

# **Lattice Boltzmann Simulation of Solid Particles Suspended in Fluid**

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*Received July 19, 1994; final February 27, 1995*

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The lattice Boltzmann method, an alternative approach to solving a fluid flow system, is used to analyze the dynamics of particles suspended in fluid. The interaction rule between the fluid and the suspended particles is developed for real suspensions where the particle boundaries are treated as no-slip impermeable surfaces. This method correctly and accurately determines the dynamics of single particles and multi-particles suspended in the fluid. With this method, computational time scales linearly with the number of suspensions,  $N$ , a significant advantage over other computational techniques which solve the continuum mechanics equations, where the computational time scales as  $N^3$ . Also, this method solves the full momentum equations, including the inertia terms, and therefore is not limited to low particle Reynolds number.

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**KEY WORDS:** Lattice Boltzmann method; suspensions; boundary conditions.

## **1. INTRODUCTION**

Understanding the macroscopic transport behavior of particles or fibers suspended in a fluid medium is important to many industries that deal with slurries, colloids, polymers, ceramics, etc. In the paper and photographic film industries the flows of suspensions occur in important manufacturing processes, including paper formation, coating, and printing applications. Effective experimental methods, such as magnetic resonance imaging, are being developed for investigation of the macroscopic behavior of suspensions. There is a great need for a theoretical approach to analyze accurately

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and predict the microstructural dynamics of flow in many manufacturing processes. The flow of suspensions under the blade in coating paper and film is a prime candidate. The small-scale structure of the coating layer on the surface of the paper and photographic films is of critical importance for the industry. Controlling and improving the surface quality and physical properties depend on understanding the microstructure of the pigment particle formation, binder migration, and interactions with the porous substrate. In a typical blade coating system, the particle Reynolds number varies from 0.1 to 5. Therefore, inertia effects need to be included in the analysis.

One of the methods that has been successful for analysis of suspensions is Stokesian dynamics.<sup>(1-3)</sup> This method solves the Stokes equations for the fluid phase and the  $N$ -body Langevin equation to obtain the motion of  $N$  particles. With this method, however, the computational time scales as  $N^2$  if the mobility matrix is directly constructed and  $N^3$  if the hydrodynamic interactions are included. Also, the method is limited to suspensions with simple geometries such as spheres or spheroids in simple shear layers. Considering that in some applications, the particles are irregularly shaped and the particle Reynolds number is not small, other methods need to be developed for analysis of various particulate transport processes.

We are developing a method for microdynamical analysis of particles suspended in liquid. This method is based on the solution of the lattice Boltzmann equation<sup>(5)</sup> for the fluid phase, which reduces to the Navier–Stokes equations with appropriate equilibrium distribution function. The equations describing the interaction of the fluid with the suspended particles are derived based on the conservation of mass and momentum. The suspended particles move based on Newton’s equation of motion.

In this study, we present the boundary collision rules, and we examine the accuracy of this method with known solutions of flow over circular particles using the finite-element solution of the Navier–Stokes equations. Single-particle sedimentations are also simulated and compared with the results of Feng *et al.*<sup>(4)</sup> We also compare the effective viscosity of suspensions with other simulation results<sup>(2, 3, 6)</sup> for multiparticle flow systems. In all cases, the results agree very well with the known results. We have also examined the computational speed as a function of the number of solid particles  $N$ . The computational time increases linearly with  $N$ , making it possible to obtain macroscopic behavior by considering a large number of suspended particles.

The reason for the remarkable computational speed is the local nature of time evolution operation with the lattice Boltzmann method.<sup>(5)</sup> At each time step, the distribution function is updated in two steps. One is the collision operation, which is completely local at each lattice and independent of

the surrounding lattices. The other step involves the streaming where mass and momentum are transported to neighboring lattice nodes. This step also involves local communication between immediate lattice neighbors. The time evolution of the solution is explicit and therefore involves no matrix solution or inversions.

