Shear viscosity of bulk suspensions at low Reynolds number with the three-dimensional lattice Boltzmann method

S. V. Lishchuk, I. Halliday, and C. M. Care
Materials and Engineering Research Institute, Sheffield Hallam University, Sheffield S1 1WB, United Kingdom
(Received 13 January 2006; published 10 July 2006)

We report three-dimensional parallel Lagrangian particle simulations using the lattice Boltzmann method, conducted at a low Reynolds number. Using modified Lees-Edwards boundary conditions and directly calculated viscous dissipation, we show that it is possible to recover excellent agreement with the Einstein viscosity formula in the low concentration limit and to predict viscosity corrections for larger concentrations.

DOI: 10.1103/PhysRevE.74.017701 PACS number(s): 47.11.−j, 47.55.Kf

I. INTRODUCTION

Aqueous and nonaqueous suspensions are of great importance in a wide range of industrial processes. Analytical and semiempirical formulas for the shear viscosity of such a suspension are well established [1,2]. These results rely on the assumption of homogeneity and are valid in the limit of small suspended solids volume fraction ϕ and small Reynolds number Re. Unfortunately, the results rely either upon a range of simplifying assumptions seldom found in practice [1] or empiricism [2]. For the larger values of ϕ and Re of typical sludge and slurry systems, the necessary suspension viscosity formulas quickly assume a complicated dependance upon flow properties as well as upon concentration.

In developing appropriate methods to model to larger ϕ and Re, it is important to have verified methods. We present a robust, efficient, and scalable technique based upon the lattice Boltzmann (LB) method. Our approach allows us viscosity data which accurately represent the bulk to be obtained; it is validated against Einstein's shear viscosity formula [1] for an infinite fluid at $\mathrm{Re}\rightarrow 0$. It is shown to be necessary to include a simple correction for the effective hydrodynamics radius of the particles. The resulting method applies to larger ϕ and Re of course.

A particular advantage of the LB method is its ability to model systems with a large number, N, of embedded Lagrangian particles. More particularly, for the simulation of suspensions, LB's general merits are (i) locality of its surface stress information, (ii) parallelizability, and (iii) the ability easily to accommodate geometrically complex boundary conditions. Simulation execution times scale with particle size and with N^2 (for our present method). However, there are strategies well known from molecular dynamics, which may easily improve the latter scaling, but which were unnecessary here (owing to the low particle volume fractions we consider).

By applying shear forces in order to obtain a suspension's shear rate response, one implicitly imposes a boundary, thereby making measurements unrepresentative of a bulk system. However, it is possible to obtain bulk information by adapting Lees-Edwards (LE) type boundary conditions, similar to those originally developed for LB by Wagner [3–5]. LE boundary conditions enable the bulk of a sheared system to be simulated [6], essentially by translating the usual periodic replicas uniformly in the direction of a (known) imposed shear. Here we report an adaptation of Wagner's approach, applicable to isothermal LB fluids containing embedded Lagrangian particles. A recent study by Hyväluoma *et al.* [10] also reports the use of the LB method to model high concentrations of sheared suspensions. However, the results of Hyväluoma *et al.* are recovered in the presence of boundaries rather than the bulk. Additionally the current work uses dissipation to measure the viscosity, an approach which becomes necessary when using LE boundary conditions.

Using the algorithm of Ladd [7], a monodisperse population of N spherical particles, radii R, was inserted into a three-dimensional (3D) LB fluid simulation with domain decomposition parallelization. The LB model used was the isothermal variant widely designated D3Q15 [8], with a single relaxation time, τ. Our chosen variant of Ladd's algorithm employs what are essentially bounce-back boundary conditions [8] to represent the suspended particles' boundaries [7]. While later versions of similar algorithms (e.g., Verberg and Ladd [9]) result in refined boundary representations, the original method [7] was chosen for this work on account of its being representative, simple, and robust.

Features of our method are discussed in Sec. III. Also described in Sec. III is the method by which the viscous dissipation in the fluid is calculated directly, then used to extract effective viscosity measurements. In Sec. IV we present results for effective viscosity (i) in the low concentration limit, which we find, on applying corrections, to be in excellent agreement with the Einstein calculation and (ii) for slightly increased concentration, which we find to be in agreement with the Krieger-Dougherty relation. We present conclusions in Sec. V.

