

Modified Multi-Relaxation-Time Lattice Boltzmann Method for Herschel-Bulkley Fluids: Postprint

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Abstract

As an important class of non-Newtonian fluids, Herschel-Bulkley fluids have been widely applied in engineering fields. To improve the stability and accuracy of LBM for simulating Herschel-Bulkley fluid flows, an improved method is proposed based on the multiple-relaxation-time LBM (MRT LBM). Taking Poiseuille flow as an example, the improved algorithm is introduced in detail, comparisons are conducted for shear-thinning and shear-thickening fluids respectively, and the variation trend of relative error with increasing grid number under different exponent conditions is analyzed, demonstrating the effectiveness of this improved method. Finally, through application in cement 3D printing nozzles and comparison with simulation results from the multiple-relaxation-time LBM (MRT LBM), the feasibility of this improved method is further validated.

Full Text

Preamble

A Modified Multiple-Relaxation-Time Lattice Boltzmann Method for Herschel-Bulkley Fluids

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Abstract

As an important class of non-Newtonian fluids, Herschel-Bulkley fluids have been widely applied in engineering fields. To improve the stability and accuracy of the Lattice Boltzmann Method (LBM) when simulating Herschel-Bulkley

fluid flows, a modified method based on the Multiple-Relaxation-Time LBM (MRT LBM) is proposed. Using Poiseuille flow as an example, the modified algorithm is introduced in detail. Comparisons are made for both shear-thinning and shear-thickening fluids, and the variation trends of relative errors with increasing lattice nodes under different power-law indices are analyzed to demonstrate the effectiveness of this improved method. Finally, through application in a cement 3D printing nozzle, the simulation results are compared with those obtained using the standard MRT LBM, further verifying the feasibility of the proposed method.

Keywords: Herschel-Bulkley fluids; modified MRT LBM; Poiseuille flow; cement 3D printing; MRT LBM

0 Introduction

The Lattice Boltzmann Method (LBM) provides an effective alternative to finite element methods for fluid flow simulation, offering clear physical processes and simple computational procedures. It has been widely applied to numerous complex fluid flows, with in-depth research conducted on non-Newtonian fluid flow simulations. When analyzing non-Newtonian fluid flows, the relaxation time varies with the local viscosity of the fluid in real time. It is well known that maintaining the relaxation time within the range of $1/2$ to 1 ensures simulation stability and accuracy; beyond this range, instability and poor accuracy readily occur. To address this issue, various scholars have proposed a series of solutions. Gabbanelli S proposed a truncated model for power-law fluids and validated its effectiveness through analysis and comparison with Poiseuille flow. Malaspina O employed a local method to conduct detailed studies on both power-law and Carreau fluids, demonstrating good stability within certain index ranges. Boyd J et al. used a local method to analyze power-law fluid flow in pipes, showing that this method's computational accuracy and efficiency were superior to Gabbanelli S's truncated model. In 2001, D' Humières D et al. proposed the Multiple-Relaxation-Time LBM for three-dimensional cavity flow, proving its superior stability compared to standard LBM. Subsequently, MRT LBM was also applied to non-Newtonian fluid simulations. CHAI Zhenhua et al. used MRT LBM to analyze power-law and Bingham fluids in non-Newtonian flows, demonstrating excellent stability and good accuracy. Fallah K et al. simulated power-law fluid flow in a rotating cylinder using MRT LBM, analyzing the effects of rotational speed and power-law index on the flow process. CHEN Songgui et al. simulated three-dimensional Bingham fluid flow between parallel plates using MRT LBM, resolving the instability issues encountered in traditional LBM simulations of non-Newtonian fluids. LI Qiuxiang et al. analyzed power-law fluid flow in a two-dimensional square cavity, showing that MRT LBM can be effectively applied to non-Newtonian fluid simulations, though Reynolds number and power-law index significantly influence the results.

Although research on non-Newtonian fluids has been extensive, it has primarily focused on common types such as power-law and Bingham fluids, with limited

investigation of less common varieties like Herschel-Bulkley fluids. This paper takes Herschel-Bulkley fluid as the research object and proposes an improved method based on MRT LBM that can more effectively enhance simulation stability. Using Poiseuille flow as an example, the method is introduced in detail and compared with analytical solutions, with relative errors analyzed. Finally, the method is applied to analyze cement paste flow in a 3D printing nozzle to further demonstrate its feasibility.

