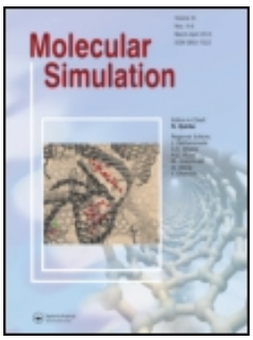

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SPECIAL ISSUE: FRONTIERS OF MOLECULAR SIMULATION IN CHINA

Drop movements and replacement on surface driven by shear force via hybrid atomistic–continuum simulations

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ABSTRACT

The movements and replacement of a nanoscale drop on a horizontal surface driven by shear force from the other immiscible fluid have been investigated by hybrid atomistic–continuum modelling in this work. The interfacial interaction near the drop, which may not be fully covered by the continuum theories, is modelled by molecular dynamics for accurate capture of transport behaviour, while the bulk flow region is simulated by the lattice Boltzmann method for high efficiency. The momentum exchange between atomistic and continuum regions is realised in a buffer region to couple the multiscale effects, where we propose an artificial solid molecular layer at the outer edge of buffer region to ensure the continuity of shear force between different regions. The influences of moving wall velocity, drop size, surface tension on resistance are examined. Our results show that the resistances increase with the moving wall velocity. A larger drop leads to a larger resistance to drop moving on solid wall, and a larger resistance to bulk flow. A higher surface tension results in a higher resistance to drop movement and bulk flow resistance over the drop because of lower deformation of drop.

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KEYWORDS
Drop movement; hybrid modelling; flow resistance; multiscale simulation

1. Introduction

Drop movements and replacement have a variety of applications including oil production,[1] industrial coating,[2,3] agricultural spraying[4] and cell biomechanics.[5] Understanding of resistance in the drop moving process has significant importance on these fields, such as enhancing oil recovery. Except experiments, simulations have contributed a lot to studies of drop moving problem, such as the computational fluid dynamics (CFD) methods. However, when the spatial scale goes down to nanometres and is comparable to the mean free path of atoms, the traditional CFD method fails down to describe fluid flow because the assumption of continuity may break down.[6] Moreover, continuum equation may have a singular point at some special area, for example on the three-phase contact line when a drop moves on the substrate.[7,8] Last but not least, sometimes it is difficult to give the exact boundary condition for continuum method in complex simulation domain, such as porous media.

Atomistic approaches, such as the molecular dynamics (MD) method, are capable to model nanoscale flows and can avoid singularity problem naturally. However, the computational time and computer resources required by a full MD simulation for a real system are unacceptable. Moreover, it is not necessary to run a full MD simulation because the continuum method just fails in a very limited domain, such as near the interface between fluids and/or fluid and solid.[9,10] Therefore, a hybrid method combining continuum and atomistic methods is of most efficiency for such cases.

Since 1995, hybrid methods have gained a lot of attention and developed rapidly over the last 20 years. Domain decomposition method is the most popular and commonly used method to combine continuum and atomistic modelling, which was first proposed by Connell and Thompson [11]. They divided the simulation domain into two parts, where MD ran in the region where continuum assumption broke down and the continuum method in the rest area. A buffer region was introduced where both MD and continuum method overlapped, to exchange information from each other. This method worked well for the demonstrated cases; however, the flow direction had to be parallel to the interface of two different methods.[9] Weinan et al. [12] presented a comprehensive review of the heterogeneous multiscale method (HMM) developed by some researchers [13–17] to couple MD and continuum method in a different way against the domain decomposition method. The simulation domain was entirely described by the continuum model, and meanwhile the embedded regions were described by atomistic method aiming to provide missing information to the continuum solution locally, such as the constitutive relations and the slip boundary condition. It is not necessary for MD to run the same time with the continuum approach so that it is timesaving compared with domain decomposition method.

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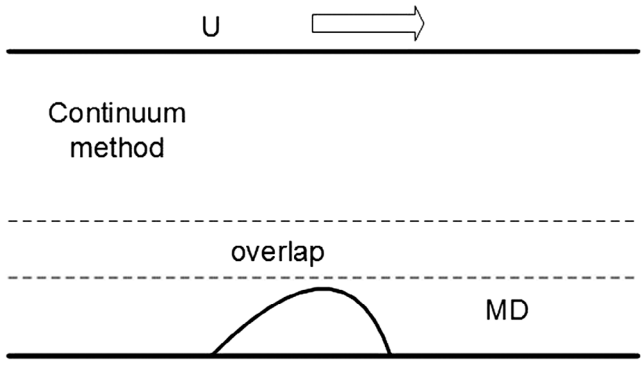

Figure 1. Physical model of drop movement and domain decomposition used in our simulation. The drop is fully covered by MD simulation. The far field is modelled by continuum method which is LBM in this study. There is an overlapped region which is called buffer region to exchange information to ensure continuities of velocity and force. The lower wall is stationary and the upper wall starts to move suddenly with a velocity *U*.

