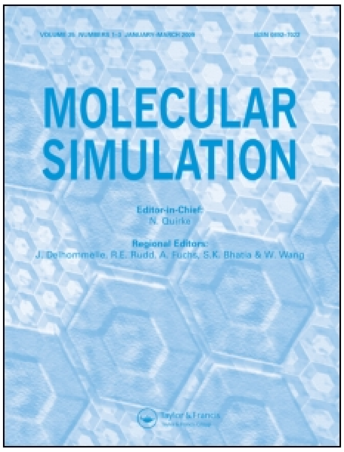

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Modification to Lees–Edwards periodic boundary condition for dissipative particle dynamics simulation with high dissipation rates

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The Lees–Edwards periodic boundary condition has been a workhorse for simulating shear flows in molecular dynamics (MD). It has also been used in dissipative particle dynamics (DPD) to calculate the rheology of complex suspensions. However, owing to the dependence of inter-particle forces on the relative velocity of the particles in DPD, this boundary condition can give rise to serious errors if the velocity dependence is not properly accounted for in its implementation. This is particularly true for higher dissipation rates. This report will explore this issue and propose a simple remedy.

Keywords: Dissipative particle dynamics; DPD; Lees–Edwards boundary condition; Molecular dynamics

1. Introduction

The Lees–Edwards (LE) boundary condition [1] was proposed to simulate shear flows using the classical molecular dynamics (MD) technique. This boundary condition enables the imposition of a constant shear rate in a Couette-type flow by a simple and ingenious modification to the standard periodic boundary condition [2]. As a result, it allows the calculation of the shear viscosity of a model fluid as a function of shear rate by simply calculating the stress tensor in response to the applied shear rate [2,3]. Using this approach, the behavior of both Newtonian and shear rate dependent non-Newtonian systems can be analyzed.

Ever since its introduction in 1992 [4], the dissipative particle dynamics (DPD) technique has also used this boundary condition. Being a particle based technique similar to MD, the implementation of the LE boundary condition in DPD has been similar to that in MD [4,5]. For the situations reported in the literature, which consist mostly of suspensions with solvents that are DPD fluids with Schmidt number (*Sc*) of the order of one, the approach has worked. However, when trying to simulate higher *Sc* number DPD fluids with higher dissipation rates using the LE boundary condition, serious problems were unearthed that stem primarily from the dependence of the dissipative force in DPD on relative velocity. This also makes numerical integration in DPD more challenging than MD [6].

The Couette flow problem, in which a constant shear rate is imposed, is used as a canonical set-up for measuring viscosity experimentally and calculating viscosity numerically. Simulating a Couette flow using the LE condition is very convenient and powerful because it mimics a constant shear viscometer and thereby enables the study of non-Newtonian systems, in stark contrast to other set-ups like the reverse Poiseuille flow approach proposed recently in Ref. [9]. Therefore, it is imperative that one should be able to use Couette flow for DPD systems with high dissipation rates. In what follows, a simple modification to the LE condition is proposed that will enable its unconditional use in DPD.

2. The problem and the proposed modification

As illustrated in figure 1, in the LE approach the standard periodic boundary condition is modified to account for the constant shear rate in a Couette flow type set-up [1]. If a linear velocity profile is to be imposed across the *Y* dimension, then in the LE boundary condition the particles leaving the *Y* boundaries are not just introduced

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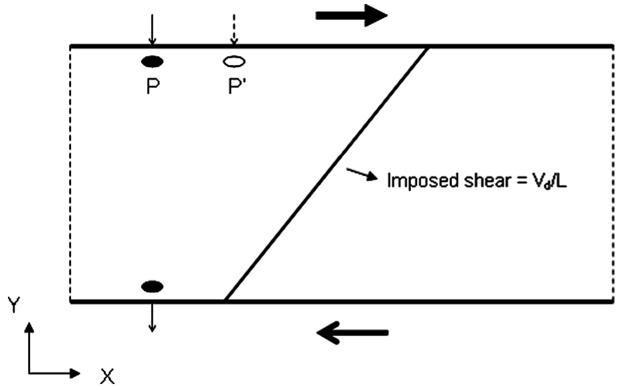

Figure 1. A Couette flow set-up for constant shear rate. L is the length in the Y direction and V_d is the velocity differential between the two parallel plates. P is the insertion point in ordinary periodic boundary condition and P' in the case of the LE condition.