1.1 Constitutive Equation of Herschel-Bulkley Fluids

The constitutive model of Herschel-Bulkley fluids is presented in piecewise function form. Due to the existence of initial yield stress, the shear rate is zero when the stress is below this threshold. The specific expression is:

$$\tau = \begin{cases} \tau_0 + K\dot{\gamma}^n & \text{if } \tau > \tau_0 \\ 0 & \text{if } \tau \leq \tau_0 \end{cases}$$

To avoid the inconvenience caused by piecewise functions during analysis, a modified constitutive equation is adopted as follows:

$$\tau = \tau_0[1 - \exp(-m\dot{\gamma})] + K\dot{\gamma}^n$$

In this equation, parameter m primarily controls stress growth to avoid the inherent discontinuity characteristics of the constitutive equation. When m approaches zero, it becomes the constitutive equation for power-law fluids; when m approaches infinity, it becomes the ideal Herschel-Bulkley fluid. When $\dot{\gamma} = 0$, it matches the original constitutive equation. In general cases, m takes a relatively large value, though it should be noted that m cannot take arbitrarily large values, as this would cause convergence issues. The apparent viscosity equation can be further derived:

$$\mu(\dot{\gamma}) = \frac{\tau_0[1 - \exp(-m\dot{\gamma})]}{\dot{\gamma}} + K\dot{\gamma}^{n-1}$$

Transforming $f(\mathbf{r}, t)$ and $f^{eq}(\mathbf{r}, t)$ into moment space yields $\mathbf{m}(\mathbf{r}, t)$ and $\mathbf{m}^{eq}(\mathbf{r}, t)$, where $\mathbf{m} = M\mathbf{f}$ and $\mathbf{m}^{eq} = M\mathbf{f}^{eq}$. Matrix M is defined as the transformation matrix, and S is a diagonal matrix related to relaxation: $S = \text{diag}(s_0, s_1, s_2, s_3, s_4, s_5, s_6, s_7, s_8)$. In the model, density and momentum are conserved quantities, so the parameters s_0 , s_3 , and s_5 related to density and momentum are all set to 0, while s_7 and s_8 are set to $1/\tau$, where τ is the relaxation time in the BGK model. The remaining parameters take values slightly greater than 1, with $s_1 = s_2 = 1.4$ and $s_4 = s_6 = 1.2$.

The evolution process of the MRT model consists of two steps: collision and streaming. The collision step differs from the BGK model and follows the equation:

$$\mathbf{f}^+(\mathbf{r}, t) = \mathbf{f}(\mathbf{r}, t) - M^{-1}S[\mathbf{m}(\mathbf{r}, t) - \mathbf{m}^{eq}(\mathbf{r}, t)]$$

where $\mathbf{f}^+(\mathbf{r}, t)$ is the post-collision density distribution function. The streaming step is the same as in the BGK model:

$$f_i(\mathbf{r} + \mathbf{e}_i\delta_t, t + \delta_t) = f_i^+(\mathbf{r}, t)$$

Compared with the BGK model, the MRT model primarily includes the transformation process between moment space and velocity space. Using Chapman-Enskog expansion, the kinematic viscosity can be obtained:

$$\nu = c_s^2 \left(\frac{1}{s_7} - \frac{1}{2} \right) \delta_t = c_s^2 \left(\tau - \frac{1}{2} \right) \delta_t$$

The macroscopic definitions of density and velocity can also be obtained, consistent with the BGK model.

1.2 MRT LBM for Fluid Analysis

The Multiple-Relaxation-Time Lattice Boltzmann equation is:

$$\mathbf{f}(\mathbf{x} + \mathbf{e}_i\delta_t, t + \delta_t) = \mathbf{f}(\mathbf{x}, t) - M^{-1}S[\mathbf{m}(\mathbf{x}, t) - \mathbf{m}^{eq}(\mathbf{x}, t)]$$

The kinematic viscosity is related to the shear rate. Traditional numerical methods require establishing appropriate difference models to solve this, while LBM can avoid this process. In the MRT model, the strain rate tensor is more complex than in the BGK model and can be derived as:

$$\dot{\gamma}_{\alpha\beta} = -\frac{1}{2\rho c_s^2} \sum_{i=0}^8 f_i^{(1)} (\mathbf{e}_{i\alpha} \mathbf{e}_{i\beta} - c_s^2 \delta_{\alpha\beta})$$

where $f_i^{(1)}$ can be approximated by $f_i^{(1)} \approx f_i - f_i^{eq}$.

