3D INTERNAL FLOW STRUCTURES OF A MOVING DROPLET ACTUATED BY WETTABILITY GRADIENT

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Summary A two-phase dissipative particle dynamics model is developed for simulating droplet movement actuated by gradient of wettability. It is found that the droplet moves in a way of rolling and sliding combined. The process of the droplet motion can be generally divided into rolling, deforming and decelerating stages. The vortex inside the droplet has a solid-core structure. The 3D movements of the flow particles are analyzed in detail by examining the streamlines obtained.

INTRODUCTION

The actuation and manipulation of a discrete droplet is one of the crucial technologies in the design and optimization of droplet-based microfluidic systems. With the scale of fluid decreasing, the specific surface area dramatically increase, thus the surface forces might have profound impact on the fluids over than inertia or body forces. The imbalance of surface tension induced by the wetting gradient can be utilized to actuate a droplet on a flat surface along the direction of wetting gradient. The idea was demonstrated by the experimental work of Chaudhury and Whitersides [1]. In their experiment, the wettability gradient was generated along a silicon wafer and it was found that a sessile droplet can move automatically uphill against gravity. Since then, a variety of technologies have been developed for adjusting wetting properties aiming at manipulating droplets.

A lot of experiments were carried out to explore the spontaneous motion of droplet actuated by wettability gradient, including the engineering prediction of the quasi-steady speed of the droplet [2]. The investigation of internal flow characteristics is of importance for understanding the mechanism of droplet movement. Das et. al. [3] and Shi et. al. [4] studied the two-dimensional internal flow structure of a liquid droplet translation on a flat surface and found a strong circulation in the droplet. However, the three-dimensional flow characteristics inside a moving droplet over a solid substrate actuated by wettability gradient have not been described yet. Based on dissipative particle dynamics (DPD), the present work developed a 3D numerical model to simulate the motion of a droplet propelled by wetting gradient.

MODEL AND NUMERICAL IMPLEMENTATION

The dissipative particle dynamics was proposed by Hoogerbrugge and Koelman [5] to take advantages of large timescale in lattice-gas automata (LGA) and mesh-free algorithm in molecular dynamics (MD). The basic component of the DPD is coarse-grained particle which represents a cluster of molecules instead of atoms/molecules themselves. Therefore it is capable of modeling systems with larger length and time scales comparing to MD. To simulate the interfacial phenomena, many-body potential for conservative force [6] is applied and given by:

$$\mathbf{F}_{ij}^{C} = A_{ij}\omega_C(r_{ij})\mathbf{e}_{ij} + B(\bar{\rho}_i + \bar{\rho}_j)\omega_d(r_{ij})\mathbf{e}_{ij} \quad (1)$$

where A_{ij} is a species-dependent constant, A_{ll} defines the interaction between liquid (*l*) and liquid(*l*) particles, while A_{sl} stands for the interaction between solid (*s*) particles and liquid (*l*) particles.

The wetting behavior is allowed to adjust from hydrophilic to hydrophobic by changing the mutual attraction between the solid and liquid particles, which results in variation of the solid-liquid interfacial tension. As displayed in Fig. 1, the static contact angle θ is a monotonous function of A_{sl}. A location-dependent A_{sl} is considered in the present study, which results in a linear variation of contact angle varying from θ_L to θ_R between -40 and 40 in x direction, as shown in Fig. 2. The static contact angle θ_L=150° for x<-40 and θ_R=40° for x>40.

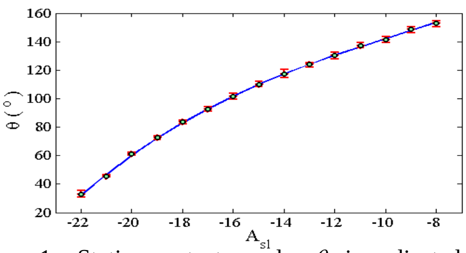

Figure 1. Static contact angle θ is adjusted from hydrophilic to hydrophobic by varying A_{sl}.

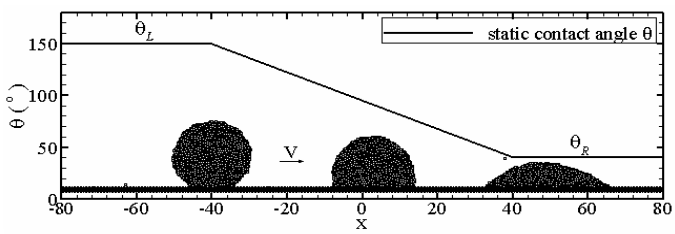

Figure 2. Wettability gradient on the flat substrate.