Ladd *et al.*<sup>(6)</sup> first applied the lattice gas automaton<sup>(7,8)</sup> to the two-dimensional flow of suspensions. Recently, Ladd<sup>(9,10)</sup> combined the lattice Boltzmann method for the fluid phase with the Newtonian dynamics of the colloidal suspension system for analysis of short-time motion of colloidal particles. Ladd's method,<sup>(10)</sup> however, allows a small amount of mass transfer across the surface of the solid particles. In other words, the lattice nodes inside and outside the particles are treated in an identical manner so that the fluid occupies the whole computational domain, inside and outside the suspended particles.

We have developed a new boundary rule for the interaction between the surface of impermeable particles and fluid. The new rule treats the suspensions as solid particles and prevents mass exchange across the suspension boundary, while taking account of the momentum exchange between the fluid and the solid particle. The particles have solid boundaries and their motion relative to the fluid phase is governed by Newton's law of motion. Following an outline of the problem formulation and the new particle/fluid interaction rule, we present the numerical results and we examine the accuracy of this method.

In this analysis, we use the Bhatnagar–Gross–Krook<sup>(11)</sup> single-relaxation-time approximation to replace the linear operator of Higuera *et al.*<sup>(12)</sup> in the lattice Boltzmann equation, proposed by McNamara and Zanetti.<sup>(5)</sup> Consider a square lattice where on each lattice node, there are pseudo fluid particles that can fall into three categories: fluid particles at rest, fluid particles moving along the off-diagonal directions, and fluid particles moving along the diagonal directions. The velocity vectors are denoted as  $\mathbf{e}_{0i}$  for the fluid particles at rest and  $\mathbf{e}_{1i}$  and  $\mathbf{e}_{2i}$  for the moving fluid particles, respectively. The velocity vectors are defined as

$$\mathbf{e}_{0i} = (0, 0) \quad (1)$$

$$\mathbf{e}_{1i} = \left( \cos \frac{i-1}{2} \pi, \sin \frac{i-1}{2} \pi \right), \quad i = 1, \dots, 4 \quad (2)$$

$$\mathbf{e}_{2i} = \sqrt{2} \left( \cos \left( \frac{i-1}{2} \pi + \frac{\pi}{4} \right), \sin \left( \frac{i-1}{2} \pi + \frac{\pi}{4} \right) \right), \quad i = 1, \dots, 4 \quad (3)$$

At each time step, the moving fluid particles will arrive only at their nearest neighbor nodes. The lattice Boltzmann equation applied to the fluid particles is given by

$$f_{\sigma i}(\mathbf{x} + \mathbf{e}_{\sigma i}, t + 1) - f_{\sigma i}(\mathbf{x}, t) = -\frac{1}{\tau} [f_{\sigma i}(\mathbf{x}, t) - f_{\sigma i}^{(0)}(\mathbf{x}, t)] \quad (4)$$

where  $f_{\sigma i}(\mathbf{x}, t)$  ( $\sigma = 0, i = 1$ ;  $\sigma = 1, 2$ ;  $i = 1, \dots, 4$ ) is the single-particle distribution function,  $f_{\sigma i}^{(0)}(\mathbf{x}, t)$  is the equilibrium distribution at  $(\mathbf{x}, t)$ , and  $\tau$  is the single relaxation time. In our simulations,  $f_{\sigma i}^{(0)}(\mathbf{x}, t)$  is taken as

$$f_{\sigma i}^{(0)}(\mathbf{x}, t) = A_{\sigma} + B_{\sigma}(\mathbf{e}_{\sigma i} \cdot \mathbf{u}) + C_{\sigma}(\mathbf{e}_{\sigma i} \cdot \mathbf{u})^2 + D_{\sigma}u^2 \quad (5)$$

