Three-dimensional Transient Motion of Spherical and Deformable Droplet in L-Shaped Rectangular Micro-channel

Chang-Wei Kang kangcw@ihpc.a-star.edu.sg +65 6419 1324

Jinsong Hua huajs@ihpc.a-star.edu.sg +65 6419 1537

Jing Lou loujing@ihpc.a-star.edu.sg +65 6419 1540

Institute of High Performance Computing
1 Science Park Road, #01-01, The Capricorn, Singapore Science Park II, Singapore 117528

ABSTRACT

Numerical simulations are conducted to examine the effects of surface tension on the transient motion and deformation of a droplet during its transit in straight and L-shaped rectangular micro-channels. This study is investigated by a three-dimensional front tracking method. The results show that in the straight channel, the droplet with higher Bond number (i.e. lower surface tension) deforms more significantly than that with lower Bond number. The droplet deformation subsequently leads to higher drag force from the flow and accelerates the elongated droplet to move faster. As a result, the deformed droplet may take shorter time to exit the micro-channel. In the case of L-shaped channel, since there is an abrupt change in flow field, the shape of the droplet with higher Bond number (0.2) is significantly affected compared to that of lower one, although both droplets travel in a similar path.

Keywords: micro-channel, deformation, surface tension, front tracking, L-shaped.

1 INTRODUCTION

In the fields of chemical and biomedical, there is a rising demand for a fast, precise and cost-effective analysis method. A concept, so-called "lab-on-a-chip" has been recommended, where aqueous droplets in an immiscible carrier fluid are applied to transport a small amount of chemical agent in the micro-channels. These droplets can provide ideal microcapsules that can isolate reactive materials, cells or drugs, but the accurate control and manipulation of these droplets set a new challenge, especially when the droplets are deformable. This is because for droplet which deforms, its shape changes continuously during its transit in the micro-channel. The change of the shape subsequently affects the flow field driving the particle and thus the trajectory of particle and time taken for particle to exit the micro-channel may differ from that of non-deformable one. The motion of droplet in a micro-channel is even more complicated when the flow path gets a sharp turn in "L" shaped channels which are quite common in micro-fluidic device.

Much of the published work was associated with the study of the effects of droplet size, droplet viscosity and distance between droplets on the droplet dynamics. In the experiments by Engl *et al*. [1], it was shown that the T-junction could act as a hydrodynamic sieve, depending on the distance between incoming droplets. Ye and Li [2] reported their numerical studies on droplet motion through T-junction channel. However, both experimental and numerical studies involve only non-deformable droplet. The research to quantify the interaction mechanism of moving deformable droplets in micro-channels, to our best knowledge, is still lacking.

In this study, our objective is to investigate the moving behavior of single deformable droplet in straight and L-shaped rectangular micro-channels. The straight channel serves as the benchmark study. As for L-shaped channel, due to the sharp turn of the flow path, the droplet motion and deformation are affected by its inertia, driving flow and interfacial tension. Droplet may impact on channel wall, even break up if handled improperly. It is quite challenging to conduct experimental study, due to the small dimensional scale and deformable droplet. In this study, numerical simulation based on the three-dimensional front tracking method, one of the promising techniques to solve the problem of this nature, is applied to explore the deformable droplet moving dynamics in micro-channel.

2 FRONT TRACKING METHOD: A BRIEF DESCRIPTION

Front tracking method is a computational technique that was conceptually designed by Tryggvason *et al*. [3] and further extended and validated by Hua and Lou [4] as a method to capture sharp interface between the fluids of different phases. In this method, one single set of Navier-Stokies equation is solved throughout the whole computational domain by treating the different phases as one fluid with variable properties. The non-dimensional Navier-Stokes equation, governing the momentum balance in the fluid domain, including the interface can be expressed as

$$\frac{\partial(\rho\mathbf{u})}{\partial t}+\nabla.\rho\mathbf{u}\mathbf{u}=-\nabla p+\frac{1}{\mathrm{Re}}\nabla.[\mu(\nabla\mathbf{u}+\nabla^{T}\mathbf{u})]+\frac{1}{\mathrm{Bo}}\kappa\mathbf{n}\delta(x-x_f) \quad (1)$$

where $\delta(x - x_f)$ is a delta function that is one only where $x = x_f$ and zero otherwise. The subscript f refers to the interface and the dimensionless Reynolds and Bond numbers are defined as follows:

$$\mathrm{Re}=\frac{\rho_l g^{1/2} D^{3/2}}{\mu_l} \quad (2)$$

$$\mathrm{Bo}=\frac{\rho_l g D^2}{\sigma} \quad (3)$$

where σ is surface tension of the droplet and subscript l refers to the liquid phase. The fluid properties, such as density, ρ and viscosity, μ are updated based on the interfacial front. The third term on the right-hand side of equation (1) represents the surface tension source term calculated from the interface and transmitted to this equation using a delta function.