1.3 Modified MRT LBM

Based on the above analysis, when MRT LBM is applied to non-Newtonian fluids, it is primarily affected by the local relaxation time, which can also be viewed as being influenced by viscosity, which in turn is related to the strain

rate through the stress tensor. For Herschel-Bulkley fluids, when $n < 1$, it corresponds to shear-thinning fluids; when $n = 1$, it corresponds to Bingham fluids; and when $n > 1$, it corresponds to shear-thickening fluids. Direct application of MRT LBM to non-Newtonian fluids with exponential terms leads to stability and accuracy issues. When the shear rate approaches zero, for shear-thinning fluids with $n < 1$, the viscosity tends to infinity, causing divergence; for shear-thickening fluids with $n > 1$, the viscosity tends to zero. Previous scholars have not mentioned solutions specifically for analyzing Herschel-Bulkley fluids.

In fact, most non-Newtonian fluids exhibit non-Newtonian characteristics only within a certain shear rate range, and typically display Newtonian-like behavior outside this range, where viscosity is constant. Based on this phenomenon, a modified MRT LBM method is proposed for Herschel-Bulkley fluids, presented in piecewise function form. Due to the yield stress in Herschel-Bulkley fluids, to ensure that viscosity remains constant when the shear rate is outside the effective range, the Bingham fluid constitutive model is used as a substitute.

MRT LBM can perform accurate and stable simulations when the dynamic viscosity is within a certain range. However, when the relaxation time approaches $1/2$, instability occurs, causing divergence, which corresponds to viscosity approaching zero ($\nu \leq 0.001$). Correspondingly, when the relaxation time exceeds 1, the accuracy of MRT LBM decreases, which corresponds to relatively large viscosity ($\nu \geq 1/6$). Therefore, upper and lower viscosity limits are set for the apparent viscosity equation as $\nu_{\min} = 0.001$ and $\nu_{\max} = 0.16$. Clearly, for shear-thinning fluids, the maximum viscosity corresponds to shear rates approaching zero, while for shear-thickening fluids, the minimum viscosity corresponds to shear rates approaching zero.

2 Flow Between Parallel Plates

Due to the existence of theoretical solutions, Poiseuille flow is often used to verify stability and accuracy issues. Here, Poiseuille flow is taken as an example to introduce the specific process of this modified model. Two parallel plates are separated by a distance H in the y -direction, with a constant pressure gradient ∇P applied in the x -direction, allowing the velocity component u_y distribution along the y -direction to be obtained. Based on symmetry, the y -direction distance is divided into $[-H/2, 0]$ and $[0, H/2]$ intervals. Due to symmetry, analyzing only the $[0, H/2]$ range yields the u_y distribution along the entire y -direction. Within the $[0, H/2]$ interval, four distinct regions A, B, C, and D can be identified. Region A corresponds to the high shear rate range near the wall, where the shear rate exceeds $\dot{\gamma}_{\infty}$, with y_h as the boundary value; in this region, the fluid is treated as Bingham fluid. Region B corresponds to the effective region of Herschel-Bulkley fluid, with y_l as the critical boundary value. Region C corresponds to the low shear rate range, where the fluid is treated as Bingham fluid. Region D corresponds to the stage where stress is less than yield stress, where the shear rate is zero, with y_{τ} as the boundary value. Combining the velocity derivation for Poiseuille flow, the theoretical function for the velocity

distribution of this modified method can be obtained:

$$u(y) = \begin{cases} \frac{\nabla P}{2\mu_\infty} (y^2 - H^2/4) + \frac{\tau_0}{\mu_\infty} (y - H/2) + u_{\text{plug}} & \text{for } y_h \leq y \leq H/2 \\ \frac{\nabla P}{2\mu_B} (y^2 - y_l^2) + \frac{\tau_0}{\mu_B} (y - y_l) + u_{\text{HB}}(y_l) & \text{for } y_l \leq y < y_h \\ \frac{\nabla P}{2\mu_0} (y^2 - y_\tau^2) + \frac{\tau_0}{\mu_0} (y - y_\tau) + u_{\text{plug}} & \text{for } y_\tau \leq y < y_l \\ u_{\text{plug}} & \text{for } 0 \leq y < y_\tau \end{cases}$$

The constant terms α_1 , α_2 , and α_3 in the above equation are expressed as follows:

$$\alpha_1 = \frac{\nabla P}{\mu_\infty}, \quad \alpha_2 = \frac{\nabla P}{\mu_B}, \quad \alpha_3 = \frac{\nabla P}{\mu_0}$$