However, this coupling method may have difficulties dealing with problems with strong force or momentum interaction or strong time consequence, in which one has to keep track of the dynamics of fluid microstructure.[12] Therefore, the domain decomposition method is more reliable even though it is more expensive and needs further development.

In this work, the movements and replacement of a nanoscale drop on a horizontal surface driven by shear force from the other immiscible fluid have been investigated by hybrid atomistic–continuum modelling. The domain decomposition method will be developed for coupling. We are concerning the macroscopic behaviour and rules of the drop movements and replacement and the resistance caused by the drops. The rest of this article is organised as follows. In Section 2, the physical and numerical models and methods used in our simulations are presented. We analyse the current challenge and limitations in the previous methods and develop a new boundary treatment for the buffer region. In Section 3, after validations, the present simulations concern the various resistances of movements or flows under different conditions. The conclusions are drawn in Section 4.

2. Model and methods

2.1. Physical model and numerical framework

The physical model of drop movements and displacement is shown in Figure 1. A nanoscale drop is sitting on the lower wall of a long channel. When a velocity is suddenly applied on the upper wall, the drop will be driven to move by shear force from the bulk fluid in the channel. Since the liquid–liquid interaction between drop and bulk fluid and the liquid–solid interaction between drop and wall surface may not be able to be described by the continuum model at nanoscale any more, a hybrid atomistic–continuum modelling that can consider the coupling effect timely becomes necessary. Based on the domain decomposition method, the whole simulation domain is divided into three parts: a pure MD simulation domain covering the nanodrop, a continuum domain for the bulk fluid where LBM is applied because of its highlight ability to deal efficiently with complex geometries and an overlap/buffer region for information exchange.

In the MD region, only simple monatomic molecules are considered for both liquid and solid for simplification with a Lennard-Jones potential for interaction:

$$\Phi\left(r_{ij}\right) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] \tag{1}$$

where r_{ij} is the distance between two different atoms, σ and ε are the characteristic parameters of length and potential, respectively. In the following discussion, we will use reduced units made up of σ, ε and m of simple atom. The reduced unit of temperature is ε/k_B, the reduced time unit is $\tau = \left(m\sigma^2/\varepsilon\right)^{1/2}$, the reduced velocity unit is σ/τ, and the reduced force unit is ε/σ.[9,18]

In the continuum region, the lattice Boltzmann method in a two-dimensional nine-speed (D2Q9) model [19,20] is used because a two-dimensional flow is actually concerned. Resistance of flow is directly obtained by averaging forces between different atoms in x direction parallel to the solid wall. For example, the resistance of drop moving caused by solid wall is obtained by averaging the forces in x direction between drop atoms and solid atoms, while the resistance of channel flow is caused by both solid walls and the drop.

Other modelling details are described as follows. The simulation domain is set as $62.56 \times 4.81 \times 54.10\ \sigma^3$, as shown in Figure 1. In z direction, the MD region is from 0 to 33.28 σ, while the LBM simulation domain is from 17.63 to 54.10 σ. In the x and y directions, periodic boundary conditions are applied. Initially, a total of about 7637 liquid atoms and 480 solid atoms are placed in a FCC lattice and the normalised density of liquid is set to 0.81 for both the drop and the bulk fluid. The solid atoms form a two-layer static wall and are fixed on their positions. The internal interaction potentials (ε_i) for bulk fluid and drop are set at 1.0 and 1.5 respectively, to get different densities and viscosities for two fluids. For the interaction between fluid molecules and the solid atoms, ε_{fs} is set at 0.6 to achieve the non-slip boundary condition.[9] We vary the interaction between the bulk fluid and the drop to get different surface tension. In order to control the system temperature, we use a stochastic dynamics method [21] as a thermostat in every time step of 0.005 τ. Parameters in LBM simulation are set consistent with MD, such as 0.81 for the dimensionless density and 2.14 for the dimensionless viscosity. The time step of LBM is set as 1.715 for the reason that the relaxation time of LBM maintains unity. After the simulation run 100 τ, the system relaxes to its equilibrium state. Subsequently, we suddenly apply a velocity on the upper wall of the channel to drive the drop to move by the shear force. To minimise the fluctuation of statistical results, each simulation is run 16 times independently, and their results are averaged.