with

$$\begin{aligned} A_0 &= \frac{\rho}{2}, & B_0 &= 0, & C_0 &= 0, & D_0 &= 0 \\ A_1 &= \frac{\rho}{12}, & B_1 &= \frac{\rho}{3}, & C_1 &= \frac{\rho}{2}, & D_1 &= -\frac{\rho}{2} \\ A_2 &= \frac{\rho}{24}, & B_2 &= \frac{\rho}{12}, & C_2 &= \frac{\rho}{8}, & D_2 &= \frac{\rho}{8} \end{aligned} \quad (6)$$

where  $\rho$  is the mass density at the node. For this model, the speed of sound is  $c_s = \sqrt{1/3}$ , and the kinematic viscosity is  $\nu = (2\tau - 1)/6$ . With this equilibrium distribution, the Navier–Stokes equations can be derived using the Chapman–Enskog expansion.

## 2. BOUNDARY RULE AND DYNAMICS FOR SOLID PARTICLES

The physical boundary condition at the solid–fluid interface is the no-slip condition, that is, the fluid adjacent to the solid surface moves with the solid surface and the velocity normal to the solid surface is zero. There are several methods to implement the no-slip boundary conditions<sup>(11)</sup> in lattice Boltzmann simulations. Here we use a modified bounce-back method with appropriate momentum exchange between the solid and the fluid.

The solid boundary is located at a distance equal to one-half the lattice space away from the lattice point. In this case, the fluid particles collide with the solid boundary in the middle of the convection process and bounce back along the same link, as shown in Fig. 1. This bounce-back process involves zero mass transfer. It works only if the boundary is stationary. Ladd<sup>(10)</sup> proposed the following rule for moving boundary

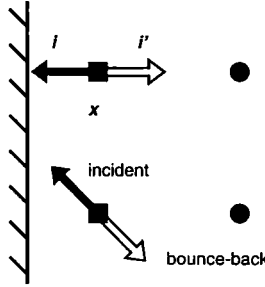


Fig. 1. Location of boundary nodes, denoted by solid squares, for a flat solid surface. The incident links are indicated by solid arrows, the bounce-back links by hollow arrows.

problems. This rule applies only to the bounce-back links (see Fig. 1) that are opposite to the incident links and is given by

$$f_{\sigma i'}(\mathbf{x}, t+1) = f_{\sigma i}(\mathbf{x}, t_+) + 2B_{\sigma}(\mathbf{e}_{\sigma i'} \cdot \mathbf{u}_b) \quad (7)$$

where  $\mathbf{x}$  is the position of the node adjacent to the wall which is moving with velocity  $\mathbf{u}_b$ ,  $i'$  denotes the bounce-back link, and  $i$  points in the opposite direction to  $i'$  and intersects the solid surface. The last term in the above equation,  $2B_{\sigma}(\mathbf{e}_{\sigma i'} \cdot \mathbf{u}_b)$ , is an additional term to the bounce-back rule, which correctly accounts for the momentum transfer between the fluid and the moving solid boundary. However, it also introduces an extra amount of mass into the boundary node  $\mathbf{x}$ . The total amount of the “extra mass” at the node is just the summation of these terms over all the bounce-back links, defined as

$$\delta\rho(\mathbf{x}) = 2 \sum_{\sigma} \sum_{i'} B_{\sigma}(\mathbf{e}_{\sigma i'} \cdot \mathbf{u}_b) \quad (8)$$

where  $i'$  denotes the bounce-back link. In most cases,  $\delta\rho(\mathbf{x})$  is nonzero for a moving solid surface. Consequently, with Ladd’s rule, the mass at the boundary node is not conserved and there has to exist fluid inside the suspended particles to allow mass to transfer across the solid boundary. Here, we propose a method to conserve mass at the solid boundary such that the solid boundary is treated as an impermeable surface. The new rule for links that are along the bounce-back directions is

$$f_{\sigma i'}(\mathbf{x}, t+1) = f_{\sigma i}(\mathbf{x}, t_+) + 2B_{\sigma}(\mathbf{e}_{\sigma i'} \cdot \mathbf{u}_b) + \varepsilon_{\sigma} \delta\rho(\mathbf{x}) \quad (9)$$

where  $\delta\rho(\mathbf{x})$  is the total “extra mass” at the node and  $\varepsilon_{\sigma}$  is a constant depending on the lattice form. For the two-speed square lattice without the

rest fluid particle, we have  $\varepsilon_\sigma = (-1/2)^\sigma$ . For the links other than the bounce-back ones, the rule is

$$f_{\sigma j}(\mathbf{x}, t+1) = f_{\sigma j}(\mathbf{x} - \mathbf{e}_{\sigma j}, t_+) + \varepsilon_\sigma \delta\rho(\mathbf{x}) \quad (10)$$