back in the same symmetric location with the same velocities (as in standard periodic boundary condition). Instead, they are introduced in a displaced location along the X direction with their velocities increased or decreased by a linear function of V_d, where V_d is the differential between the imposed velocities of the upper and lower plates. If L is the distance between the plates, then V_d/L is the imposed shear rate and the velocity variation between the plates is linear. For the situation shown in figure 1, the particle leaving the lower Y boundary is introduced back to the upper boundary at the location P'. P' is appropriately displaced to the right of the symmetric location P, at which the particle would have been introduced in the case of an ordinary periodic boundary condition. The distance between the points P' and P and their relative locations depend on the magnitude of V_d and the direction of the plate velocity. In figure 1, P' is to the right of P because the upper plate is moving to the right and therefore [1,2],

$$x_{P'} = x_P + f(V_d)t, \tag{1}$$

where $x_{P'}$ and x_P are the x-coordinates of P' and P, respectively, $f(V_d)$ is a linear function, and t is the time.

In DPD, unlike in MD, there is a dissipative component to the inter-particle force. This force, which is of the form,

$$F_D \propto -\gamma V_{ij}, \tag{2}$$

serves to reduce the relative velocity (V_{ij}) between the two interacting particles. The coefficient, γ, is therefore a measure of the dissipation rate and hence a measure of the viscosity of the fluid. The Sc, which is the ratio of momentum diffusivity of the fluid to its self (particle) diffusivity, is a more appropriate parameter in this context and it has been shown that a DPD fluid has the following dependence of Sc on γ [7,8]:

$$Sc \propto \sqrt{\frac{m}{kT}} r_c \gamma. \tag{3}$$

In equation (3), r_c is the cut-off radius, m is the mass of a DPD particle, and kT is the thermal energy. From this dependence, it can be seen that one convenient way of increasing Sc is by increasing γ.

Typically, the value of γ used in contemporary works is in the range of 5–6 [5,8]. As has been shown in Refs. [8,10], these values yield a Sc number of $O(1)$ for the DPD fluid, and the rheology of non-dilute suspensions of water-like solvents has been successfully simulated as reported in Refs. [5,8], for instance, and many other works. For this value of γ, the use of the LE boundary condition to mimic Couette flow set-up yields acceptable results as is seen in figure 2. A 10 by 10 by 10 system is simulated by using the set-up described in figure 1. The value of V_d—the velocity difference between the parallel plates—is 1.4 and the number density of the particles is 3. As can be seen, the expected linear velocity profile is obtained for $\gamma = 5.6$. But as the value of γ increases, the linear regime of the velocity profile gets more and more compressed. Meanwhile, the velocity differential diminishes as seen in figure 3(a) and (b) for the values of γ of 50 and 100, respectively. Clearly, the desired shear rate is not imposed in these simulations.

This behavior can be attributed to the presence of the dissipative force, F_D, in DPD, which becomes more and more conspicuous with higher values of γ (equation (2)). As explained above, in the LE boundary condition, particles leaving the Y boundaries undergo an artificial change in their velocities by a linear function of V_d to maintain the imposed shear rate. In DPD, because of the presence of F_D—whose strength increases with γ—this change is mitigated immediately by F_D because the sole purpose of this force is to reduce the relative velocity. Thus, the velocity-altering operation in the LE condition gets progressively annulled by the dissipative force component of DPD. Therefore, as seen in figure 3(a) and

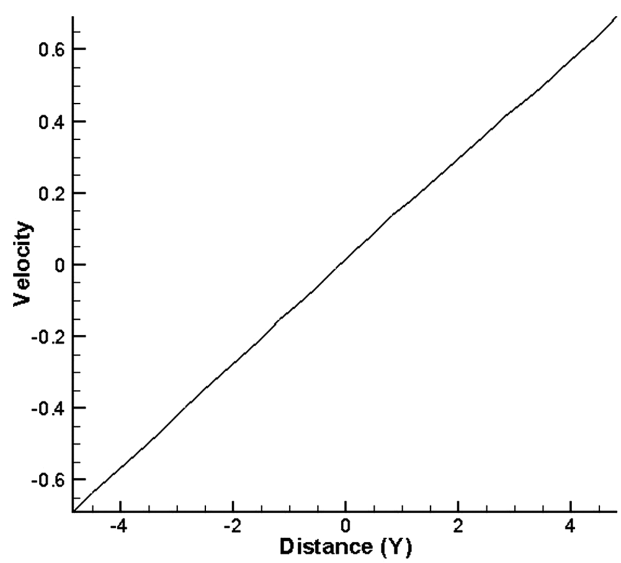

Figure 2. Linear velocity profile obtained for the Couette flow set-up in figure 1 for low value of γ (= 5.6).