1.2. Domain decomposition introduction and challenge analysis

For coupling MD and continuum method, the most important thing is to exchange information between both sides correctly and timely with conservations guaranteed. Hadjiconstantinou and Patera [22] developed a Schwarz alternating method based on domain decomposition to exchange variables. The diagram of this method is shown in Figure 2. The process of Schwarz

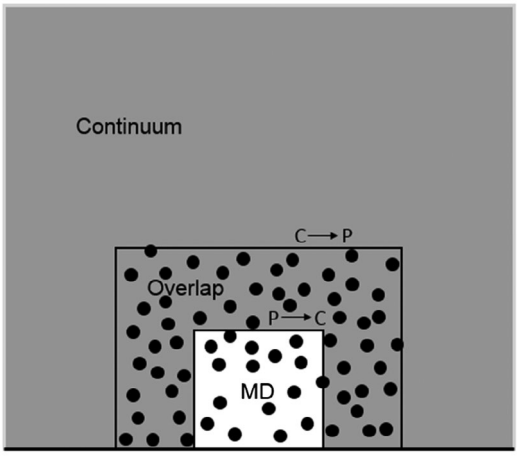

Figure 2. The domain decomposition and Schwarz alternating method.

alternating method is as follows: first, the MD and continuum methods initialise in their own regions; second, at the P–C boundary, MD gives macroscopic variables in buffer as the boundary condition to the continuum model; third, after one time step of continuum simulation, it feeds back values to MD at the C–P boundary, and MD starts to perform simulation again. Repeating step 2 and 3, the alternating procedure will go on until convergence. The flux continuity was said to be automatically ensured when convergence was reached.[23] Wagner and Flekkoy [24] suggested another method based on flux exchange. Instead of preforming MD and continuum simulation alternatively, the flux exchange method imposes the arithmetic mean of the fluxes measured at the interface, as new boundary condition on both systems, and runs MD and continuum simulation at the same time. This method seemed to guarantee flux conservation naturally; however, it could involve large noise and sometimes fails to couple time evolution.[25]

To impose boundary condition for the Schwarz alternating method from MD to continuum method at P–C boundary, statistics is widely used by previous researchers. The expressions for density and momentum are shown below.

$$\rho = \frac{1}{V}\sum_{i=1}^{N} m_i \tag{2}$$

$$\rho \mathbf{u} = \frac{1}{V}\sum_{i=1}^{N} m_i \mathbf{u}_i \tag{3}$$

where ρ is the density, m the mass of atom, $\mathbf{u}$ the drift velocity, V the bin volume and N the atom number in the volume. Imposing boundary condition at C–P boundary is not as simple as at the opposite side because one has to assign every atom at the boundary, a discrete velocity. Nie et al. [9] used a constraint-force method which applied a force on each atom at the C–P boundary to modify the acceleration rate of atoms. This constraint force was to make sure that the statistical velocity of atoms at the boundary can match the macroscopic velocity of the continuum simulation. The formation of the constraint force is:

$$\ddot{x}_i = \frac{F_i}{m} - \frac{1}{N_J m}\sum_{i=1}^{N_J} F_i + \frac{Du_J(t)}{Dt} \tag{4}$$

where $\ddot{x}$ is the acceleration of atom, F_i the force applied on atom i from other atoms, m the atom mass, N_J the number of atoms at boundary and u_J the drift velocity. Fluid flowing across the boundary was achieved by injecting or removing atoms from the boundary region. Hadjiconstantinou [22] used a Maxwellian distribution method to translate boundary condition from continuum method to MD simulation. In their method, at each time step, a velocity drawn from a Maxwellian distribution with mean and variance consistent with the desired velocity and temperature of the fluid would be given to the molecules at the boundary. The disadvantage of this method is that if there is fluid flux across the boundary, a particles pool has to be introduced with artificial periodic boundary. It will introduce more particles than the constraint-force method so that reduces the efficiency of hybrid simulation.

Different with a pure MD method, an important problem in hybrid simulation is how to prevent molecules from drifting away freely at the interface of continuum and atomistic method. Connell and Thompson [11] first applied a constant force at the particles in boundary region to keep atoms stay in the simulation domain.

$$F_b = -ap\rho^{-2/3} \tag{5}$$

where F_b is the constant force they proposed, p the pressure, ρ the density and a the coefficient. This constant force successfully prevented molecules from drifting; however, it imposed a large fluctuation of density at the boundary. Following works proposed many other types of force to minimise the density fluctuation. Flekkoy et al. [26] used a weight factor instead of the constant coefficient. Nie et al. [9] used the force as a function of distance between the atom and interface. When the distance approaches to zero, the force approaches to infinity. Zhou et al. [27] proposed a complicated force which took into account the forces from artificial atoms outside the boundary. They got the force as a function of density and temperature through a lot of simulations with fitting parameters. Nearly no fluctuation was found using this method; however, much preparation and fitting work had to be done before.

