Free-surface Simulations of Newtonian and Non-Newtonian Fluids with the Lattice Boltzmann Method

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Abstract: This paper describes the application of a three-dimensional lattice Boltzmann method (LBM) to Newtonian and non-Newtonian (Bingham fluid in this work) flows with free surfaces. A mass tracking algorithm was incorporated to capture the free surface, whereas Papanastasiou’s modified model was used for Bingham fluids. The lattice Boltzmann method was first validated using two benchmarks: Newtonian flow through a square cross-section tube and Bingham flow through a circular cross-section tube. Afterward, the dam-break problem for the Newtonian fluid and the slump test for Bingham fluid were simulated to validate the free-surface-capturing algorithm. The numerical results were in good agreement with analytical results, as well as other simulations, thereby proving the validity and correctness of the current method. The proposed method is a promising substitute for time-consuming and costly physical experiments to solve problems encountered in geotechnical and geological engineering, such as the surge and debris flow induced by a landslide or earthquake.

Key words: Newtonian and non-Newtonian flows, free surface, lattice Boltzmann method, mass tracking algorithm

1 Introduction

Free-surface flows are ubiquitous in both nature and industrial applications. Landslides and debris flows are typical free-surface flows that are common in many regions, especially in areas of southwest China (Chen et al., 2011; Zhang et al., 2013). Both can be treated as “granular flows”, i.e., large collections of discrete solid particles with fluids (water and air) filling the interstices, flowing at a high velocity down a slope channel because of gravity (Zhou and Ng, 2010; Zhou et al., 2014). In many cases, a granular flow can be regarded as a single-phase flow and treated with continuum fluid methods if its macroscopic effect is the main concern. Some free-surface flows like landslides, debris flows, and dam breaks may cause an inestimable loss of human life (Cui et al., 2013), whereas others are related to beneficial industrial products, such as concrete casting and mold filling. Therefore, efforts should be made to study and describe free-surface flows. On the one hand, doing so can help predict the area of influence of natural disasters, thereby playing an important role in reducing the loss of life and property. Conversely, production technology involving free-surface flow can be optimized with the assistance of studies and an accurate description of such flow. Concerning landslides and debris flows, most of the research has been conducted by the macroscopic geophysical survey (Chen et al., 2009; Liu et al., 2001; Zhang et al., 2013; Ni et al., 2014; Yang et al., 2015), including physical experiments (Zhou et al., 2013) and theoretical analysis (Sun et al., 2009; Tang et al., 2014; Sun 2015). In this regard, it should be mentioned that analytical and experimental approaches are relatively expensive in terms of financial and computational costs. Instead, numerical modeling can provide a reasonable substitute (Fei et al., 2012; Švec et al., 2012; Zhou and Sun, 2014).

Many numerical methods have been developed to treat free-surface problems, including the marker-and-cell method (Harlow, 1964), the volume-of-fluid method (Hirt and Nichol, 1981), the height function method (Frederiksen and Watts, 1981), the smoothed particle hydrodynamics (Monaghan, 2005), and the moving particle semi-implicit method (Koshizuka and Oka, 1996). These methods can be divided into two categories: Lagrangian surface-tracking methods and Eulerian surface-capturing methods (Ginzburg and Steiner, 2003); both categories have advantages and disadvantages.

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The interface of most free-surface problems that concern us is usually formed by air and fluid. Compared to fluid, the density of air is so small that its influence on the movement of the fluid can be neglected. Thus, we employ the newer and simpler mass tracking algorithm (Körner et al., 2005; Thürey and Rüde, 2009) to describe the free surface. Unlike the volume-of-fluid method, a parameter representing the mass of the interface cell is used as a substitute for the volume of fluid in the interface cell, making it easier to implement. Because there is no need to simulate the gas phase, much computational cost is saved. Thus, Švec et al. believe that this method is one of the simplest and fastest algorithms that conserves mass precisely (2012), a condition generally required for large-scale simulations.