RESULTS AND DISCUSSION

When a spherical droplet is released on a heterogeneous substrate, the Marangoni effect due to the wettability gradient

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will haul the droplet towards the hydrophilic end, and hence actuates the self-transportation of droplet. The droplet moves towards the right side in Fig. 2. Fig. 3 plots the time variation of the location of droplet centroid X_{CM} and its speed V. An aspect ratio $\alpha=H/L$, which is defined as the maximal vertical height H over maximal horizontal length of the liquid droplet L, is used to analyze the deformation of the droplet as it advancing. α=1.0 represents a sphere while small α means flat spherical cap. Results show that the process of self-transportation can be generally divided into three stages, i.e., rolling, deforming and decelerating stage. In the initial stage, the substrate is hydrophobic and rolling dominates the motion, the speed of droplet increases rapidly while the deformation of droplet is small. Then, the speed of droplet V reaches its maximum and starts to decrease while the aspect ratio α declines significantly when the droplet contacts with the hydrophilic surface. The droplet deforms dramatically and it advances in a way of rolling and sliding combined. The driving force acting on the drop due to wetting gradient can not overcome the drag force causing by viscous dissipation, which results in the reduction of translation speed V. Finally, when X_{CM} is large than 30, some part of the droplet move out of the region with wetting gradient, and the droplet decelerates until it comes to halt.

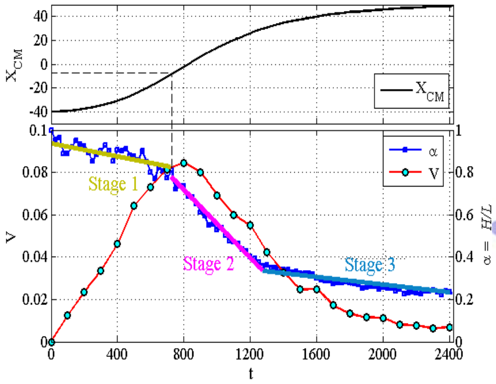
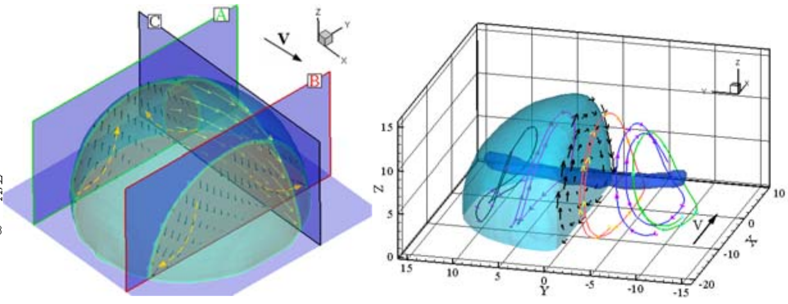


Figure 3. The time variation of the location of droplet centroid X_{CM} and its speed V



(a) (b)

Figure 4. The three-dimensional flow structure inside the moving droplet. Vector **V** denotes the moving direction.

When the droplet moves to the location of X_{CM}=-5.8, the static contact angle across the droplet varies from hydrophobic to hydrophilic in x direction. Fig. 4(a) illustrates the three-dimensional flow structure of the moving droplet at this moment, in which the velocity vectors are shown in cross-section A, B and C. It is found that in the front part (section B), the droplet contacts with the hydrophilic area of the solid in an acute angle, and the fluid particles spread on the substrate; whereas in the back part (section A), the angle of the droplet contacting with the solid wall is comparatively large, and the flow particles tend to leave the substrate and behave like dewetting. Consequently, the flow particles generally move forwards and the liquid droplet advances towards the hydrophilic region (section C).

A vortical structure of internal flow is presented in Fig. 4(b) after subtracting the translation speed of droplet from the three-dimensional velocity filed, which reveals that the movement of the droplet is a combination of rolling and translation. The velocity vectors in the figure show a solid core vortex structure on the central section Y=0. The streamlines splay out as they approaching the substrate, manifesting three-dimensionality substantially. The more the streamlines lie away from the central section Y=0, the more oblique they are. This result indicates the role of the flow in y direction, which is perpendicular to moving direction of the droplet.

CONCLUSIONS

When a spherical droplet is released onto a surface with gradient of wetting property, the difference of wettability across the droplet will actuate it to move towards the hydrophilic end. Based on DPD simulations, we show that the kinds of movements, i.e. the rolling and the sliding, might have different roles during the process of droplet movement. The former dominates the motion when the droplet lies on hydrophobic surface, while the combination of rolling and sliding plays a crucial role when the droplet contacts with the hydrophilic surface. The three-dimensional flow field inside the moving droplet is presented and reveals a solid-core vortical structure.

References

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