Although the previous studies have contributed significantly to developments of hybrid atomistic–continuum methods, there are still big challenges and difficulties for popular usage. The *first* one is the computational efficiency. The low efficiency of current hybrid modelling comes from two aspects: one from the inherent characteristics of MD and the other from the exchanging information algorithm. For reduction of the statistical fluctuation of MD, we use multiple independent threads running at the same time to increase the sample size. Most of the previous algorithms for information exchange between continuum and MD are based on macroscopic thermodynamic parameters, such as velocity and pressure, used as boundary condition at the interface. It needs huge amount of collisions and time steps for the molecules near interface to really catch the macroscopic information. Although the gradient of macroscopic parameters was used to accelerate this process by some researchers including ourselves, the numerical stability is still troubling. The *second* challenge of hybrid modelling comes from the shear force when transfers from continuum to MD. As we described before, in the Schwarz alternating algorithm of domain decomposition, a preventing force was added to prevent molecules in the buffer region from drifting

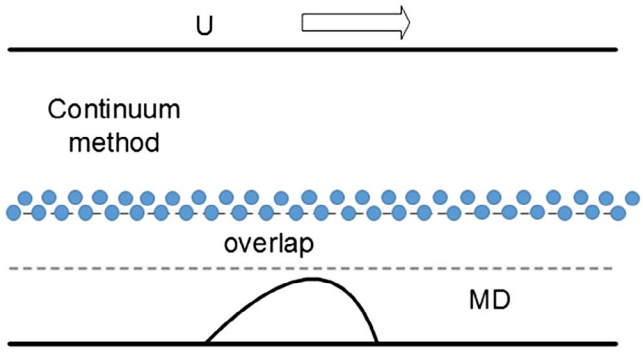

Figure 3. (Colour online) Arrangement of an artificial solid molecular layer (represented by blue circles) at the outer edge of buffer region to ensure the continuity of shear force between different regions. This layer should result in a non-slip and non-stick condition for MD side. This layer obtains macroscopic moving velocity at each time step but never participates continuum modelling as a solid wall.

away. The algorithm ensured correctly the velocity transferred from the continuum to MD; however, the shear force deviates from the analytical solution even for a standard Couette flow. The reason lies in that the preventing force disturbs the shear stress of molecules group in the buffer region besides holding molecules in the region. Therefore, this algorithm works well for weak interactions between continuum and MD, such as the rough wall channel flows, but is not suitable for fluid–fluid interface with relatively strong force interactions, such as drop deformation, movement and displacement. Therefore, a new treatment at the buffer edge is required to ensure both the flow velocity and the shear force correctly exchanged between continuum and MD. We propose one which is described as follows.

2.3. Boundary treatments for buffer region

As we learn from a typical MD modelling for a Couette flow, the moving upper wall can transfer its velocity and the shear force accurately to the fluid by molecular collisions. Meanwhile, the wall molecules prevent naturally fluid molecules from flying outside the channel as well. Inspired by this, we propose an artificial solid molecular layer at the edge of the buffer region. The artificial layer has no effects on the continuum modelling. When C–P process stars, the layer participates in MD collisions with a moving velocity from the continuum (LBM) modelling at the position, as shown in Figure 3. The molecule type and configuration of the layer will surely influence the results, as well as the layer number. In this work, we just simply copy the lower wall with bi-layer molecules of MD region as the artificial solid molecular layer and set the interaction potential between the layer and bulk fluid at 0.6 for a non-slip and non-stick condition. By this treatment, both the macroscopic fluid velocity and shear force can be transferred from continuum to MD correctly. It is simple and practicable. If there is any fluid flux across this artificial solid layer, atoms will be added or removed at the boundary region as the previous works.[9] Any other acceleration technique for information exchange can be integrated into this treatment as well. Our simulations will validate this treatment in the next section.

3. Results and discussion

In this part, the algorithm and code are validated first. Subsequently for the drop movement driven by the shear force from a moving upper wall, the influence of drop size, moving wall velocity and surface tension on resistance is examined. We consider the resistance to drop movement, the resistance to channel flow and the partial resistance to flow caused by drop. The resistance to drop movement and the resistance to channel flow are caused by solid wall and calculated by averaging the forces parallel to the wall between solid wall and drop or bulk fluid, respectively. The partial resistance to flow caused by drop is calculated by averaging forces parallel to the wall between drop and bulk fluid. All the resistances are calculated at steady state and averaged over 16 independent simulations to minimise the fluctuation.