The last terms of the above equations are isotropic. By addition of these terms, not only is momentum transfer correctly accounted for, but also mass is conserved along the boundary and no fluid mass is transferred into the solid particle, since

$$2 \sum_{\sigma} \sum_{i'} B_{\sigma}(\mathbf{e}_{\sigma i'} \cdot \mathbf{u}_b) + \sum_{\sigma} \sum_i \varepsilon_{\sigma} \delta\rho(\mathbf{x}) = 0 \quad (11)$$

An alternate way to prevent mass flux across the solid surface at the boundary nodes is to include the rest fluid particles. With  $\varepsilon_1 = \varepsilon_2 = 0$ , the “extra mass”  $\delta\rho(\mathbf{x})$  is balanced by the rest particle, i.e.,

$$f_{01}(\mathbf{x}, t+1) = f_{01}(\mathbf{x}, t_+) - \delta\rho(\mathbf{x}) \quad (12)$$

where  $\delta\rho(\mathbf{x})$  is the total “extra mass” at the node.

The fluid particles collide with each other at each time step, while the interaction between the fluid and the suspended particles takes place in the middle of the convection time step. The solid boundary is impermeable and therefore no fluid can penetrate into it. Due to the impermeable feature of the solid particles, our simulation involves two basic steps for the interactions between suspended particles and fluid. The first step is the impact of fluid particles on the wall of the moving solid particle. The second step is the displacement of the fluid particles due to the motion of the solid particle. In contrast, Ladd’s method<sup>(10)</sup> does not include the second step.

The velocity vector  $\mathbf{u}_b$  depends on the translational and angular velocities of the solid particle, as well as the position where the fluid particles collide with the solid particle, and the direction of the collision, that is,

$$\mathbf{u}_b = \mathbf{U} + \boldsymbol{\Omega} \times (\mathbf{x} + \frac{1}{2} \mathbf{e}_{\sigma i} - \mathbf{X}) \quad (13)$$

where  $\mathbf{U}$  is the translational velocity of the suspension,  $\boldsymbol{\Omega}$  is the angular velocity with respect to the center of mass, and  $\mathbf{X}$  is the position vector of the center. In the second step, as the solid particle moves through the domain, mass is displaced, accordingly.

For a given link ( $\sigma i$ ) at a node, the force on the solid particle is given by

$$\mathbf{F}_{\sigma i} = \begin{cases} 2(f_{\sigma i} + B_{\sigma} \mathbf{u}_b \cdot \mathbf{e}_{\sigma i}) \mathbf{e}_{\sigma i}, & \text{incident links} \\ 0, & \text{otherwise} \end{cases} \quad (14)$$

whereas the torque  $\mathbf{T}_{\sigma i}$  with respect to the center of mass  $\mathbf{X}$  is given by

$$\mathbf{T}_{\sigma i} = (\mathbf{x} + \frac{1}{2} \mathbf{e}_{\sigma i} - \mathbf{X}) \times \mathbf{F}_{\sigma i} \quad (15)$$