After differentiating the above velocity distribution function and applying stress continuity conditions, the corresponding boundary values are obtained:

$$y_\tau = \frac{\tau_0}{|\nabla P|}, \quad y_l = \left(\frac{\mu_B |\nabla P|}{K} \right)^{1/(n-1)}, \quad y_h = \left(\frac{\mu_\infty |\nabla P|}{K} \right)^{1/(n-1)}$$

where μ_B is the Bingham viscosity and μ_0, μ_∞ are the limiting viscosities. Different values of $\partial P/\partial x = \nabla P$ yield different region divisions. According to the velocity distribution equation, four main factors affecting the final simulation results are considered: initial yield stress τ_0 , pressure gradient ∇P , power-law index n , and number of lattice nodes N . Examination of the boundary conditions reveals that to ensure the existence of y_l and/or y_h , the following condition must be satisfied:

$$\frac{|\nabla P|H}{2\tau_0} > 1$$

To investigate the effectiveness of this truncated model for different indices n , the range of n is taken as $0.2 \sim 5$. Here, the power-law index n is taken as 0.5 and 1.5, corresponding to shear-thinning and shear-thickening fluids respectively, which more clearly demonstrates the influence of initial yield stress on simulation results.

When $n = 0.5$, the pressure gradient $\nabla P = -1.5 \times 10^{-6}$, fluid viscosity coefficient $K = 0.001$, plate height $H = 10$, number of lattice nodes $N = 200$, fluid density $\rho = 1$, kinematic viscosity limits $\nu_{\min} = 0.001$ and $\nu_{\max} = 0.16$. Since $n < 1$, $\nu_0 = 0.16$ and $\nu_\infty = 0.001$, with initial yield stress $\tau_0 = 3.0 \times 10^{-6}$. The comparison between numerical and simulation results is shown in Figure 1 [Figure 1: see original paper]. The solid line in the figure depicts the velocity distribution according to the analytical solution, circles represent results

obtained through LBM simulation, dashed portions represent the extensions corresponding to Bingham fluid and Herschel-Bulkley fluid respectively, and vertical dashed lines represent boundaries between different regions.

When the power-law index $n = 1.5$, the pressure gradient $\nabla P = -2 \times 10^{-6}$, fluid viscosity coefficient $K = 0.01$, plate height $H = 10$, number of lattice nodes $N = 200$, fluid density $\rho = 1$, kinematic viscosity limits $\nu_{\min} = 0.001$ and $\nu_{\max} = 0.16$. Since $n > 1$, $\nu_0 = 0.001$ and $\nu_{\infty} = 0.16$, with initial yield stress $\tau_0 = 4.0 \times 10^{-6}$. The comparison between numerical and simulation results is shown in Figure 2 [Figure 2: see original paper]. The solid line depicts the velocity distribution according to the analytical solution, circles represent LBM simulation results, dashed portions represent extensions corresponding to Bingham fluid and Herschel-Bulkley fluid, and vertical dashed lines represent boundaries between different regions.

Observation of Figures 1 and 2 reveals that regardless of how the initial yield stress changes, the numerical solution shows good agreement with the analytical solution. The initial yield stress τ_0 and pressure gradient ∇P determine the size of the yield stage, i.e., region D.

3 Simulation Application in Cement 3D Printing Nozzle

During cement 3D printing, screw extrusion is used to achieve the extrusion molding of cement paste, making it particularly important to understand the flow behavior of cement paste within the nozzle. Under certain water-cement ratios, cement paste exhibits obvious Herschel-Bulkley fluid characteristics. At room temperature of 20°C, with a water-cement ratio of 0.5 and hydration time of 5 minutes, the paste displays typical Herschel-Bulkley rheological behavior, described by the rheological equation:

$$\tau = 3.899 + 1.103\dot{\gamma}^{0.5}$$

A series of simulations were conducted for four fluids with different indices, comparing the relative errors between MRT LBM simulations and analytical solutions. The relative error is calculated as:

$$\text{Error} = \frac{\sum |u_{\text{num}} - u_{\text{ana}}|}{\sum |u_{\text{ana}}|}$$

Since LBM simulation accuracy is related to viscosity, to ensure discussion focuses only on the relationship between relative error and number of lattice nodes, during unit conversion the viscosity in the model is set as $\nu^* = \nu(\delta x^2/\delta t)$, with $\delta x^2/\delta t$ held constant. When increasing the number of lattice nodes N in LBM, δx and δt are scaled proportionally to maintain constant viscosity. Since $1/\delta x \propto N$, according to the previous relationship, N is gradually increased from 10 to 200. The relative errors under different indices and pressure gradients are

shown in Figure 3 [Figure 3: see original paper]. The solid line in the figure represents a straight line with slope -1. In the legend, 'a' represents cases where the low shear rate region C is small, while 'b' represents cases where region C is large. Comparison shows that the relative errors produced in both cases are essentially the same, and as the number of lattice nodes increases, the relative error continuously decreases. If the number of lattice nodes is further increased, the error can be controlled within 0.01%. The figure further shows that when the index n takes different values, the differences in relative error are more pronounced.