3.1. Benchmark and validations

To validate our code, we simulate a single-phase sudden-start Couette flow as shown in Figure 4(a) and compare the time-dependent velocity profiles and the steady-state shear force with the analytical solution. The shear force for a steady Couette flow is calculated by:

$$f = A\mu\frac{\mathrm{d}u}{\mathrm{d}y} \tag{6}$$

where f is the shear force, A the area, μ the viscosity of fluid, u the velocity along the channel and y the coordinate vertical to the channel. The analytic solution of a sudden-start Couette flow comes from Mendiburn et al. [28]. Figure 4(b) shows that the velocity profiles at different time predicted by our hybrid modelling agree well with the analytic solution, which validates our algorithm at the first stage.

Furthermore, as we discussed about the challenges of previous algorithms, the shear force has to be examined carefully. In Figure 5, the calculated shear force using our proposed treatment at interface in the particle region (buffer region and MD region) is compared with analytical solution, as well as the shear forces obtained by other methods, including the constraint-force method and the Maxwellian distribution method. Only our modelling results match the analytical shear force well, and the previous methods overrate the shear force. This means that even though the previous methods for information exchange can reserve the velocity well, they lead to incorrect shear force transfer from continuum to MD; and therefore they are not suitable for drop movement modelling driven by shear force.

3.2. Resistance variations

3.2.1. Drop size effects

Drop size has significant effects on the resistance to channel flow because clearly a larger drop has a larger shape resistance. However, since the liquid drop is different from a solid rough or obstacle, this effect has seldom been studied yet. To clarify this effect quantitatively, we vary the initial radius of semicircular drop from 8 to 11 unit of length, as shown in Figure 6(a). The cross interactive potential parameter between molecules of bulk fluid and drop is set at 0.4, and the upper wall velocity is set at 0.4

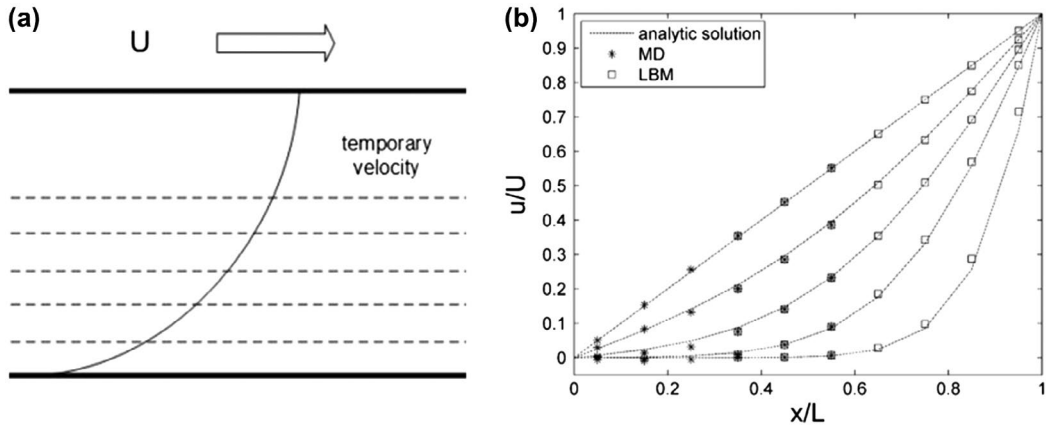

Figure 4. (a) Single-phase sudden-start Couette flow to validate our code. The solid cure shows the temporary velocity along the height at a time. Dash line shows the position where we calculate the shear force, together with the lower wall. (b) Validation of velocity profile in sudden-start Couette flow. Squares and asterisks show results from LBM and MD respectively, and the dotted lines show analytic solution at different time.

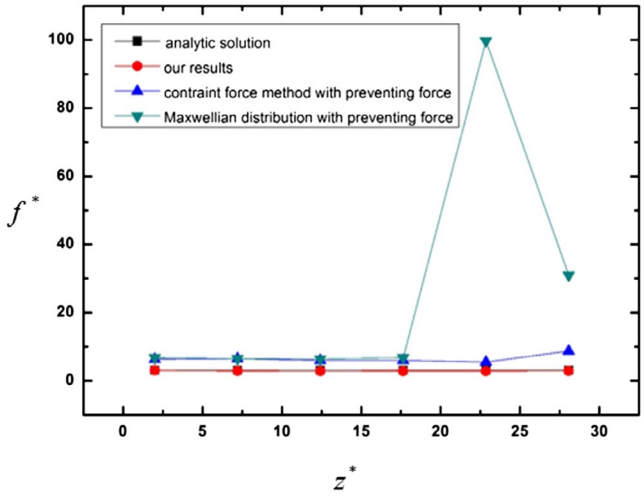

Figure 5. (Colour online) Shear force at different position. Black squares show the analytic solution, and are covered by red circles, which mean our results. Up triangles and down triangles show constraint-force method and Maxwellian distribution method with preventing force, respectively. The shear force is normalised by ε/σ, i.e. $f^* = f/(\varepsilon/\sigma)$ and z position is normalised by σ, e.g. $z^* = z/\sigma$.

