NUMERICAL STUDY OF NANO-PARTICLE ADSORPTION METHOD BY LATTICE BOLTZMANN SIMULATION

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Summary The dynamics of two-phase flows with a constant driving force inside a micro-channel was studied by Lattice Boltzmann Method. Flow regimes under different wall wettabilities and over grooved geometric surfaces were investigated. It is found that slip lengths on different surfaces are found to collapse nearly onto a single curve as a function of the static contact angle, and flow behaviors are strongly affected by the wall wettability and topography.

Numerical model

To simulate non-ideal multiphase fluids, the attractive or repulsive interaction among molecules, which is referred to as the non-ideal interaction, should be included in the LB model. The interparticle-potential model proposed by Shan & Chen is to mimic microscopic interaction forces between the fluid components, and modified the collision operator by using an equilibrium velocity that includes an interactive force, which guarantees phase separation and introduces surface-tension effects[1]. In the Shan-Chen model[2, 3], the fluid-fluid interaction is obtained by using an attractive short-range force[2]

$$\mathbf{F}(\mathbf{x}) = -G\psi(\mathbf{x},t)\sum_i w_i\psi(\mathbf{x}+\mathbf{c}_i\Delta t,t)\mathbf{c}_i . \tag{1}$$

Where G is the interaction strength, that is used to control the two-phase liquid interaction, and is negative for particle attraction. ψ is the interaction potential, defined as $\psi(\mathrm{x},t) = \psi_0 e^{-\rho_0/\rho}$, where ψ_0 and ρ_0 are constants.

It is simple to describe the interaction between a fluid and a wall by introducing an extra force, and this method is first used by Martys and Chen[4]. The idea is to create an analogue to the particle-particle interaction force used to induce phase separation, and in this paper the equation describing this is[5]

$$\mathbf{F}_{ads}(\mathbf{x}) = -G_{ads}\psi(\mathbf{x},t)\sum_i w_i s(\mathbf{x}+\mathbf{c}_i\Delta t,t)\mathbf{c}_i , \tag{2}$$

Here s =0, 1 for the fluid and the solid phase, respectively, the adhesion parameter G_{ads} is used to control the wettability behavior of the liquid at solid surfaces. It is visible that the Eq. (2) incorporates an adhesive interaction between fluid and surfaces.

Contact angle simulation

Contact angle is a static parameter of measuring the wettability of a liquid on a solid surface, and it can be easily measured. Fig. 1 shows different static contact angles by simulation.

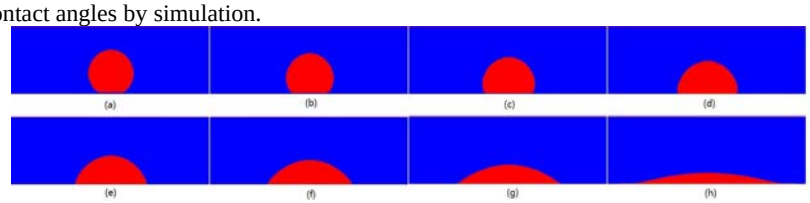

Fig.1 Static contact angle

As shown in Fig.1, G_{ads} and G determine the value of contact angle in the Shan-Chen-type LB method. G_{ads} represents the strength of interaction between fluid and solid surface and G represents the strength of interaction between liquid and gas. A negative G_{ads} indicates attractive interaction. When G is determined, the greater the magnitude of $|G_{ads}|$, the stronger the reaction, and thus resulting in smaller contact angle. So we can change parameter G_{ads} and parameter G to simulate contact angle for arbitrary surface condition, and then obtain different wall wettabilities.

Numerical simulation

Numerical results of contact angles and slip lengths, represented by different symbols with different colors shown in Fig. 2. From the results shown in Fig.2, it is easily and clearly to found that the slip length is a function of contact angle (as shown by the solid curve in Fig.2),

$$\delta_L = 0.1441(e^{\theta/56.06} - 1) . \tag{3}$$

where θ is contact angle (in degree), and δ_L is slip length in lattice unit.