Converting the above equation into the form of the apparent viscosity equation, parameter m primarily controls stress growth, with $m = 500$ taken here:

$$\tau = 3.899[1 - \exp(-500\dot{\gamma})] + 1.103\dot{\gamma}^{0.5}$$

Cement paste flows in the screw channel region shown in Figure 4 [Figure 4: see original paper], where the screw rotates at constant speed N . Assuming the screw is stationary, the barrel can be considered to rotate in the opposite direction at speed N . Expanding the entire structure forms a rectangular cross-section cavity. Ignoring the slight inclination of the screw flights, the expansion schematic is shown in Figure 5 [Figure 5: see original paper]. Thus, the flow analysis of cement paste in the screw is transformed into flow analysis of cement paste in the rectangular cavity shown in Figure 5.

According to the nozzle expansion schematic, the central cross-section $(Y-Z)_{\text{Center}}$ is taken, using the D2Q9 model. Only the top surface is assigned velocity along the Z-direction at $y = h$, while the other three surfaces have zero velocity. Wall slip effects are neglected. The actual cross-section dimensions are $W = 16$ mm and $h = 6$ mm. Considering the nozzle scanning speed requirements and cement paste setting time, the paste extrusion speed is relatively low. The screw rotation speed is taken as 30 r/min, with a screw lead angle $\theta = 20^\circ$. Using similarity criteria with Reynolds number Re as the key dimensionless parameter for scaling, various parameters in the simulation model can be obtained. The viscosity is then corrected using the modified viscosity equation to ensure stability and accuracy, yielding the streamline diagram shown in Figure 6 [Figure 6: see original paper]. The fluid flow presents a circulation pattern, with the circulation center near $(0.5W, 0.7h)$. No obvious fluid flow exists in the lower left and right corners.

Using the modified MRT LBM, simulations were performed with different numbers of lattice nodes and compared with standard MRT LBM, yielding the corresponding velocity field distributions shown in Figure 7 [Figure 7: see original paper]. The modified MRT LBM used lattice numbers of 288×108 and 160×60 , while standard MRT LBM used 288×108 for comparison. Figure 7(a) shows the relationship between velocity component u and channel depth at a channel width of 8 mm. Figure 7(b) shows the relationship between velocity component

u and channel width at a channel depth of 5.4 mm. Figure 7(c) shows the relationship between velocity component v and channel depth at a channel width of 14.4 mm. Figure 7(d) shows the relationship between velocity component v and channel width at a channel depth of 3 mm. The results demonstrate that this modified method can effectively simulate velocity field distributions. Although some errors exist when using different numbers of lattice nodes, the results are essentially consistent.

4 Conclusions

A modified MRT LBM method is proposed for Herschel-Bulkley fluids in generalized Newtonian fluids, which can effectively improve the divergence issues that easily occur during simulation.

- (1) The method is discussed in detail through Poiseuille flow, with theoretical solution formulas derived. Relative errors are calculated, showing that as the number of lattice nodes increases, the relative error continuously decreases, reaching approximately 0.05%. Both shear-thinning and shear-thickening fluids exhibit the same trend. It is further demonstrated that the size of the low shear rate region has almost no effect on the relative error, while the value of index n has a significant influence.
- (2) The method is applied to analyze the flow of cement paste in a 3D printing nozzle and compared with the standard MRT LBM method. The velocity field distributions are found to be essentially consistent, further proving the effectiveness of this improved method.
- (3) Analysis of the flow in the cement 3D printing nozzle shows that due to the paste viscosity and nozzle structure, the paste flow in the nozzle cross-section exhibits circulation characteristics, with the circulation center approximately at $(0.5W, 0.7h)$. The flow region can be determined from the streamline diagram. The flow analysis reveals that no obvious fluid flow exists in the lower left and right corners of the cavity. To ensure fluid flow velocity, the screw rotation speed can be appropriately increased on one hand, and the channel width can be appropriately increased on the other hand.

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