unit of velocity. The temperature of system is fixed to 1.1 unit of temperature through a thermostat. It is worth mentioning that the resistance calculation may meet large fluctuations when the drop is crossing inlet or outlet boundary. Therefore, we just use the calculated resistance when the drop is moving near the centre of the channel, as shown in Figure 6(b).

The three kinds of resistance forces varying with drop size are shown in Figure 7. Unsurprisingly, both the resistance forces of drop to bulk flow and wall to drop increase continuously with the drop size. At the current parameters, the resistance of wall to drop is larger than that of drop to bulk flow. The resistance from wall surface to bulk flow decreases with the drop size. The reason may lie in that the contact area between bulk fluid and solid wall decreases with a larger drop, and therefore weakens the effective resistance to the bulk fluid in channel.

3.2.2. *Moving wall velocity effects*

For a single-phase Couette flow, the shear force increases linearly with moving wall velocity. How the resistance respects to moving wall velocity with a soft drop on substrate is not clear, and the linear relationship needs to be examined for such a multiphase case. The modelling parameters are as follows: the cross

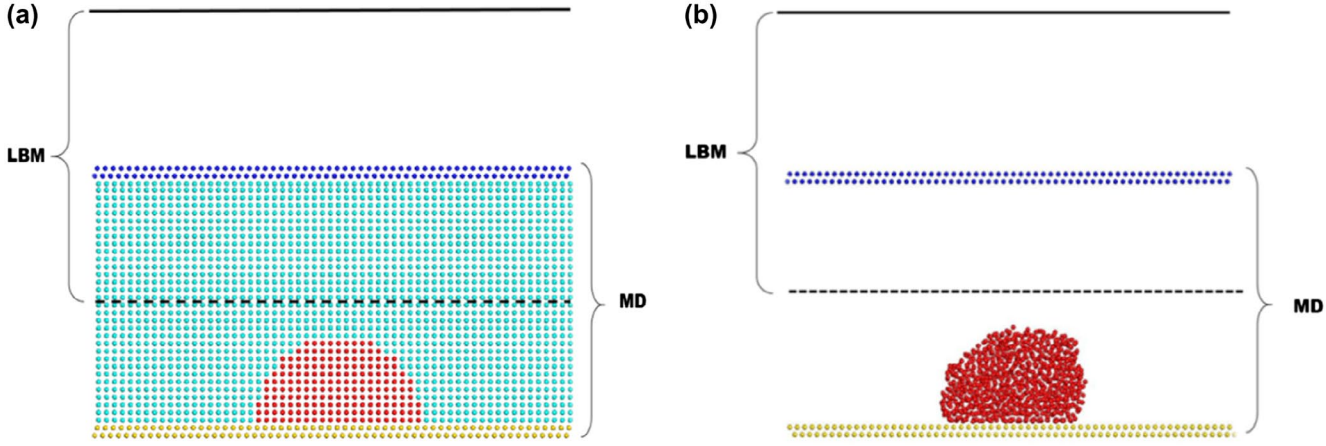

Figure 6. (Colour online) (a) Initial position of semicircular drop on the surface. Atoms of drop are shown in red, those of bulk fluid in green, those of solid lower wall in yellow and those of artificial solid molecular layer in blue; (b) the moving drop near the centre of the channel, where the calculation of resistances has the least fluctuation.

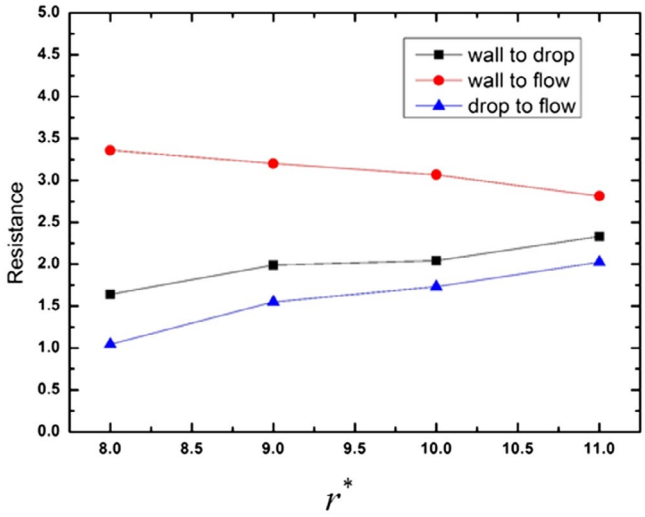

Figure 7. (Colour online) Resistances as a function of drop size. Red circles are resistance from wall to bulk flow, black squares are resistance from solid wall to drop movement and blue triangles are the resistance fraction from drop to bulk fluid flow. The resistance is normalised by ε/σ and the radius of drop is normalised by σ, e.g. $r^* = r/\sigma$.