Both Newtonian and non-Newtonian fluids play important roles in most engineering issues, and sometimes their effect can be crucial. For example, water has an important influence on both the macroscopic and microscopic properties of granular flows, and most granular flows can be simplified to flows of non-Newtonian fluids. The most traditional method used to simulate fluid flows is computational fluid dynamics. However, such a traditional method often works inaccurately with complex geometries and moving boundary conditions, which occur often in geotechnical and geological engineering situations. The lattice Boltzmann method (LBM) is a new computational fluid dynamics approach, developed within the last 20 years, which is a meso-scale model between microscopic molecular dynamics and the macroscopic continuum model. He and Luo (1997) were the first to derive the lattice Boltzmann equation from the continuous Boltzmann equation, thereby laying a solid physical basis for the development of the lattice Boltzmann method. The microparticle background of the lattice Boltzmann method makes it more intuitive and convenient for handling interactions between a fluid and its surrounding environment (e.g., boundary), resulting in more advantages than those of traditional numerical methods used for handling multiphase systems, interface kinetics, and other complex flow phenomena. Furthermore, the evolution equations of the lattice Boltzmann method are clear and simple, and the computation is local (i.e., parallel and scalable), which has a great advantage for simulating large-scale flow problems (Guo and Zheng, 2008). Ever since its introduction, the development of the lattice Boltzmann method has continuously progressed, and at present, it has become a viable tool that is widely used in many regions of research (Feng et al., 2007; Aidun and Clausen, 2010; Han et al., 2010; Feng et al., 2010; Owen et al., 2011).

Developing numerical methods, which can be used to simulate free-surface flows and interactions between a fluid and its surrounding boundaries, has important value in terms of both scientific research and engineering applications. In the present paper, a three-dimensional (3D) lattice Boltzmann method for free-surface flow of both Newtonian and non-Newtonian fluids is presented. The paper has been organized as follows: section 2 describes the 3D lattice Boltzmann method algorithm and introduces the rheological model for Newtonian and non-Newtonian fluids, as well as the mass tracking algorithm that is used to capture free surfaces. Section 3 presents the validation of the test results, using the proposed method; while section 4 offers conclusions from these analyses.

2 Numerical Models

2.1 D3Q19 LBM

In the lattice Boltzmann method, almost all continuous physical quantities are transformed into discrete quantities. The physical domain is divided into a fixed regular or irregular lattice, whereas the velocity, which originally has infinite possible directions, is also simultaneously broken into discrete velocities with finite directions. Similarly, the continuous time is subdivided into discrete time steps, and the fluid is modeled as a group of fluid particles that are allowed to move between the adjacent lattice nodes or stay at rest (Feng et al., 2010). There are several types of lattices, differentiated according to their shape. In this paper, the D3Q19 lattice model has been used (Fig. 1), with D and Q representing the dimension of the problem and the number of lattice velocities, respectively.

The lattice Boltzmann equation for the lattice Bhatnagar–Gross–Krook model can be expressed as

![Fig. 1. D3Q19 lattice model.](image-url)
\[ f_i(x + \epsilon, \Delta t, t + \Delta t) - f_i(x, t) = - \frac{1}{\tau_{BGK}} \left[ f_i(x, t) - f_i^{eq}(x, t) \right] \]

where \( f_i(x, t) \) is the density distribution function of a particle moving with velocity \( \epsilon \) at position \( x \) and time \( t \). \( \tau_{BGK} \) is the relaxation time, which is the most important parameter of the lattice Boltzmann–Gross–model, and \( f_i^{eq}(x, t) \) is the equilibrium distribution function of \( f_i(x, t) \) given by

\[ f_i^{eq}(x, t) = \omega_i \rho \left[ 1 + \frac{\epsilon \cdot \mathbf{u}}{c_i^2} + \frac{2 \epsilon^2 - \mathbf{u}^2}{2c_i^2} \right] \]

with \( \rho \) being the fluid density, \( \mathbf{u} \) being the fluid velocity, \( c_i \) being the speed of sound in the lattice, and \( \omega_i \) being the weighting factors related to the lattice speeds.