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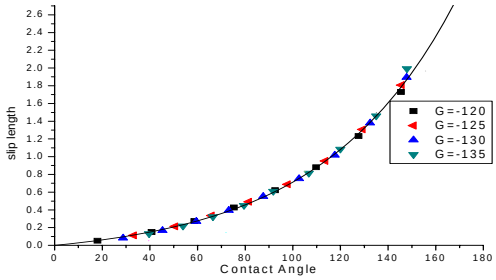

Fig.2 the slip length against contact angle

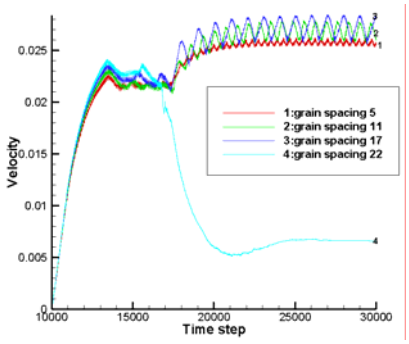

Fig.3 Comparison of the average liquid velocity under different grain spacing

Form Fig.2 we can see that slip lengths on different surfaces are found to collapse nearly onto a single curve as a function of the static contact angle characterizing the surface wettability. The slip length is the result of interaction between the liquid and the wall surface, and it depends on the properties of the liquid (e.g. G) and the wall surface (e.g. G_{ads}). So the simulation of slip length should take into account all parameters of the interaction objects, but it is a very hard task [6] to do this. In fact, the contact angle is a more comprehensive expression of interactions between liquid and solid surface, and the weaker the solid-fluid interaction is, the larger the contact angle is. So it may be a feasible and advisable way to use contact angle as control parameter to simulate the slip length. The result listed in Fig.4 shows that this method is feasible, practical and much simpler.

We simulate a droplet moving inside a grooved channel to study the effects of roughness as shown in Fig.3 and Fig.4. From the image sequences we can see that the grain spacing alters the droplet dynamics properties.

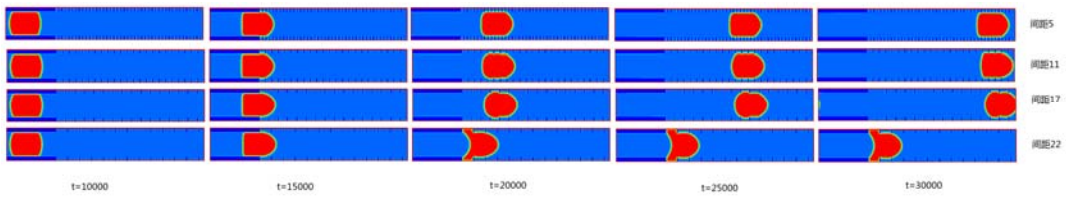

Fig.4 Comparison of snapshots of the liquid positions and configurations

A general trend shown in Fig.3 is that in each case the time series of the average liquid velocity are similar to those of a sin curve when grain spacing is 5 to 17, and we also can see that, when the grain spacing is wider, the average liquid velocity is greater, the frequency of the curve is smaller and the amplitude of the curve is greater. This may be due to the fact that a non-continuous solid-liquid contact line in the roughness wall is made by the gas trapped by nano-structured boundary. When the solid-liquid contact line is continuous the liquid velocity is slower, and when the solid-liquid contact line is non-continuous the liquid velocity is faster. It also can be seen from Fig.3 that the speed of the droplet varies with the grain spacing. There is a critical grain distance. When the grain spacing is less than the critical distance (as shown in Fig.8 grain spacing is between 5 and 17), the average liquid velocity increases as the distance between nanoparticles increases, this may be due to the fact that when the distance between neighboring is wider, the more gas will be trapped by the nano-structured and the solid-liquid contact line will become shorter, which will make the drag on the droplet decrease. When grain spacing is more than the critical distance such as 22 lattice unit, the droplet will contact the bottom and the average liquid velocity will decrease greatly.

CONCLUSIONS

The lattice Boltzmann method is successfully applied in this work to simulate contact angle of a fluid on a solid surface and the slip length of a fluid flowing over a solid surface, and the results show that wettability boundary is proposed to control slip length in the numerical simulation. It is also found that flow behaviours are strongly affected by the wall wettability and topography, and the LBM is efficient and accurate, has very good application prospect in the study of drag reduction of microscopic seepage of reservoir.

References

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