II. BACKGROUND

The single relaxation time LB method [8] may be defined by the evolution equation for its primary quantity, the momentum distribution function f_i:

$$f_i(\mathbf{r}+\mathbf{c}_i,t+1)=f_i(\mathbf{r},t)-\frac{1}{\tau}[f_i(\mathbf{r},t)-f_i^0(\rho,\rho\mathbf{u})]. \qquad (1)$$

f_i represents a population of particles with velocity $\mathbf{c}_i$. The set $\mathbf{c}_i, i=0..14$ defines the lattice. Associated with link i is weight t_p. Corresponding t_ps and $\mathbf{c}_i$s for the D3Q15 variant used here are defined in Table I. The nodal density ρ and the

TABLE I. Velocities and corresponding weights for the D3Q15 lattice.

i	0	1–6	7–14
$\lvert\mathbf{c}_i\rvert$	0	1	$\sqrt{3}$
t_i	$\frac{2}{9}$	$\frac{1}{9}$	1/72

nodal momentum $\rho\mathbf{u}$ are defined by the moments of f_i with $\mathbf{c}_i$. In Eq. (1), the f_is are relaxed towards the *equilibrium population* $f_i^0(t_p,\rho,\mathbf{u})$, which is a polynomial in $\mathbf{u}$. Parameter τ in Eq. (1) determines the kinematic viscosity $\nu=\frac{1}{6}(2\tau-1)$ [8].

No-slip, boundary conditions in LB emerge from a *midlink bounce-back* lattice closure rule, in which the f_is on a boundary node at $\mathbf{r}_w$ are subject to a specular reflection, taken to occur at the midpoint $\mathbf{r}_w+\frac{1}{2}\mathbf{c}_i$ of the link $\mathbf{c}_i$:

$$f_{-i}(\mathbf{r}_w,t+1)=f_i(\mathbf{r}_w,t),\quad (\mathbf{c}_{-i}\equiv-\mathbf{c}_i). \tag{2}$$

This rule was generalized by Ladd [7] to boundaries with velocity $\mathbf{u}_w$; he replaced the evolution in Eq. (1) with

$$f_{-i}(\mathbf{r}_w,t+1)=f_i(\mathbf{r}_w,t)+\frac{2\rho t_p}{c_s^2}(\mathbf{w}_w\cdot\mathbf{c}_1), \tag{3}$$

where the speed of sound $c_s=1/\sqrt{3}$ for our model.

Equation (3) is useful in representing the effect of moving particles boundaries on the embedding fluid. It can also be used to compute the forces and torques impressed upon the particles by the fluid [7]. Emphasizing that later versions of Ladd's method [9] result in refined boundary representations, we note that the sublattice lubrication force for particles in close approach, inserted into this algorithm by Nguyen and Ladd [11], was omitted from our model, which is aimed at the low concentration limit.

III. SIMULATION METHOD

The D3Q15 model and Ladd's representation of moving particle boundaries are outlined in Sec. II. Ladd's algorithm [7] treats the particle interior as being occupied by an *interior fluid*. For our model, the interior fluid was considered to be in a state of uniform translation and rotation, determined by the motion of the particle boundary. Let $\mathbf{r}$ be a location inside a particle centered on the origin, with translational velocity $\mathbf{u}_0$, angular velocity ω; the interior fluid was described by the equilibrium population $f_i^0(t_p,\rho,\mathbf{u}_0+\boldsymbol{\omega}\times\mathbf{r})$.

LE boundary conditions [6], after Wagner [3,4], were applied. For embedded particles migrating across the LE boundary, any portion of the particle surface which had passed the boundary was reintroduced (from the periodic replica) having been displaced and accelerated. For a boundary parallel to the shear direction, $\hat{e}_x$, the reentrant portion of a crossing particle was (i) displaced (advected) by the action of the LE velocity $v_{LE}\hat{e}_x$ [3–5] through distance $v_{LE}\hat{e}_x\Delta t$, with $\Delta t=1$ the simulation time step and (ii) accelerated by an addition of the LE velocity $v_{LE}\hat{e}_x$. Wagner's method was applied to all (including interior) fluid at the LE boundary, which, to facilitate parallel implementation, coincided with a boundary of the domain decomposition. The update of particle position and velocity on the LE boundary was made after the LB collision step; information on the LE boundary being updated in the interprocess communication routine. This precaution ensured that each process knew of the data in its own domain and in that neighboring layer required for the LB propagation step and for calculating velocity derivatives, Eq. (5).