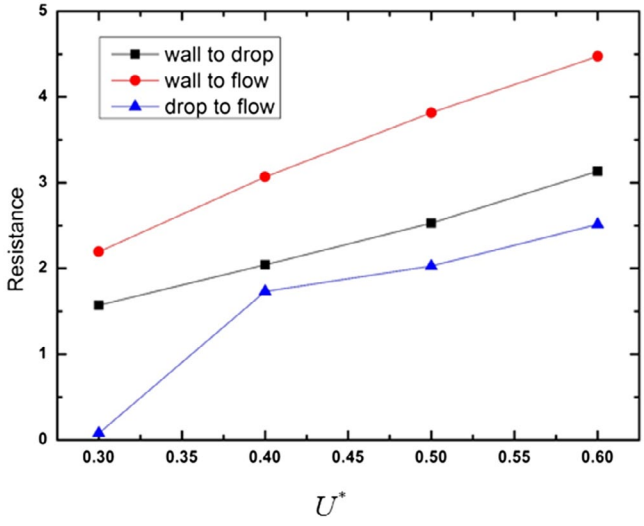

Figure 8. (Colour online) Resistance as a function of the upper wall velocity. Red circles are resistance from wall to bulk flow, black squares are resistance from solid wall to drop movement and blue triangles are the resistance fraction from drop to bulk fluid flow. The resistance is normalised by ε/σ and the moving wall velocity is normalised by σ/τ, e.g. $U^* = U/(\sigma/\tau)$.

interaction between the bulk fluid and the drop is set at 0.4, and the initial radius of drop is set at 10 unit of length. The moving wall velocity varies from 0.3 to 0.6 unit of velocity.

Figure 8 shows that all three kinds of resistance increase with moving wall velocity. For Couette flow even in multiphase cases, the shear force increases with the moving wall velocity. The resistance from wall to bulk fluid is still perfectly linear for a given drop size, as the red circles line shows in Figure 8. The resistance from wall to drop is lower than that from wall to bulk fluid, but is still nearly linear with the moving wall velocity, as the black squares line shows. For the resistance to bulk fluid flow by the drop, as the blue triangles line shows, the curve is far deviated from linearity, because the strong shear force will cause the drop

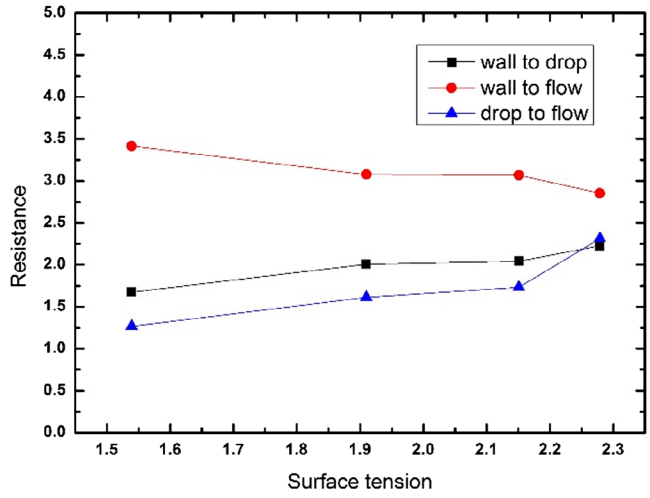

Figure 9. (Colour online) Resistance as a function of surface tension. Red circles are resistance from wall to bulk flow, black squares are resistance from solid wall to drop movement and blue triangles are the resistance fraction from drop to bulk fluid flow. The resistance is normalised by ε/σ, and the surface tension is normalised by ε/σ^2. The radius of drop is set at 10 unit of length and the velocity of upper wall is set at 0.4 unit of velocity.

to deform significantly. For the current surface tension, the drop will be torn into two parts if the velocity of upper wall is higher than 0.6 unit of velocity.