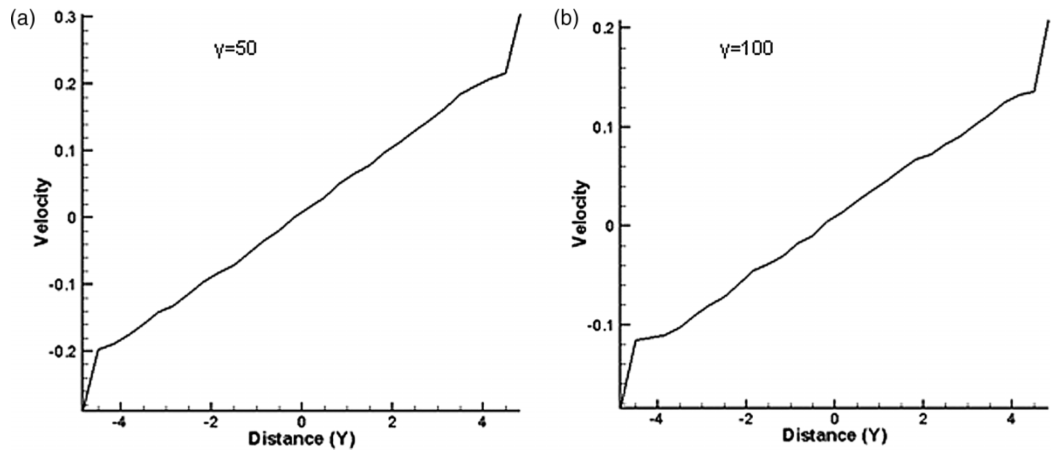

Figure 3. Erroneous velocity profiles using the unmodified LE condition in a Couette flow set-up for (a) $\gamma = 50$ and (b) $\gamma = 100$.

(b), the velocity differential diminishes with higher dissipation rates.

A possible remedy to this problem is to identify that the effect of velocity alteration in the LE condition has to be preserved to let it serve the intended purpose and the DPD forces have to be modified in accordance. This can be done by letting the particles whose velocities (and position along the *X* direction) have been artificially modified by the LE periodic boundary condition interact with other particles across the *Y*-edges through the conservative force only. Referring to figure 4, if particle A is inserted near the top edge using the LE condition, then its interactions with particles like D and E (if they are within the interaction range) are modified, but not its interactions with particles like B or C. This can be easily accomplished by letting the value of γ for these interactions become zero, thus removing any kind of dissipative (and random) force between them. This way, the LE condition is allowed to play out as originally intended and overall momentum is conserved.

When this modification was applied to the cases of $\gamma = 50$ and 100 (figure 3(a) and (b)), linear velocity profiles corresponding to the imposed gradient were obtained as shown in figure 5(a) and (b). These were similar to the profile in figure 2 (the case of low value of γ), and the effect of high values of γ were no longer seen. In figure 6, the density profile was plotted for the modified LE case of $\gamma = 100$ and a near-constant particle density (~ 3) was obtained across the domain. Further, the DPD viscosities calculated using this modification for the different values of γ compared well with the corresponding viscosities calculated for a similarly sized system using the reverse Poiseuille flow set-up [9] as shown in table 1. In the reverse Poiseuille flow set-up, it should be noted, only pure periodic boundary condition is used and hence is very accurate; but only for a Newtonian system as the shear rate is not a constant in the system. The DPD fluid system we considered here is purely Newtonian.

It should be noted that the proposed modification does not alter the basic behavior of the original LE boundary condition from a theoretical perspective. In fact, it reinforces the theoretical premise of LE boundary condition [1] for DPD-type systems, which is: the purpose of altering particle reinsertion point and particle velocity is to maintain the shear rate in a consistent manner. From algorithmic implementation point of view, absolutely no penalties are paid. This modification does not impose any additional limit to the applicability of LE boundary condition.