The weighting factors \( \omega_i \) in the D3Q19 model are given as

\[ \omega_i = \begin{cases} 
\frac{2}{9}, & i = 0, \\
\frac{1}{9}, & i = 1, \ldots, 6 \\
\frac{1}{72}, & i = 7 \ldots 18 
\end{cases} \]

and the 19 discrete velocities are

\[ c_i = \begin{cases} 
(0, 0, 0) & i = 0, \\
\pm(1, 0, 0), (0, \pm 1, 0), (0, 0, \pm 1) & i = 1, \ldots, 6 \\
\pm(1, \pm 1, 0), \pm(1, 0, \pm 1), (0, 0, \pm 1) & i = 7, \ldots, 18 
\end{cases} \]

During each discrete time step of the simulation, the evolution of the lattice Boltzmann–Gross–model can be considered to occur in two stages: collision and streaming. In the collision step, the particle distribution function is modified by

\[ f_i(x, t) = f_i(x, t) - \frac{1}{\tau_{BGK}} \left[ f_i(x, t) - f_i^{eq}(x, t) \right] \]

where \( f_i(x, t) \) denotes the density distribution function after the collision. After collision, the density distribution function advances to the next lattice node along the directions of their motion without a change in their values, i.e.,

\[ f_i(x + \epsilon, \Delta t, t + \Delta t) = f_i(x, t) \]

As the time step is normalized to a unit length within the lattice unit, the particles directly move to the neighboring cell along their velocity direction, as shown in Fig. 1. Thus, after each streaming step, all the cells again have a complete set of density distribution functions. As can be seen from the evolution equation, all the computations are local, thus the lattice Boltzmann method can be easily parallelized.

The macroscopic variables can be obtained as

\[ \rho = \frac{1}{3} \sum_{i=0}^{18} f_i, \quad \rho u = \sum_{i=0}^{18} \epsilon_i f_i, \quad p = c_s^2 \rho \]

where \( c_s = 1/\sqrt{3} \) for the D3Q19 model. The kinematic viscosity \( v \) of the fluid is determined by

\[ v = \frac{1}{3} \left( \tau_{BGK} - \frac{1}{2} \right) (\Delta h)^2 \]

where \( \Delta h \) is lattice spacing and \( \Delta t \) is the discrete time step.

2.2 Rheological model

It is well known that fluids can be divided into two categories: Newtonian and non-Newtonian. The viscous stresses of a Newtonian fluid are proportional to the local strain rate, and the viscosity is constant when the viscosity of non-Newtonian fluids is dependent on the shear rate. In this paper, Bingham fluid, a non-Newtonian fluid, has been focused on because of its practical engineering demands.

The behavior of these viscoplastic fluids is well described by several mathematical models, including the Bingham model, the Casson model, and the Herschel–Bulkley model, among which the Bingham model is the simplest and perhaps the most commonly used. The ideal Bingham model can be expressed as

\[ \tau = \tau_0 + \mu_\gamma \gamma \quad \text{for} \quad |\gamma| \geq \gamma_0 \]

\[ \tau = \tau_0, \quad \text{for} \quad |\gamma| < \gamma_0 \]

where \( \tau \) is the shear stress, \( \tau_0 \) is the yield stress \( \mu_\gamma \) is the plastic viscosity, and \( \gamma \) is the shear rate. As can be seen from Equation 9, the model is inherently discontinuous at the yield stress \( \tau_0 \) and may bring certain difficulties in numerical simulations. To work around this issue, Papamastasiou (1987) modified the equation by introducing a material parameter \( m \). The modified equation can be expressed as

\[ \tau = \left( \frac{\tau_0}{\gamma} - 1 - e^{-\gamma} \right) \mu_\gamma + \mu_\gamma \gamma \]

where \( m = \mu_\gamma \) is the stress growth exponent. Our previous work (Chen et al., 2014) has proven that Papamastasiou's model can accurately calculate the ideal Bingham model when the value of \( m \) is sufficiently high, and so for this paper, a value of \( m = 10^8 \) is chosen.

The apparent viscosity of Bingham fluids can be derived from Equation 10;

\[ \mu = \frac{\tau}{\gamma} = \mu_\gamma + \tau_0 \left( 1 - e^{-\gamma} \right) \]

where \( |\gamma| = \sqrt{\sum_{\alpha=1}^{n} \sum_{\beta=1}^{n} S_{\alpha \beta} S_{\beta \alpha}} \) and \( \mu_\gamma \) is the second invariant of the strain rate tensor \( S_{\alpha \beta} \). Moreover, in 3D LB formulations, \( S_{\alpha \beta} \) can be locally obtained from the nonequilibrium part of the density distribution function,

\[ f_i(x, t) = f_i(x, t) - f_i^{eq}(x, t) \]

(12)

Therefore, the apparent viscosity \( \mu \) can also be locally
calculated. According to Equation 8, the relaxation factor can be derived as
\[
\tau_{BGK} = \frac{1}{2} + \frac{3\mu \Delta t}{\rho (\Delta h)^2}
\]  
(13)

From Equation 13, we observe that \( \tau_{BGK} \) is constant for a Newtonian fluid; however, it changes with the apparent viscosity \( \mu \) for non-Newtonian fluids, which precisely reflects the different natures of these two kinds of fluids. However, the value of \( \tau_{BGK} \) must be within a limited range for stability and accuracy reasons (Latt, 2007). In this paper, we chose \( 0.501 \leq \tau_{BGK} \leq 8 \).