Knowing the net force and the torque, we have that the motion of the solid particle is governed by the Newtonian equations, given by

$$\mathbf{U}(t + \frac{1}{2}) - \mathbf{U}(t - \frac{1}{2}) = M^{-1} \sum_{\text{BN}} \sum_{\sigma} \sum_i \mathbf{F}_{\sigma i}(\mathbf{x}, t + \frac{1}{2}) \quad (16)$$

for translation, where BN stands for the boundary nodes, and

$$\mathbf{\Omega}(t + \frac{1}{2}) - \mathbf{\Omega}(t - \frac{1}{2}) = I^{-1} \sum_{\text{BN}} \sum_{\sigma} \sum_i \mathbf{T}_{\sigma i}(\mathbf{x}, t + \frac{1}{2}) \quad (17)$$

for rotation. Here  $M$  is the mass of the suspension and  $I$  is the moment of inertia. Equations (13)–(17) completely prescribe the motion of the suspended solid particles in the fluid. In the following section, we use several examples to show the accuracy and robustness of this method.

### 3. RESULTS AND DISCUSSION

The new collision rule between the fluid and the suspended solid particles satisfies the conservation of mass and momentum at all solid boundaries. Furthermore, the suspended particles are treated as real solid particles with impermeable boundaries. To demonstrate the accuracy of this method, we apply this method to simulate several 2D problems.

In order to examine the accuracy of the boundary rule, we apply this method to two different forms of the same hydrodynamic problem. Consider the flow over a cylinder placed at the middle of a straight channel, as shown in Fig. 2. If the cylinder is fixed and the channel walls move in the  $x$  direction with constant velocity  $u_w$ , then the problem has no moving boundaries and conventional methods can be applied. An alternative form of this problem is to fix the coordinate system with the channel walls and to allow the cylinder to move freely inside the channel as a suspended solid particle would (Fig. 2b). If the body force exerted on the freely moving cylinder is equal to the force that the fixed cylinder experiences when the channel walls move with velocity  $u_w$ , then the terminal velocity of the moving cylinder  $u_c$  should be equal to  $-u_w$ . To examine the boundary rule for a moving solid particle, we apply the lattice Boltzmann method and solve the fixed cylinder problem first to compute the hydrodynamic force per unit area of the cylinder. We then apply the same force on the freely moving cylinder and compute the cylinder's

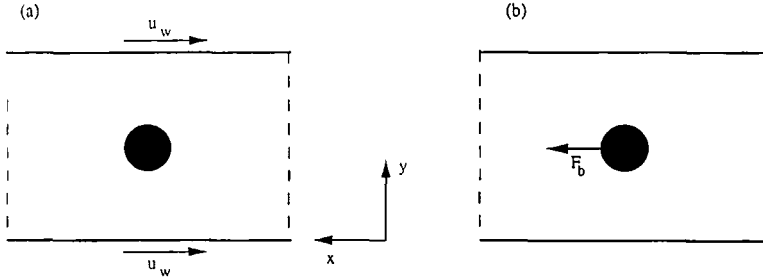


Fig. 2. Flow over a circular cylinder inside a straight channel; (a) fixed cylinder where the channel walls move with velocity  $u_w$ ; and (b) cylinder free to move under the body force  $F_b = -f_c A$ , where  $A$  is the surface area of the cylinder.

terminal velocity using the lattice Boltzmann method with the new boundary rule presented above. We also solve the fixed cylinder problem directly from the Navier–Stokes equations, using finite-element discretization with Galerkin projection<sup>(14)</sup> examine the accuracy of the lattice Boltzmann method in general.

The drag on the surface is computed for cylinders with radius 5.4, 10.4, and 30.4 lattice dimensions. The width of the channel is 128 and in all cases periodic boundary conditions are imposed on the two sides of the channel as shown by the dashed lines in Fig. 2. For each case, the time relaxation parameter  $\tau$  is adjusted to keep the Reynolds number, defined as  $Re = 2u_w r/\nu$ , equal to 1. The hydrodynamic force per unit area on the cylinder and the shear stress per unit area on the wall are listed in Table I along with results from finite-element solutions of the Navier–Stokes equations. For each case, the first and second rows correspond to the solution of the Navier–Stokes equation and the lattice Boltzmann equation, respectively.  $f_w$  and  $f_c$  represent the dimensionless force per unit area of the channel wall and the cylinder surface, respectively. The pressure scale  $\rho_f \mu_w^2$  is used to nondimensionalize the stress at the wall and the cylinder. The agreement between the Navier–Stokes solution and the lattice Boltzmann solution is within the numerical deviation of  $\pm 5\%$ . The error is believed to be mainly due to the ill-defined shape and roughness of the circular boundary of the cylinder with a square lattice. This effect will diminish as finer lattices are used. To examine the new rule for the moving solid particles, we impose a body force on the moving cylinder equal to the force computed for the fixed-cylinder case and solve for the terminal velocity of the moving cylinder. The results for each case are listed in Table I. Again, in all cases the results agree very well. This example confirms the correctness and the reliability of our lattice Boltzmann boundary rule.