To solve the Navier-Stokes equation, equation (1) is discretized on the staggered and structured grids and subsequently worked out numerically by a projection-correction scheme. In order to rapid the solution with higher accuracy, advanced modeling techniques such as adaptive mesh refinement (AMR) and parallel computing have been implemented using PARAMESH [5].

Once the fluid velocity is solved on the regular finite difference grid, the velocity of the moving interface is computed by interpolating from the fixed grid so that the interfacial front moves at the same velocity as that of the surrounding fluid. Then, the front is advected normally in a Lagrangian manner;

$$x_f^{t+1}-x_f^{t}=\Delta t\mathbf{u_f}.\mathbf{n} \quad (4)$$

After the interfacial front moves to the new location, the elements used to mark the interface are modified to keep a good geometric resolution, and thus ensure better accuracy of the simulation results.

3 OPERATING CONDITIONS AND CHARACTERIZATION OF A DEFORMED DROPLET

Table 1 summarizes the set of parameters applied in this study. All parameters are remained constant for both straight and L-shaped channels, except for Bond number. The Bond number of 0.02 refers to droplet with higher surface tension and Bond number of 0.2 indicates that the droplet is easier to deform. With higher Bond number, it is expected that there will be topological change, which can be quantified by a parameter, so-called elongation factor, E.

The elongation factor is defined as the ratio between the length of the longest axis to that of the shortest axis, i.e. E = b/a. Fig. 1 shows the schematic diagram of an elongated droplet in a moving fluid flow.

Channel	Re	$\rho_r=\rho_l/\rho_d$	$\mu_r=\mu_l/\mu_d$	Bo
Straight	20	0.5	0.02	0.02
				0.2
L-shaped	20	0.5	0.02	0.02
				0.2

*Subscript l refers to liquid phase and subscript d is for droplet phase.

Table 1: Summary of parameters applied for this study

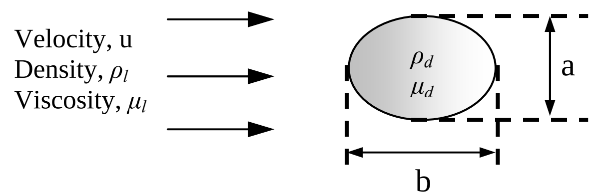


Figure 1: Illustration of a droplet with its elongation factor, E = b/a.

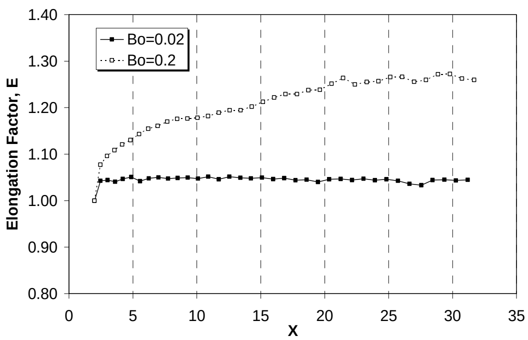
4 RESULTS AND DISCUSSION

Velocity inlet and outflow boundary condition are applied at the inlet and outlet of the channel, respectively. Non-slip velocity condition is implemented on all sides of the wall. Since the droplet motion is strongly dependent on its initial position, we locate a spherical droplet at X=2, Y=2 and Z=2 for all cases so that we can isolate and study the effects of surface tension on the droplet dynamics and deformation.