It is noteworthy that other types of non-Newtonian fluids can also be simulated like Bingham fluid, as long as their apparent viscosities are calculated by their corresponding rheological model and linked with the relaxation factor.

### 2.3 Mass tracking algorithm

The free-surface capturing algorithm was derived by Körner et al. (2005) and Thürey and Rüde (2009). At the free surface, lattice cells are divided into three categories: fluid, interface, and gas, as shown in Fig. 2. Compared with normal lattice Boltzmann method cells, the mass of the fluid cell, \( \rho(x, t) \), does not vary, whereas the mass of interface cell is defined as \( m(x, t) \), where \( 0 < m(x, t) < \rho(x, t) \). Because the influence of the gas is neglected, the mass of the gas cell is 0 and has no other information.

Consider one interface cell at position \( x \) (see Fig. 2). During the streaming step, some particle distributions coming from the neighboring cells arrive at this interface cell, whereas some density functions of this cell stream to other cells. The difference between the inflow and outflow of the density distribution functions results in a change in the mass of the current interface cell (Švec et al., 2012), which can be represented by
\[
m(x, t+\frac{1}{2}) = m(x, t) + \sum b_i \left[ f_i(x + e_i, t) - f_i(x, t) \right]
\]  
(14)

where \( f_i \) and \( f_j \) are the density distribution functions with opposite directions, and

\[
\begin{pmatrix}
\frac{1}{2}[m(x, t)+m(x+e_i, t)] & \text{if } (x+e_i, t) \text{ is an interface cell} \\
1 & \text{if } (x+e_i, t) \text{ is a fluid cell} \\
0 & \text{if } (x+e_i, t) \text{ is a gas cell}
\end{pmatrix}
\]  
(15)

In terms of the change of state of the cells, the interface cell becomes a fluid cell when \( m(x, t) \geq \rho(x, t) \), and becomes a gas cell when \( m(x, t) \leq 0 \). In such cases, the mass of the surrounding cells would be changed as well and converted into interface cells. The interface cells must form a completely closed boundary to separate the gas cells and the fluid cells to assure the conservation of mass and momentum (Körner et al., 2005).

It is noteworthy that some of the density distribution functions from the gas cells should arrive at the current interface cell during the streaming step. These functions do not exist and need to be reconstructed, which can be found in the work of Švec et al. (2012).

### 3 Validation and Discussion

As described in this section, the applicability of the proposed method was demonstrated using four examples. The first two benchmarks were a Newtonian flow through a square cross-section tube and a Bingham flow through a circular cross-section tube, both of which were utilized to validate lattice Boltzmann method model. Subsequently, the dam-break problem for Newtonian fluid and the slump test for Bingham fluid were simulated to validate the free-surface-capturing algorithm.

#### 3.1 Newtonian flow through a square cross-section tube

To test the 3D lattice Boltzmann method model, a Newtonian flow through a square duct was simulated, because this problem possesses analytical solutions that could be used for further comparison with the simulation results. The quasi-parabolic axial velocity distribution for flow in a rectangular duct is given by the series approximation
\[
u_z(y, z) = -\frac{16a^2}{\rho
\sum_{n=1}^{\infty}\frac{(-1)^{n+1}2n}{\cosh(\pi k b / 2a) - \cosh(\pi n b / 2a)} \frac{\cos(\pi y / 2a)}{k^2}}
\]  
(16)
in which, \(-a < y < a, -b < z < b\). The size of the computation domain was 0.2 m × 0.2 m × 0.2 m. The pressure boundary conditions, put forward by Zou and He (1997) were used at the inlet and outlet at an equivalent pressure gradient of \( G = 10^5 \) in lattice units, whereas halfway bounce-back boundary conditions were applied to
the other walls of the tube. The fluid density, kinematic viscosity, and relaxation parameters used were 1000 kg/m³, 10⁻⁵ m²/s, and 0.51, respectively. Fig. 3(a) is a contour plot of the axial velocity in the duct when a lattice spacing of 0.004 m was used, whereas the simulation and analytical velocities at the cross-sections with z = 0.1 m, y = 0.1 m and z = 0.1 m, y = 0.05 m are shown in Fig. 3(b). The characteristic quasi-parabolic flow profile is evident, and the simulation results fit well with the analytical results, proving the accuracy of the 3D lattice Boltzmann method.