Total dissipation was calculated from a discrete approximation to the usual volume integration for dissipation in incompressible fluids [12,13]:

$$\dot{E}_{kin}(t)=\frac{\eta}{2}\sum_{\mathbf{r}}\left[\left(\frac{\partial u_\alpha}{\partial x_\beta}+\frac{\partial u_\beta}{\partial x_\alpha}\right)^2\right]_{\mathbf{r},t}, \tag{4}$$

where $\mathbf{r}$ excludes nodal positions inside particle boundaries. The derivatives in (4) were evaluated nonlocally using the isotropy properties of the D3Q15 lattice:

$$\frac{\partial u_\alpha}{\partial x_\beta}=\frac{1}{c_s^2}\sum_i t_p u_\alpha(\mathbf{r}+\mathbf{c}_i)c_{i\beta}+o(\mathbf{c}_i^3). \tag{5}$$

Although it is more computationally convenient to calculate dissipation from the product of the stress and velocity (both being local functions of f_i in the LB method [7]) we found this approach to give noisy results.

For the given LE velocity $v_{LE}\hat{e}_x$, $\dot{E}_{kin}(t)$ in Eq. (4) was calculated for (i) a continuous fluid and (ii) a fluid containing particles. Note, in (i) the result coincided with the theoretical value for a continuous LB fluid; $\eta_0=(\rho/6)(2\tau-1)$, [8]. For LB nodes with links across a particle boundary, the nearest-neighbor velocity, $u_\alpha(\mathbf{r}+\mathbf{c}_i)$, in Eq. (5) was taken to be the velocity of the interior fluid, the motion of which, we recall, reflects that of the particle.

Denote the total dissipation for the continuous (particulate) system $\dot{E}_{Ckin}$ ($\dot{E}_{Dkin}$). For an unbounded, sheared, dilute suspension of spheres at Re=0, Einstein showed $\dot{E}_{Dkin}=\eta\dot{\gamma}/2$, where η is the effective suspension viscosity [1,12]; for the corresponding sheared bulk fluid $\dot{E}_{Ckin}=\eta_0\dot{\gamma}/2$. η may therefore be calculated from

$$\frac{\eta}{\eta_0}=\frac{\dot{E}_{Dkin}}{\dot{E}_{Ckin}}. \tag{6}$$

IV. RESULTS AND DISCUSSION

Ladd's method [7] for inserting the particle surface is efficient and robust. However, its use of what is effectively a bounce-back closure leads to a displacement of the Dirichlet boundary imposed by the particles on the fluid; the essential problem is well known in LB. For stationary plane boundaries, depending upon the value of τ and boundary orientation, a closure imposed by bounce back locates a zero of velocity 0.5 lattice spacings into the flow domain [8]. It follows that particles' effective radius is not well defined. By increasing the particle number and decreasing the particle radius, this effect must increase in importance. We show in

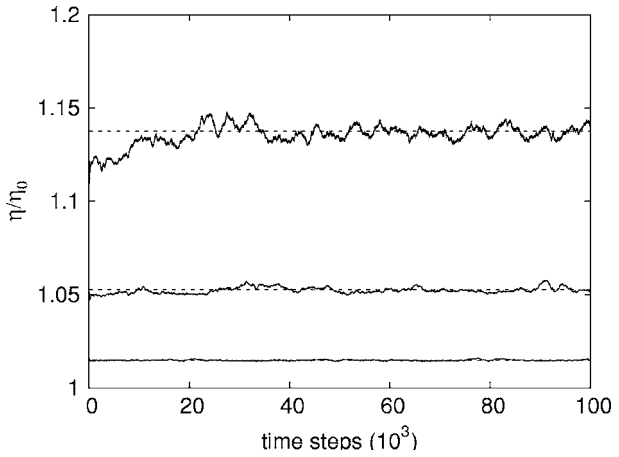

FIG. 1. Time variation of the ratio η/η_0 for $N=8$ (lower branch), 27 and 64 (upper branch), and particles of radius $R=8$.

this section that one can overcome "hydrodynamic misfit" in the dilute systems under study, by straightforward recalibration, down to a surprisingly small particle radii $R>3$.