**Table I. Comparison of the Finite-Element Solution of Navier-Stokes Equation for the Fixed-Cylinder Case with the Lattice Boltzmann Solution of the Fixed and Moving Cylinders<sup>a</sup>**

Case	Cylinder	$\tau$	$\rho_c/\rho_f$	$u_w$	$u_c$	$f_w$	$f_c$
I ( $r = 5.4$ )	Fixed	N/A <sup>b</sup>	$\infty$	-0.04	0.0	0.137	0.966
		1.796	$\infty$	-0.04	0.0	0.132	1.022
	Moving	1.796	2.0	0.0	0.040 <sup>c</sup>	0.133	1.022
II ( $r = 10.4$ )	Fixed	N/A <sup>b</sup>	$\infty$	-0.02	0.0	0.316	1.158
		1.748	$\infty$	-0.02	0.0	0.313	1.229
	Moving	1.748	2.0	0.0	0.020 <sup>c</sup>	0.307	1.229
III ( $r = 30.4$ )	Fixed	N/A <sup>b</sup>	$\infty$	-0.01	0.0	1.543	2.067
		2.324	$\infty$	-0.01	0.0	1.532	2.054
	Moving	2.324	2.0	0.0	0.010 <sup>c</sup>	1.523	2.054

<sup>a</sup> The full domain is  $128 \times 128$  lattice nodes and the Reynolds number  $Re = 1$  for all cases.

<sup>b</sup> Result from the finite-element solution.

<sup>c</sup> Result for the moving cylinder where input is the body force per unit area on the cylinder in the  $x$  direction and output is the terminal velocity of the cylinder.

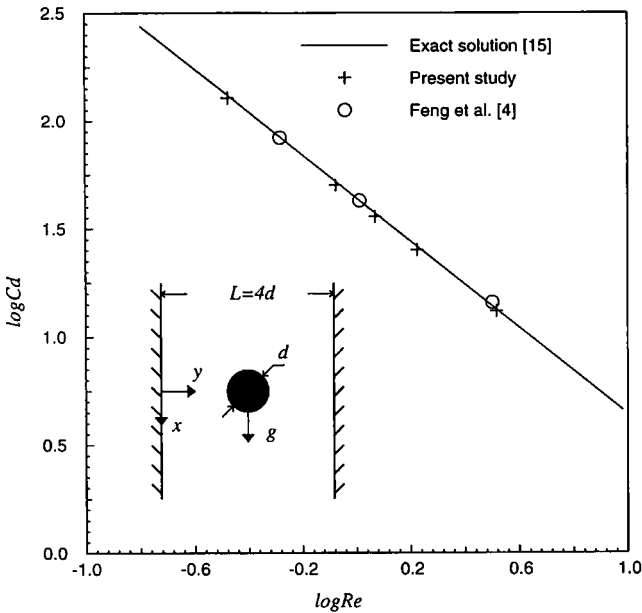


Fig. 3. Drag coefficient of a circular particle settling in a 2D channel as compared to the numerical result of Feng *et al.*<sup>(4)</sup> and the exact solution of the Stokes equation.<sup>(15)</sup>