We further investigated the error between the simulation and analytical results against lattice spacing, which is shown in Fig. 3(c). The error was evaluated as

$$
\varepsilon = \sum \sqrt{\frac{(u_{BM} - u_A)^2}{u_A^2}}
$$

(17)

in which $u_{BM}$ is the simulation result under the lattice Boltzmann method, whereas $u_A$ is the analytical result from Equation 16. More accurate simulation results can be obtained with smaller lattice spacing with an approximate second-order convergence, implying a second-order accuracy of the proposed 3D lattice Boltzmann method in space, which can satisfy the accuracy requirements for most problems.

3.2 Bingham flow through a circular cross-section tube

In this section, a 3D Bingham flow through a linear tube with a constant circular cross-section (approximated by a series of stairs) was simulated to further validate the 3D lattice Boltzmann method. All conditions for this simulation were dimensionless. The simulation domain comprised 48×60×60 uniform lattices (i.e., $Z=2R×2R$). The pressure boundary conditions (Zou and He, 1997) were used at the inlet and outlet at an equivalent pressure gradient of $G = -8.33×10^{-6}$ in lattice units, and halfway bounce-back boundary conditions were applied to the other walls of the tube. To save calculation time, the lattices outside the tube were considered unchanged. The plastic viscosity $\mu_p$ was set to 0.2, and Reynolds number was fixed at 0.95, whereas the yield stress $\tau_0$ increased

from 0 to 0.00010. The steady-state solution for the ideal Bingham model is given by (Chatzimina et al., 2005);

$$
u_r(r) = \begin{cases} 
-\frac{G}{4\mu}(R-r_0)^2, & 0 \leq r \leq r_0 \\
-\frac{G}{4\mu}(R^2-r^2)-\tau_0 \frac{r_0}{\mu}(R-r), & r_0 < r \leq R
\end{cases}
$$

(18)

where $r_0$ is the yield point and is given by $r_0 = -2\tau_0/G$, and $u_{max} = -G(R-r_0)^2/4\mu$.

The results from the numerical simulations (dots) and the corresponding analytical solutions (solid lines) of the middle slice are shown in Fig. 4. The velocity profile changed from a parabola to a flat plateau (i.e., an “unyielded region”) as the yield stress increased. When $\tau_0=0$, the Bingham fluid was reduced to a Newtonian fluid. It is noteworthy that the numerical results are consistent with the analytical solutions. Therefore, the proposed 3D lattice Boltzmann method can also be considered to be an effective tool for simulating Bingham fluids.

Comparing the velocity profile of Newtonian flow through a square duct in Section 3.1 with that of Bingham flow through a circular cross-section tube, big differences caused by the existence of yield stress $\tau_0$ can be seen. Bingham plasmas, or viscoplastic materials, behave as solids when the magnitude of the viscous stress is less than its
yield stress; however, above the yield stress these materials behave as liquids with an effective (apparent) viscosity dependent on the magnitude of the rate of strain. In the Bingham flow through a circular cross-section tube, on the one hand, the viscous stress next to the tube wall is greater than its yield stress, leading to a nonzero velocity gradient, which is related to the rate of strain. Conversely, the viscous stress in the center is less than its yield stress, and the rate of strain in this zone equals zero, implying that the fluid of this zone moves forward with a constant velocity like the movement of a solid. This zone is called the unyielded region, and would never exist in a Newtonian flow because the yield stress of a Newtonian fluid is zero.

3.3 Dam break of Newtonian fluids

Dam break is an important type of discontinuous flow encountered in practical engineering. This particular test example is utilized to validate our method, because it includes most flow structures, including shocks, rarefaction waves, and contact discontinuities (Tubbs and Tsai, 2011); moreover, predictions of such flows are benchmark tests for the capability of a numerical scheme (Zhou, 2007). Besides, experimental data (Martin and Moyce, 1952), as well as numerical calculations (Hirt and Nichols, 1981; Pan et al., 1993; Shao and Edmond, 2003), are available for comparison with our method.