First consider unadjusted results. Data for a range of particle sizes were obtained on a lattice of $128\times128\times128$. The fluid was initialized to a uniform density $\rho=1.8$; the value of the relaxation parameter $\tau=1.0$ used corresponds to an optimum of performance in locating the boundary using bounce-back boundary conditions [8]. A number $N=1..216$ of particles of radii $R=3$, 6, 8, 12, and 16 were considered. Note that the low concentration limit of a suspension is widely assumed to correspond to a system with an average interparticle spacing $>6R$. LE boundary conditions were imposed by a LE velocity $v_{LE}=0.05$ [3,4]. In all cases Re $\equiv v_{LE}R^2/(L_x\nu)$, L being the size of the simulation box in the direction of the velocity gradient, did not exceed the value 0.6; a value small enough to signify a linear rheological response.

The instantaneous suspension viscosity η and the corresponding viscosity η_0 of the pure fluid, were determined from the direct measurement of dissipation, as discussed in Sec. III. Figure 1 displays the time dependence of the dimen-

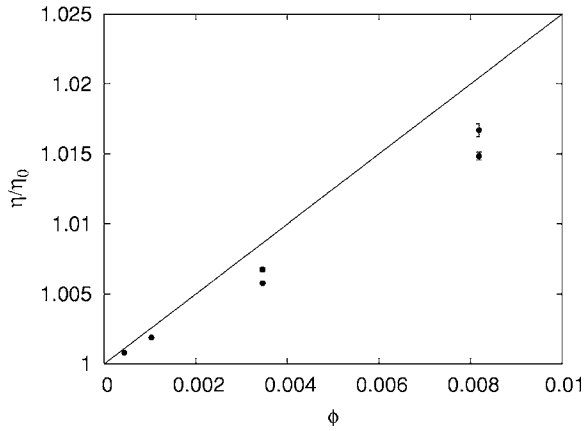

FIG. 2. Viscosity ratio η/η_0 at a small particle volume fraction ϕ. No correction has been applied to the particles' radius R. The solid line corresponds to the Einstein formula.

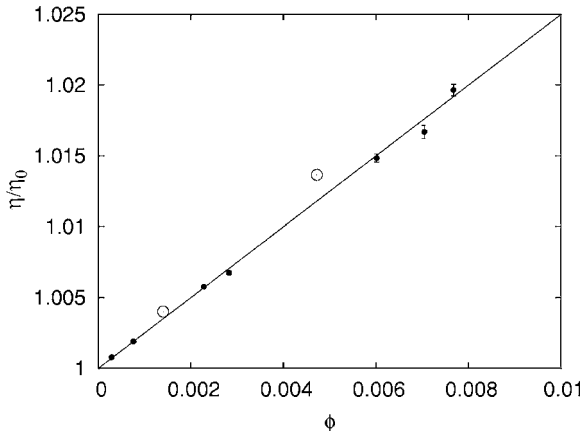

FIG. 3. Relative viscosity versus particle volume fraction, ϕ, with ϕ adjusted for particles' radius correction, $\Delta R=-0.78$. Empty circles correspond to our smallest value of $R=3$.

sionless viscosity ratio η/η_0 for $R=8$ lattice units, $N=8$, $N=27$, and $N=64$.

Steady-state, short-time averaged values of ratio η/η_0 are plotted against solid particles' volume fraction:

$$\phi=\tfrac{4}{3}\pi R^3 N, \tag{7}$$

in Fig. 2; the solid line is the Einstein formula [1]:

$$\frac{\eta}{\eta_0}=\left(1+\tfrac{5}{2}\phi\right). \tag{8}$$

In Fig. 2 no correction to the particles' radius has been applied; it shows increasing departure from the expected trend [Eq. (8)] with increasing ϕ, for $\phi<0.01$ (while still retaining the low concentration approximation). This we attribute to the increasing total surface area of the particles. In fact, the location of a particle boundary is indeterminate; with the method used, the positions at which the LB fluid velocity equates to that of a given particle (radius R) do not lie in a spherical surface, radius R, about the particle center of mass. A simple solution is to assume an effective particle radius, although this approach neglects shape fluctuations. A correction $R\rightarrow R+\Delta R$ was found to be sufficient for the data of our study. Radial correction ΔR was determined by least squares fitting of relative viscosity data like that in Fig. 2, with the Einstein formula, for $\phi<0.01$. The optimum correction is $\Delta R=-0.78$ lattice units, which value accords with typical bounce-back boundary displacements [8].

Figure 3 shows relative viscosity after applying this correction; the solid line corresponds to Einstein formula. The small value of $R=3$ produces data which testifies to the robustness of Ladd's algorithm.