We use this method to simulate the sedimentation of a circular solid particle in a two-dimensional channel. A circular particle of diameter  $d$  is released from different lateral positions, with zero initial velocity, in a channel of width  $4d$ . The coordinate system is shown in Fig. 3. The density of the solid particle is two times larger than the fluid density. The inlet of the domain where zero velocity is applied uniformly is always  $10d$  away from the moving particle, whereas the downstream boundary is  $15d$  from the solid particle. The normal derivative of velocity is set to zero at the downstream boundary. Feng *et al.*<sup>(4)</sup> recently simulated the same problem by solving the Navier–Stokes equation for fluid phase and implementing Newtonian dynamics for the solid particle. Our simulation results of drag coefficients are compared in Fig. 3 with the numerical results from Feng *et al.*<sup>(4)</sup> as well as the exact solution<sup>(15)</sup> of the Stokes approximation. The settling trajectories of the circular particle released at two off-centerline positions in the channel are presented in Figs. 4 and 5 for  $Re = 1.03$  and  $3.23$ , respectively, along with the same results from Feng *et al.*<sup>(4)</sup>. Due to the presence of inertia, the particle drifts horizontally toward the equilibrium centerline position with a counterclockwise rotation. For the case

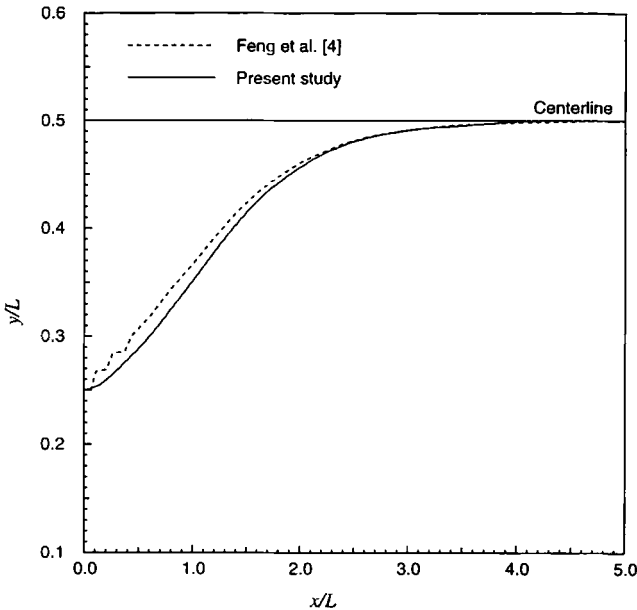


Fig. 4. Settling trajectories for particles with Reynolds number 1.03 released from different initial positions in a narrow channel with width  $L$ . The simulation result of Feng *et al.*<sup>(4)</sup> is also shown.

of  $Re = 3.23$ , there is an overshoot for the lateral migration. All our results are in good agreement with the simulation results of Feng *et al.*<sup>(4)</sup>.

We extend this method to many particles suspended in a Couette system, that is, between two parallel plates where the top plate moves with a constant velocity  $U$  relative to the lower plate. In our computations, the domain is either the  $128 \times 128$  or  $512 \times 512$  lattice and the upper wall moves with the speed of 0.08 lattice unit per time step. Identical suspensions with radius of 5.4 are uniformly suspended in the domain. The results for the effective viscosity, relative to the pure fluid viscosity, versus area ratio are shown in Fig. 6, which also shows other simulation results<sup>(2, 3, 6)</sup> for comparison. In the low- to intermediate-concentration regions, the agreements are very good. Our simulations show that the new boundary rule outlined in this paper can be used very effectively for simulation of solid particles suspended in fluid. Furthermore, this method is more practical for analysis of suspensions because of the linear relation between the cpu time  $t_{cpu}$  and the number of suspensions  $N$ . This relation is given by  $t_{cpu} = 600 + 3.4N$  (sec) for a  $128 \times 128$  system with 10,000 time steps on an IBM RS/6000.