First, a rectangular column of water (0.1 m-width and 0.2 m-height) was confined between two vertical walls (Fig. 5); then, the right wall was instantaneously withdrawn and the water inside flowed out freely. In the computation, the spatial resolution Δh was 2.5×10^-3 m and the time step Δt was 2×10^-4 s. As suggested by Shao and Edmond (2003), to account for the influence of the turbulent nature of the broken-dam flow, the kinematic viscosity in simulation was considered to be 1000 times greater than that of the constant laminar value, i.e., ν=10^-3 m²/s. The boundary condition between the fluid and bottom wall was the halfway bounce-back condition.

The fluid configurations of the flow at different times, t = 0.05 s, 0.1 s, 0.15 s, and 0.18 s, are shown in Fig. 5(a)–(d). The simulated flow patterns were very similar to those under other numerical approaches (Hirt and Nichols, 1981; Pan et al., 1993; Shao and Edmond, 2003). It was also found that water at the back end of the reservoir adhered to the back wall, forming a “tail.” This was caused by the adjusted viscosity, which was assumed to be 1000 times greater. In this context, it can be said that, although a tail should not appear for low-viscosity fluids including water, it is common for simulated fluids with high viscosity. To this end, the proposed method can demonstrate the influence of different viscosities, thereby proving its validity.

Another important index for checking the accuracy is the relationship between the normalized time \( T = t\sqrt{gh} \) and the leading edge \( X = x/H \) (note that the origin of \( x \) is defined at the dam site). Fig. 6 indicates the comparison of the temporal variation of the position of the leading edge from the dam site with experiment (Martin and Moyce, 1952) and other numerical results (Hirt and Nichols, 1981; Pan et al., 1993; Shao and Edmond, 2003). It can be seen that the relationship between \( T \) and leading edge \( X \) match with each other.

The velocity fields after the collapse of the dam at time \( t = 0.05 \) s, \( 0.1 \) s, \( 0.15 \) s, and \( 0.18 \) s are given in Fig. 7. An instantaneous jet could also be seen at the lower right corner on the free surface, caused by the imbalance of pressure after the removal of the right wall, which was similar to that observed experimentally by Stansby et al. (1998) and Shao and Edmond (2003). The magnitude of velocity in the x and z directions at the above-mentioned time are further illustrated in Fig. 8 and Fig. 9, respectively. The velocity on the free surface possessed higher values, whereas the fluid at large distances from the
Fig. 7. Evolution of the magnitude of velocity after dam break. (a) $t = 0.05 \text{ s}$, (b) $t = 0.10 \text{ s}$, (c) $t = 0.15 \text{ s}$, and (d) $t = 0.18 \text{ s}$.

Fig. 8. Magnitude of velocity in $x$ direction after collapse of dam at time (a) $t = 0.05 \text{ s}$, (b) $t = 0.10 \text{ s}$, (c) $t = 0.15 \text{ s}$, and (d) $t = 0.18 \text{ s}$.

surface remained almost stationary because of the constraint from the stationary solid walls. Both the maximum velocity and the velocity in the $x$ direction appeared in the wave front while the water in the upper right corner possessed the largest velocity in the $z$ direction.

The above case was a good test, because the appearance of both a vertical and horizontal free surface provided a
good check on the capability of the proposed method for free-surface treatment (Hirt and Nichols, 1981). Dam-breaking problems also involve rapidly varying, unsteady flows and provide extreme cases for examining the numerical stability and efficiency of numerical methods (Duan and Liu, 2007). Because the results of our simulation are in accord with those of the experiment and other numerical methods, it could be concluded that the proposed 3D lattice Boltzmann method incorporating the mass tracking algorithm can capture free-surface flows precisely and is capable of simulating unsteady flows with free surfaces stably and effectively.

Note that in order to account for the influence of the turbulent nature of the broken-dam flow, the kinematic viscosity in the simulation considered was 1000 times greater than that of the constant laminar value for easy comparison with the results of existent references. However, there are other mature methods to account for the effect of the turbulence without changing the kinematic viscosity. The most commonly used is that of incorporating large eddy simulations (LES) into the lattice Boltzmann method, which can be easily implemented in the LBE method (Krafczyk et al. 2003; Yu et al., 2005; Feng et al., 2007; Feng et al., 2010).

