Simulation of mixing inside a micro-droplet in baffled microchannel by lattice Boltzmann method

Yuhang Fu, Lin Bai, Yong Jin, Yi Cheng*

Department of Chemical Engineering, Tsinghua University, Beijing 100084, P. R. China

**Corresponding author: Dr. Yi Cheng, Email: yicheng@tsinghua.edu.cn*

Highlights

- Established a multiphase LB model to simulate the deformable droplets moving in microchannels
- Investigated the mixing performance inside droplet passing through a baffled channel
- Analyzed the influences of channel geometry and initial distribution of solute inside droplet on mixing efficiency

1. Introduction

Droplet-based reactor is a kind of *soft* reactor that series of single droplets with *deformable shape* move regularly at microlevel, which offers versatile control and flexibility for chemical process with potential applications in fast reactions [1]. Furthermore, the shear force between the rigid channel walls and moving droplets/slugs generates internal recirculation flow, which greatly enhances the species homogenization in the microdroplet reactor. This internal circulation motion has drawn a lot of interest, and various microchannel structures have been designed to introduce extra circulation inside droplets. Considering the complexity of the interfacial dynamics between different phases, especially of micro-droplets in complicated microchannels, theoretical modeling and numerical simulations are necessary to understand the details of multiphase flows. In recent years, there have been some numerical studies focusing on droplet mixing in straight channel, but the mixing study inside deformable droplet is rare.

This work aims to reveal mixing details of microdroplet passing through a baffled microchannel by a multiphase lattice Boltzmann method. Influences of the channel geometry would be discussed. The simulation results are considered to be helpful in strengthening our understanding of internal circulation inside deformable droplet, and also in better guidance of geometry design for enhanced mixing inside droplets.

2. Methods

Lattice Boltzmann (LB) method is implemented here to model the mixing behavior inside a soft droplet-based reactor. This method is a meso-scale one with features of easy parallelization and constitutive versatility. As for simulation of mixing in a micro-droplet system, one LB framework is chosen to catch the fluid dynamic of two-phase flow and another LB model is selected to capture the mixing behavior inside microdroplet. Several LB frameworks have been developed for immiscible two-phase flow, among which an improved color-gradient model [2] is more suitable to simulate micro-droplet system in microfluidics with good implementation of appropriate surface tension term in the macroscopic equations, where each component has different physical properties, i.e. viscosity and surface tension. A LB approach proposed in our previous work is applied for modeling dilute solute here, which modifies a collision operator derived from macroscopic transport equations [3,4]. It has been successfully implemented to study the internal mixing of droplets and slugs moving in microchannel [5].

3. Results and discussion

Microchannel structures studied in this work are shown in Figure 1(a). There are two straight channels with different channel width, and then there is one baffled channel, which is an interval combination of the former two. As can be imaged, the shape of a droplet would change dynamically when it passes through the baffle. The revolution of fluid circulation inside droplet has a great impact on the mixing performance. As one of the examples shown in Figure 1(b), the circulation becomes stronger due to the existence of the baffle, while the solvent transport between the upper part and the lower part of droplet is still not obvious and therefore solute positions inside droplet is another key point for mixing intensification.

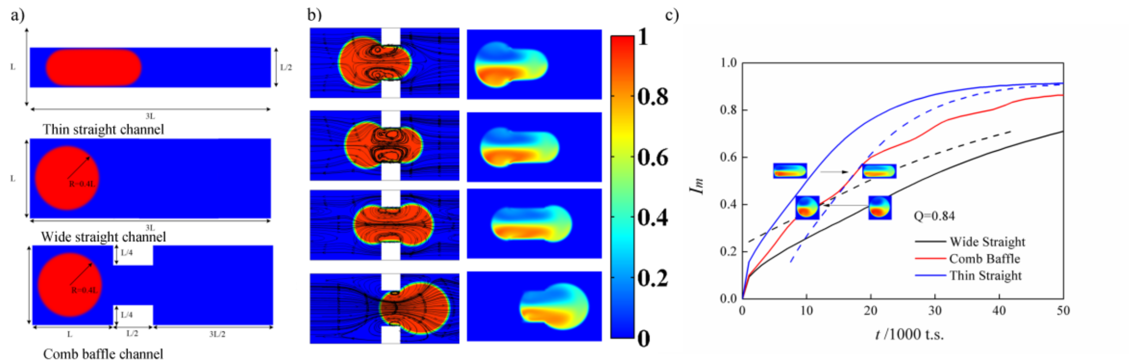

Figure 1. (a) Geometry setting (b) Typical view of streamline and solvents distribution (c) Evolution of Intensity of mixing

In order to quantify the mixing performance, we employ the intensity of mixing (I_m) (ranging from 0 to 1, value 0 represents a total segregation state whereas value 1 represents a homogeneous mixture state) to evaluate the mixing performance with the same Peclet number equal to 200, as shown in Figure 1(c). According to our numerical results, some of the well acknowledged principles for droplet moving in straight channel are validated and considerable findings for designing or optimizing baffled channel are demonstrated. First, I_m increases as the channel width decreases. The I_m of the baffled channel would locate between the I_m of two straight channels. The growth rate of I_m of baffled channel changes regularly and is the same as that in the equal width channel. Therefore, the growth rate and involving time of I_m could be adjusted by the baffle width and length respectively. On the base of the above droplet moving study, we further investigate the effect of initial distribution of solute inside droplet. The results confirm that initial distribution of solute is another factor to determine the mixing efficiency. Mixing between the upper part and the lower part of droplet can be modulated by adjusting the distribution of solute. Detailed results will be given in a full manuscript.

4. Conclusions

We established a multiphase LB model for describing the mixing behavior in a soft droplet-based reactor passing through baffled microchannel. Two LB model frameworks were adopted for bulk phase and solvent respectively. Influence of baffle length and solvent initial positions were investigated in detail. Results show that the mixing performance could be modulated by changing baffle structure after knowing the mixing performance in the straight channel without baffle, which were directed to design and optimize baffle structure and length with desired mixing conditions.

References

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Keywords

Microfluidics, Soft droplet-based reactor, Lattice Boltzmann method, Mixing performance