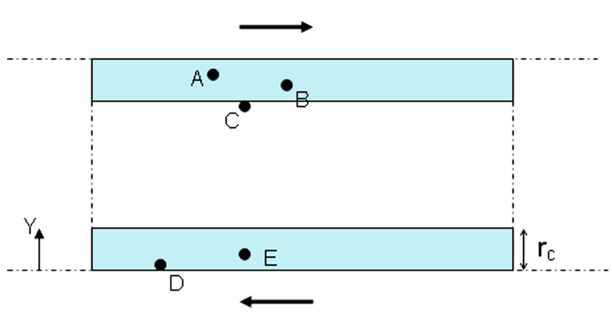

Figure 4. The proposed modification applies to the interactions of inserted points like A with points like D and E, and not with points like B and C. r_c is the cut-off radius and the horizontal arrows indicate the directions of plate-velocities.

3. Conclusion

In this article, the limitation of the classical LE condition for DPD problems with high dissipation rates was addressed and a simple modification was proposed. The proposed modification enables the unconditional use of the DPD technique for a Couette flow set-up, with both Newtonian and non-Newtonian fluids, and with high dissipation rates. This can be extremely beneficial when dealing with non-Newtonian suspensions with highly viscous solvents.

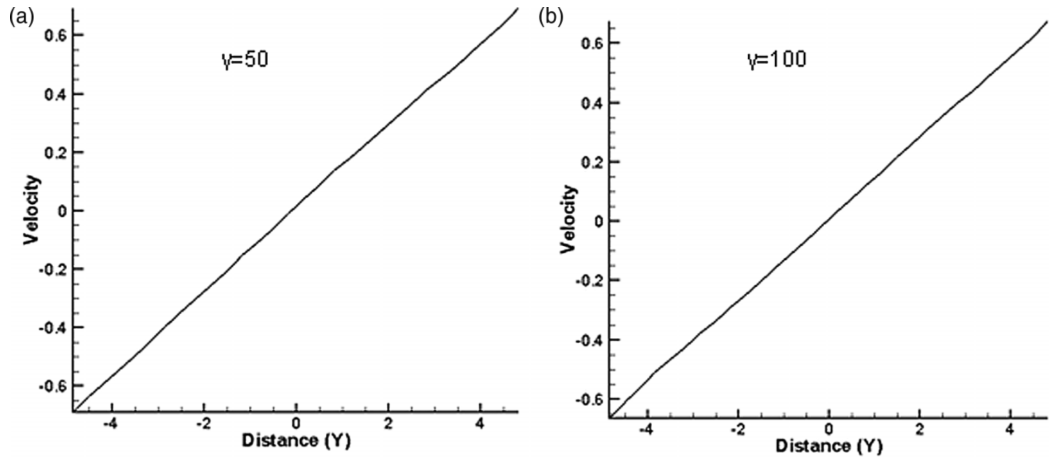

Figure 5. Linear velocity profiles using the proposed modified LE condition in a Couette flow set-up for (a) $\gamma = 50$ and (b) $\gamma = 100$.

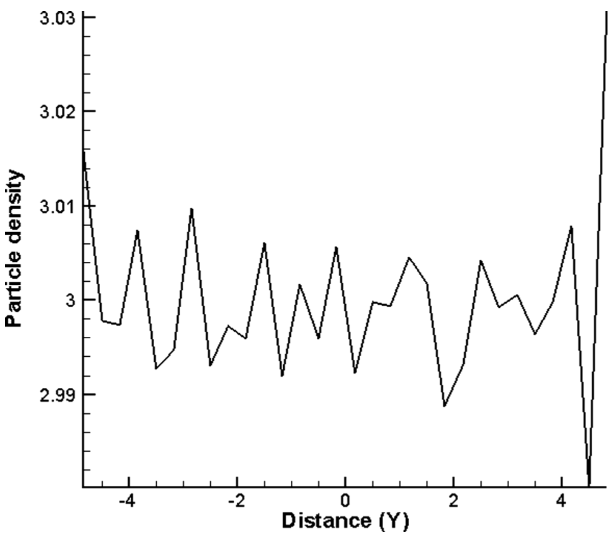

Figure 6. Particle number density variation for the case of $\gamma = 100$ using the modified LE condition.

Table 1. Comparison of DPD viscosity.

γ	*DPD viscosity using Poiseuille flow*	*DPD viscosity using modified LE condition*
6	0.77	0.73
50	1.63	1.59
100	2.4	2.33
200	3.7	3.56

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