3.4 Slump test of non-Newtonian fluids

Fresh cement mortar is a classic Bingham plastic and is widely used in hydraulic and civil engineering. It plays an important role in the rehabilitation and repair of reinforced concrete structures. The workability of cement mortar is a vital factor in ensuring the quality of any construction and is normally evaluated by a slump test. The slump test of fresh cement mortar was simulated in the current work, to verify the validity and accuracy of the free-surface algorithm and the feasibility of its coupling with the lattice Boltzmann method for non-Newtonian fluids.

Roussel and Coussot (2005) developed an analytical solution for the slump test, and the final shape at stoppage and the yield stress can be described by

$$h(r) = \left( \frac{2\tau_0(R-r)}{\rho g} \right)^{1/2} \quad \text{and} \quad \tau_0 = \frac{225\rho g \Omega^2}{128\pi^2 R^2} \quad (19)$$

respectively, where $\tau_0$ is the yield stress, $\rho$ is the density of the sample, $\Omega$ is the volume of the slump cone, $R$ is the final radius of the slump test, $r$ is the distance from the cone center, and $h(r)$ is the height of the sample at $r$ used to represent the final shape. Furthermore, $\tau_0$ can be calculated from Equation 19 and then used as an input parameter in the numerical simulation.

In the current work, the slump test was simulated using the following proposed method. The slump cone was subdivided into height $\times$ bottom diameter $\times$ top diameter (75$\times$50$\times$20) discrete lattice units, with a spatial resolution of $\Delta x = 5\times10^{-3}$ m. The time step was of $\Delta t = 8\times10^{-3}$ s. The physical yield stress, kinematic viscosity, and density of the fluid were 48 Pa, 0.012 $m^2$/s, and 2400 $kg/m^3$. 

Fig. 9. Magnitude of velocity in $z$ direction after collapse of dam at time (a) $t = 0.05$ s, (b) $t = 0.10$ s, (c) $t = 0.15$ s, and (d) $t = 0.18$ s.
respectively. According to dimensional analysis, the lattice yield stress, kinematic viscosity, density of the fluid, and acceleration due to gravity were set to $8 \times 10^{-5}$, 0.06, 1, and $1.6 \times 10^{-5}$, respectively. The boundary condition between the fluid and the bottom wall was a halfway bounce-back condition. The slump cone was first filled with fresh cement mortar, and then the simulation commenced with the instantaneous release of the slump cone. For the purpose of comparison, all the parameters and simulating conditions were kept the same as those of Švec et al. (2012). The simulation was terminated when the relaxation time of 90% of the fluid cells reached $\tau_{\text{f0K}} = 8$ (Švec et al., 2012) (see Section 2.2).

The whole simulated slump process has been illustrated in Fig. 10, which is similar to that described by Švec et al. (2012). The final shapes of the slump tests obtained by our simulation, Švec’s simulation, and the analytical solution are compared in Fig. 11. The final shape of our simulation is almost the same as those of both the analytical solution and Švec’s results, proving the correctness and the accuracy of the developed method for simulating a free-surface flow of the Bingham fluid. Note that there is a small deviation in the results, which is caused by inertia. Equation 19 is obtained by ignoring the effect of inertia (Roussel and Coussot, 2005) when the effect of inertia could not be neglected in the simulation, because the slump cone was released instantaneously, resulting a much greater falling velocity of the Bingham fluid. As a result, the final shape obtained by simulation is flatter than those of the analytical results.

It is noteworthy that our simulation result looks uneven with small steps, which results from the relatively large spatial resolution; this can be smoothed artificially. The curve would become more even if the spatial resolution was increased; however, the cost of calculation would increase as well.

Yield stress is the main difference between Newtonian fluid and Bingham fluid and many other non-Newtonian fluids. With the existence of yield stress, the behavior of a non-Newtonian fluid is more complicated and diverse, which makes it more difficult to study non-Newtonian fluids and at the same time more extensively to use them in civil and chemical engineering. For example, there exists some unyielded region like a solid in the Bingham flow, thus this means that the fluid would not flow even under a pressure gradient. Thus, the flow of Bingham fluid would stop when the stress generated by the pressure gradient was less than the yield stress, and would not flow as flat as possible like a Newtonian fluid.