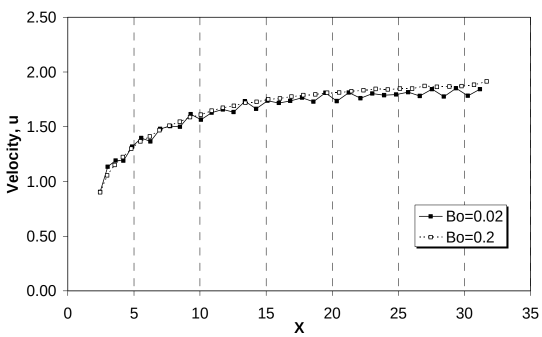
4.1 Droplet Dynamics and Deformation in Straight Channel

Fig. 2(a) shows the effect of surface tension on the deformation of droplet. For droplet with smaller surface tension (i.e. Bo=0.2), due to the drag force from the incoming flow initially exceeding the surface tension force, the droplet deforms continuously. But until X=20, where both forces are equal in magnitude, the droplet starts showing oscillatory deformation. This oscillatory deformation is also observed for droplet with higher surface tension (i.e. Bo=0.02). In this case, the droplet oscillatory deformation occurs during the entire course of travel. However, compared to the droplet with higher surface tension, droplet deforms more significantly for the case with smaller surface tension.

The effect of surface tension on the droplet velocity is shown in Fig. 2(b). It is noted that both droplets of different surface tensions travel in the same path at the same speed initially. After reaching X=15, droplet with higher Bo number accelerates, indicating that the momentum transfer from flow to droplet with higher Bo number is faster than that of the case with lower Bo number. It can also be concluded that total drag depends strongly on the droplet deformation.



(a)

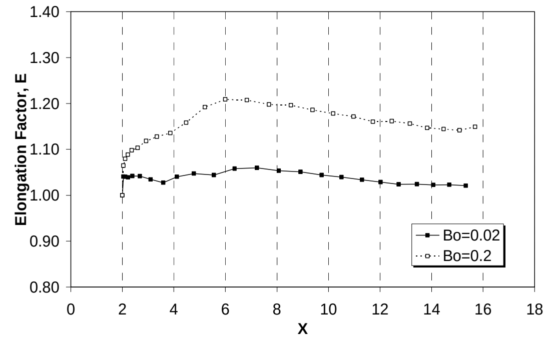


(b)

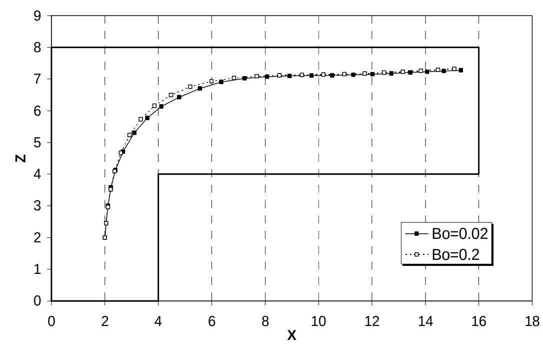
Figure 2: Effects of surface tension on droplet (a) deformation and (b) velocity in straight rectangular channel.

4.2 Droplet Dynamics and Deformation in L-Shaped Channel

Fig. 3 shows the changes of elongation factor and droplet trajectory in an L-shaped channel due to the effect of surface tension. In Fig. 3(a), the elongation factor for droplet with Bo=0.2 starts off at unity (i.e. spherical shape) and rises to a maximum of 1.20 at X=6. Beyond this location, the elongated droplet retracted to a less deformed shape. The change of elongation factor can be explained by the path taken by the droplet in the L-shaped channel. Refer to Fig. 3(b), the droplet, initially, is placed at the middle of the channel where the flow velocity is at the maximum. After a sharp turn in the L-shaped, the droplet is pushed towards the near-wall region, where the flow velocity is smaller. Therefore, the droplet becomes less elongated. But, for droplet with lower Bo number, the degree of deformation remains almost constant although the droplet follows the similar path due to higher surface tension. The evolution of droplet locations and shapes in L-shaped channel due to the effect of Bond numbers is shown in Fig. 4.



(a)



(b)

Figure 3: Surface tension effects on (a) elongation factor and (b) trajectory for droplet travels in L-shaped rectangular channel.

5 CONCLUSION

A three-dimensional front tracking method was utilized to investigate the effects of droplet surface tension on its transient motion and deformation in micro channels. Two channels; i.e. straight and L-shaped were selected as the housing for this investigation. The simulated results showed that the droplet surface tension had significant effect on its deformation. Droplet with lower surface tension (i.e. higher Bond number) deformed more significantly than that with higher surface tension (i.e. lower Bond number); regardless which channel the droplet was traveling in. The deformation subsequently affected the flow field driving the droplet, and as a result, the droplet with elongated shape moved faster than the spherical droplet. It was also found that in the L-shaped channel, as there was a sudden change of flow path, the droplet deformation was varied. Larger droplet deformation was caused by higher flow velocity. When the droplet was dragged towards near-wall region where the flow velocity was lower, the droplet retracted to a shape with less deformation.