Figure 4 shows data for higher concentrations. The solid line is the Einstein formula, the dashed line the Krieger-Dougherty [2] formula:

$$\frac{\eta}{\eta_0}=\left(1-\frac{\phi}{\phi_c}\right)^{-2.5\phi_c}, \quad \phi_c=0.65. \tag{9}$$

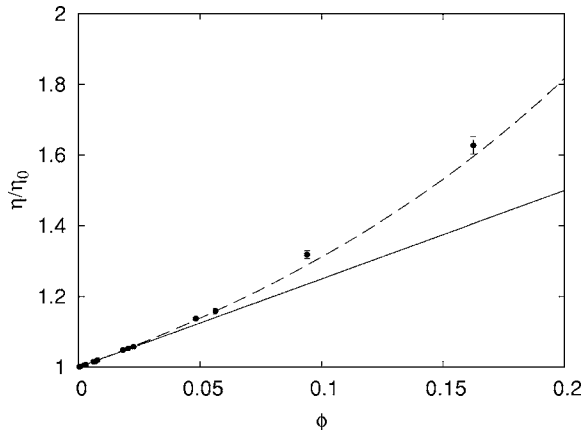

FIG. 4. Relative viscosity versus particle volume fraction, ϕ for a larger range of ϕ. The solid (broken) line is the Einstein (Krieger-Dougherty) formula.

V. CONCLUSION

We have presented quantitative results from efficient, 3D LB simulations of monodisperse bulk suspensions of spherical particles. Relative suspension viscosity has been calculated in the low concentration limit using a direct method of calculating dissipation in simulations bounded by modified LE periodic boundary conditions.

The particular Lagrangian particle algorithm used with our LB simulations is Ladd's simplest, oldest, fastest, and surprisingly robust variant [7]. It suffers from an inaccurate location of the particle boundary but we have demonstrated that this can be corrected by adjusting the Lagrangian particles' radius R, for $R>3$ (a surprisingly small value). It is unlikely that our particular calibration will remain valid for a different choice of the LB collision parameter τ since the value of τ is known to affect the location of the no-slip boundary created by a bounce-back rule, like that used here [7]. The corrected results show excellent agreement with the Einstein calculation in the low concentration limit and with the Krieger-Dougherty relation at an increased concentration.

Ladd [14] originally developed, and Adhikari *et al.* [15] have recently improved, an LB with stress fluctuations which invest the method with a Green-Kubo formula for viscosity [14]; this may be applied to particulate suspensions under periodic boundary conditions [16], to calculate an effective suspension viscosity, comparable to which we present here, but by what is a correlation measurement.

ACKNOWLEDGMENT

Thanks to Nexia Solutions UK, for the funding of this work.

[1] A. Einstein, Ann. Phys. **19**, 289 (1906).
[2] I. M. Krieger and T. J. Dougherty, Trans. Soc. Rheol. **3**, 137 (1959).
[3] A. J. Wagner and J. M. Yeomans, Phys. Rev. E **59**, 4366 (1999).
[4] A. J. Wagner and I. Pagonabarraga, J. Stat. Phys. **107**, 521 (2002).
[5] P. Stansell, K. Stratford, J.-C. Desplat, R. Adhikari, and M. E. Cates, Phys. Rev. Lett. **96**, 085701 (2006).
[6] A. W. Lees and S. F. Edwards, J. Phys. C **5**, 1921 (1972).
[7] A. J. C. Ladd, J. Fluid Mech. **271**, 285 (1994).
[8] S. Succi, *The Lattice Boltzmann Equation for Fluid Dynamics and Beyond* (Oxford University Press, Oxford, 2001).
[9] R. Verberg and A. J. C. Ladd, Phys. Rev. Lett. **84**, 2148 (2000).
[10] J. Hyväluoma, P. Raiskinmäki, A. Koponen, M. Kataja, and J. Timonen, J. Stat. Phys. **121**, 149 (2005).
[11] N. Q. Nguyen and A. J. C. Ladd, Phys. Rev. E **69**, 050401(R) (2004).
[12] L. D. Landau and E. M. Lifshitz, *Fluid Mechanics* (Butterworth-Heinemann, London, 1995).
[13] P. B. Warren (private communication).
[14] A. J. C. Ladd, J. Fluid Mech. **271**, 271 (1994).
[15] R. Adhikari, K. Stratford, M. E. Cates, and A. J. Wagner, Europhys. Lett. **71**, 473 (2005).
[16] A. J. C. Ladd, J. Fluid Mech. **271**, 311 (1994).