (12)$$

where ρ is density, g is ground acceleration, w is the width of tube, σ is surface tension, θ is contact angle, and h is capillary height. Figure 4, shows the initial and stable conditions of four different capillary rise problems with four P_{red} values of 0.2, 0.5, 0.7, and 1.0. Although the new model simulated the capillary rise for different wetting tendencies, it did not necessarily predict the contact angle from Eq. (11) for non-identical fluids at high density ratios. The more promising method to calculate the contact angle (θ) is therefore to input the height of capillary rise (h) obtained from simulation to Eq. (12).

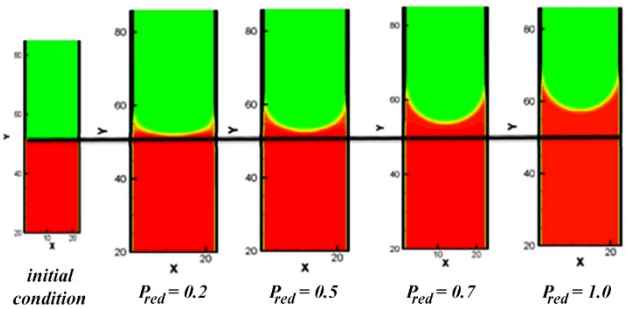

Fig. 4. Initial condition and capillary rise for different P_{red} values while density ratio = 1000, and kinematic viscosity ratio = 0.1.

3 CONCLUSIONS

A newly developed two-phase Lattice Boltzmann numerical C++ code was presented and validated. This model is based on improved Rothmann-Keller (RK) formulation of Leclaire et al. (2011) which is capable of simulating the simultaneous flow of two immiscible fluids at the pore scale with high density and viscosity ratios in the order of 1000, and 100, respectively. Afterwards, a new red percentage parameter (P_{red}) was introduced to the formulation which makes the original model capable of simulating wetting tendency of two fluids -with water-air density and viscosity ratios- near solid boundaries (wall). The performance of new parameter in simulating wetting tendency was studied through simulating two types of problem namely, static contact angle and, capillary rise. The obtained results demonstrated that the improved RKLBM is a powerful method, capable of simulating the behavior of two immiscible -high density and viscosity ratio- fluid flows near the solid phase. In addition to these fundamental problems, further developments of the method are under way for studying more complex flow phenomena such as relative permeability.

REFERENCES

Ghassemi, A., Pak, A. (2011). Numerical study of factors influencing relative permeabilities of two immiscible fluids flowing through porous media using lattice Boltzmann method. Journal of Petroleum Science and Engineering, 77(1), 135-145.

Gunstensen, A.K., Rothman, D.H., Zaleski, S., Zanetti, G. (1991). Lattice Boltzmann model of immiscible fluids. Physical Review A, 43(8), 4320-4327.

Joseph, D.D., Renardy, Y.Y. (1993). Fundamentals of Two-Fluid Dynamics, Springer, New York, U.S.A.

Latva-Koko, M., Rothman, D.H. (2005). Static contact angle in lattice Boltzmann models of immiscible fluids. Physical Review E, 72(4), 046701.

Leclaire, S., Reggio, M., Trepanier, J.Y. (2011). Isotropic color gradient for simulating very high-density ratios with a two-phase flow lattice Boltzmann model. Computers & Fluids. 48(1), 98-112.

Sadeghi, H., Chiu, C.F., Ng, C.W.W., Jafarzadeh, F. (2018). A vacuum-refilled tensiometer for deep monitoring of *in-situ* pore water pressure. Scientia Iranica. DOI: 10.24200/sci.2018.5052.1063.

Sadeghi, M. (2013) Evaluation of efficiency of RK chromodynamic model for simulation of two-fluid flow in porous media. MSc Thesis, Sharif University of Technology.

Shan, X., Chen, H. (1993). Lattice Boltzmann model for simulating flows with multiple phases and components. Physical Review E, 47(3), 1815-1819.

Sheikh, B., Pak, A. (2015). Numerical investigation of the effects of porosity and tortuosity on soil permeability using coupled three-dimensional discrete-element method and lattice Boltzmann method. Physical Review E, 91(5), 053301.

Sukop, M.C., Thorne, D.T. (2006). Lattice Boltzmann Modeling: An Introduction for geoscientists and engineers, Springer, Heidelberg, Berlin, New York.

Swift, M.R., Orlandini, E., Osborn, W.R., Yeomans,J.M. (1996). Lattice Boltzmann simulation of liquid-gas and binary fluid systems. Physical Review E, 54(5), 5041-5052.

Rothman, D.H., Keller, J.M. (1988). Immiscible cellular-automaton fluids. Journal of Statistical Physics, 52(3-4), 1119-1127.