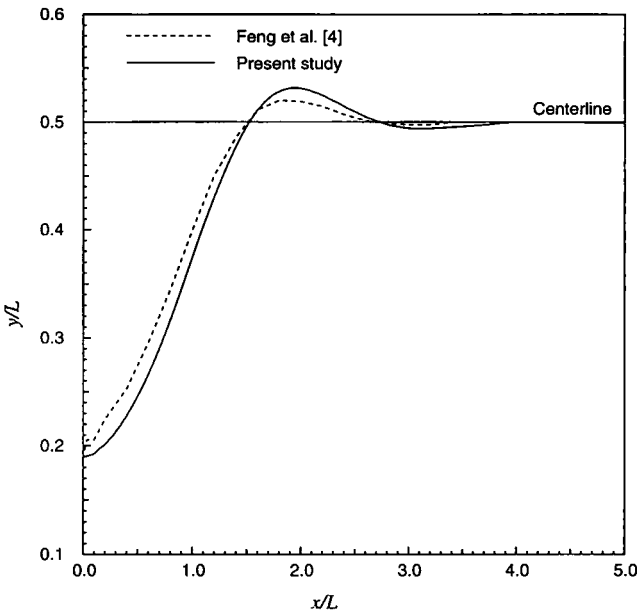


Fig. 5. Settling trajectories for particles with Reynolds number 3.23 released from different initial positions in a narrow channel with width  $L$ . There is an overshoot across the centerline. The simulation result of Feng *et al.*<sup>(4)</sup> is also shown.

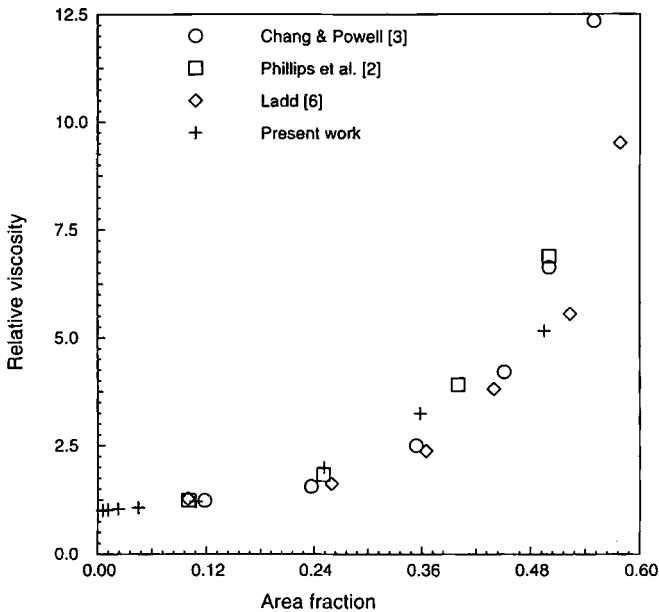


Fig. 6. Relative viscosity of 2D suspensions in a Couette flow as a function of area ratio. The simulations are carried out for systems of  $128 \times 128$  and  $512 \times 512$  lattice nodes. The number of particles ranges from 16 to 64.

In conclusion, we have developed a new boundary collision rule based on the lattice Boltzmann method for the transport of solid particles suspended in a fluid. Lattice Boltzmann simulations with the new boundary rule have been carried out for the 2D channel flow with moving particles. Results of the simulations with the new method are in good agreement with direct solutions of the Navier–Stokes equations and the exact asymptotic results. The boundary rule presented above has been extended to three-dimensional flow and the results will be presented in the near future.<sup>(16)</sup>

## ACKNOWLEDGMENTS

We acknowledge helpful discussions with Dr. Anthony J. C. Ladd, Dr. Gary Doolen, Dr. Li-shi Luo, Dr. Shuling Hou, Dr. Shiyi Chen, and Dr. Jimmy Feng. This study has been supported by the National Science Foundation's Young Investigator Award (C.K.A.) through grant CTS-9258667, and by industrial matching contributions. The calculations

were conducted, in part, using the National Center for Supercomputing Applications, a resource at the University of Illinois at Urbana-Champaign, which is funded by the National Science Foundation.

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