REFERENCES

[1] W. Engl, M. Roche, A. Colin and P. Panizza, "Droplet Traffic at a Simple Junction at Low Capillary Numbers", *Physical Review Letters*, 95, 208304-1 – 208304-4, 2005.

[2] C. Ye and D. Li, "3D Transient Electrophoretic Motion of a Spherical Particle in a T-shaped Rectangular Microchannel", *Journal of Colloid and Interface Science*, 272, 480-488, 2004.

[3] G. Tryggvason, B. Burner, O. Ebrat and W. Tauber, "Computations of Multi-Phase Flows by a Finite Difference/Front Tracking Method. I. Multi-Fluid Flows", *Von Karman Lectures Notes*, *the Von Karman Institute*, 1998.

[4] J.S. Hua and J. Lou, "Numerical Simulation of Bubble rising in Viscous Liquid", *Journal of Computational Physics*, 222, 769-795, 2007.

[5] P. MacNeice, K. M. Olson, C. Mobarry, R. de Fainchtein and C. Packer, "PARAMESH: A Parallel Adaptive Mesh Refinement Community Toolkit", *Computer Physics Communications*, 126, 330-35, 2000.

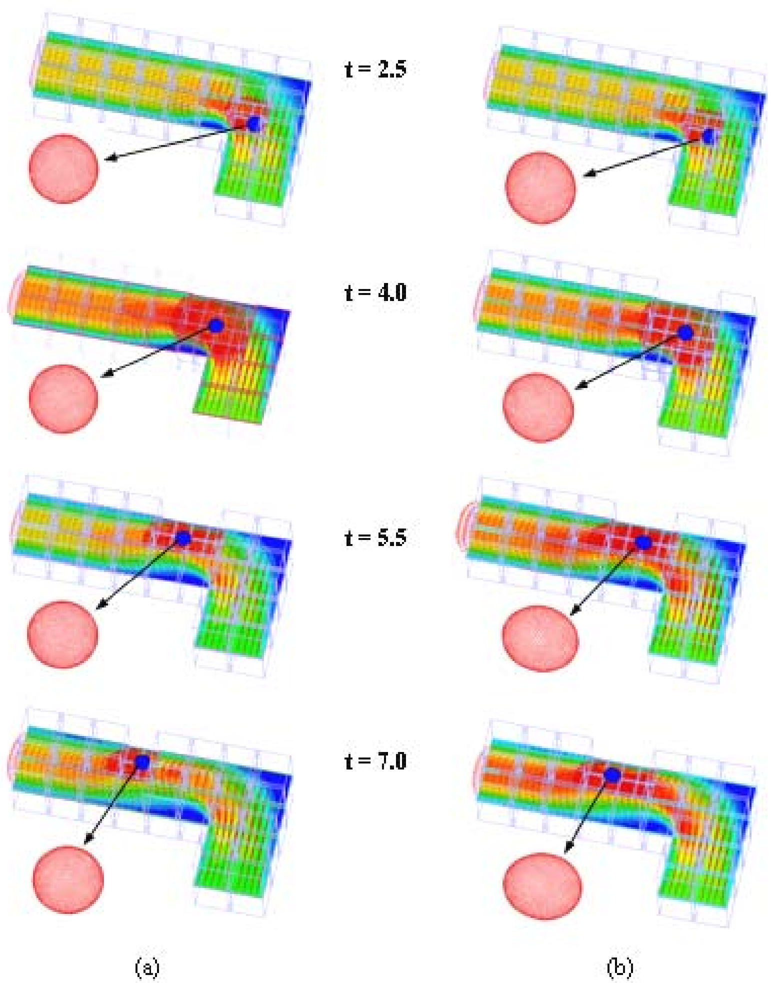


Figure 4: The change of droplet locations and shapes in the L-shaped channel due to the effect of Bond numbers: (a) Bo=0.02, (b) Bo=0.2. The cross-sectional plane indicates the flow velocity contour in the channel.