3.2.3. Surface tension effects

Following the analysis for Figure 8, the drop deformation plays an important role on resistance and drop movement and replacement process. In this subsection, we focus on the surface tension effects that dominate the drop deformation or even break-up. As we know from the molecular kinetics that the surface tension is the macro appearance of atoms interaction between fluids. For a given molecular interaction within drop, a higher atoms interaction between drop and bulk fluid leads to a lower surface tension and vice versa. A virial expression [29,30] has been used to calculate the surface tension based on the cross interactive potential between drop and bulk fluid. Here, we vary the cross interaction from 0.3 to 0.6 to change the surface tension of drop, and the results are show in Figure 9.

Variation in all the resistance forces with surface tension appears to have three stages. When the drop surface tension is extremely low, which means the repulsion interaction between drop and bulk fluid is very high, the drop is easier to deform by shear force from bulk flow, as shown, nearly breaks up, in Figure 10(d), so that the resistance forces relative to the drop are lower, as the black squares and blue triangles show in Figure 9 at surface tension = 1.539. On the other side, when the surface tension is extremely high, which means the repulsion between molecules of drop and bulk fluid is very low, the drop maintains its round shape when moving, as shown nearly keeps its initial shape in Figure 10(a), so that the resistance forces relative to the drop are higher, as shown in Figure 9 at surface tension = 2.279. Otherwise, when the surface tension is moderate, the drop may maintain a drop shape with an advancing angle and a receding angle when moving for a given shear force, as shown in Figure 10(b) and (c). For such cases, the resistance forces relative to the drop are nearly changeless, as shown in Figure 9 at surface tension from 1.9 to 2.2.

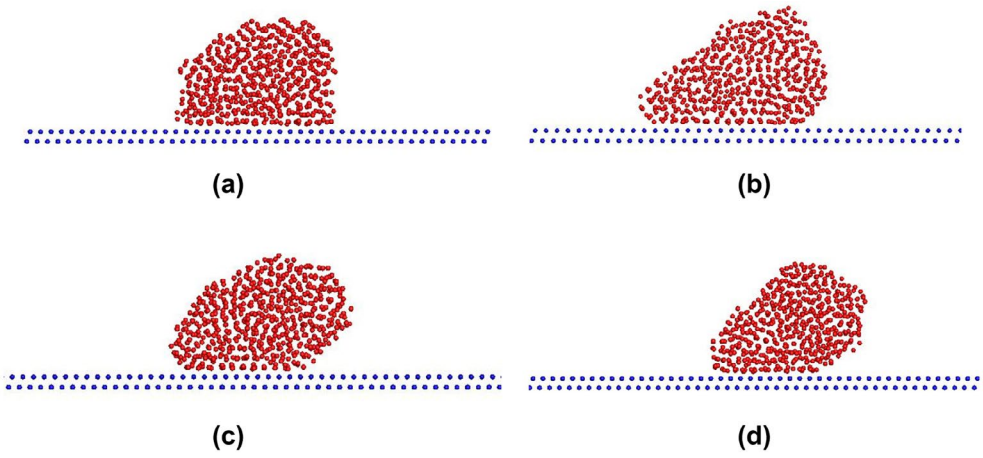

Figure 10. (Colour online) Deformations of drop for different surface tension. (a) surface tension is 2.279 ε/σ^2, when cross interaction is 0.3; (b) surface tension is 2.151 ε/σ^2, when cross interaction is 0.4; (c) surface tension is 1.910 ε/σ^2, when cross interaction is 0.5; (d) (a) surface tension is 1.539 ε/σ^2, when cross interaction is 0.6.

4. Conclusions

When the interfacial interaction near the drop is not able to be fully covered by the continuum theories, a hybrid atomistic–continuum simulation is necessary. We develop a hybrid framework in which the drop is modelled by molecular dynamics for accurate capture of transport behaviour, while the bulk flow region is simulated by the lattice Boltzmann method for high efficiency. The momentum exchange between atomistic and continuum regions is realised in a buffer region to couple the multiscale effects. To ensure the continuity of shear force between different regions, we propose an artificial solid molecular layer at the outer edge of buffer region. Our algorithm and code are validated well by comparisons between our predictions and the analytical solution for a single-phase Couette flow. The modelling results indicate that the moving wall velocity, the drop size and the surface tension have significant influences on the resistance forces, which include resistance to drop movement, resistance to channel flow caused by solid wall and the partial resistance to flow caused by drop. The results show that all resistances increase with the moving wall velocity. A larger drop leads to a larger resistance for drop moving on the solid wall, and a larger partial resistance for bulk flow. Different surface tensions result in different resistance forces to drop movement and bulk flow over the drop because of different deformations of drop.

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Disclosure statement

No potential conflict of interest was reported by the authors.

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