4 Conclusions

In the current paper, a 3D lattice Boltzmann method approach has been proposed to model the free-surface flow of both Newtonian and non-Newtonian fluids. This approach uses the mass tracking algorithm to capture the free surface. Conclusions were drawn as follows:

(1) The proposed the lattice Boltzmann method model was validated by Newtonian flow through a square cross-section tube and Bingham flow through a circular cross-section tube. In addition, the dam-break problem for Newtonian fluid and the slump test for Bingham fluid were simulated to validate the free-surface capturing algorithm. The numerical results were in good agreement with analytical or other simulation data, proving the validity and correctness of our model and the method.

(2) The advantages of numerical simulation are that it can reveal many details that cannot be acquired via experiment or theoretical analysis and that it is relatively inexpensive. Thus, the developed method can be used in many fields, including civil engineering and geomechanics problems. For example, the presently proposed method can be used as a substitute for expensive and time-consuming experiments and to simulate the gap-filling
processes in reinforced concrete structures or between the rocks to form rock-filled concrete by fresh cement mortar or self-compacting concrete, respectively. Furthermore, granular flows, which may result in large amount of damage, can be simplified as uniform non-Newtonian fluids. The mechanics of their occurrence and movement can be simulated and investigated with the help of the developed method, which may deepen the understanding of granular flows and other disasters. Related research is being conducted. All these possible applications can significantly affect engineering and scientific research in a positive way.

(3) Besides easy coupling with the LES to solve turbulence problems, the lattice Boltzmann method has other advantages over other numerical schemes for fluid flows like the computational fluid dynamics, the smoothed particle hydrodynamics, the marker-and-cell, and the volume-of-fluid. First, the boundary treatment is simple because of its micro-particle background. Other than conventional pressure, velocity, or periodic boundary conditions, there are many ways to account for the interactions between a fluid and structures or suspended particles, among which the bounce-back scheme (Frisch et al., 1987; Gallivan et al., 1997) and the immersed boundary method (Noble and Torczynski, 1998; Aidun et al., 1998; Peng and Luo, 2008) are most commonly used. The bounce-back scheme simply enforces the no-slip condition at fluid-solid interfaces by reflecting particle distribution functions from the boundary nodes in the direction of incidence, which is especially suitable for straight walls, whereas the implementation of the immersed boundary method is a bit more complicated but with better accuracy. It is frequently used for complex geometries and moving boundary conditions, like spheres and porous media. Conventional numerical schemes often work inaccurately with complex geometries and moving boundary conditions, which often occur in geotechnical and geological engineering. Secondly, the lattice Boltzmann method can easily be coupled with the discrete element method (DEM) to simulate particle suspension flow or multiphase flow. Because the fluid grid is an order of magnitude smaller than the size of the particle, the interactions between fluid and suspended particles and the movement of particles can be precisely described and solved, which are essential issues in many geotechnical problems. Third, because the evolution equations of the lattice Boltzmann method are simple and local, the lattice Boltzmann method can easily be parallelized with both CPU and GPU, offering great advantages for simulating large-scale flow problems.

(4) Note that there are also some shortcomings with the lattice Boltzmann method. The most critical one is numerical instability when the relaxation time gets very close to 0.5, which means that the lattice Boltzmann method needs special treatments to deal with low-viscosity fluids like water. This weakness can be overcome using a smaller lattice spacing and discrete time step, which conversely leads to greater computational cost. The other shortcoming is that the lattice Boltzmann method is only suitable for problems of low Mach number without special treatments.

The proposed lattice Boltzmann method may be utilized in the research of granular flows in the future, which is our main study area. Most granular flows can be simplified as non-Newtonian flows in porous media, or with complex boundaries and free surfaces where the lattice Boltzmann method can exploit its advantages to the fullest. Because most granular flows are viscous and their velocities are far smaller than the acoustic speed, no special treatments are needed for dealing with these problems with the lattice Boltzmann method. The main aim of this paper is to develop and validate the 3D lattice Boltzmann method, which can be used to simulate free-surface flows of both Newtonian and non-Newtonian fluids. The coupling with DEM, the parallel efficiency, and the application of the lattice Boltzmann method to some granular problems will be presented later.

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