Abstract
Mixing of analytes and reagents in microfluidic devices is often crucial to the effective functioning of lab-on-a-chip. It is possible to affect the mixing in microfluidics by intelligently controlling the thermodynamic and chemical properties of the substrate surface. Numerous studies have shown that the phase behavior of mixtures is significantly affected by surface properties of microfluidics. For example, the phase separation between the fluids can be affected by heterogeneous patterns on the substrate. The patterned surface can offer an effective means to control fluid behavior and in turn to enhance mixing.

In this study, we numerically studied the effect of optimum surface pattern on mixing in a microchannel and found that the flow oscillation was enhanced apparently when the ratio of hydrophobic and hydrophilic boundary follows certain ratios.

1 Introduction
It is well known that the Reynolds number Re is low in typical microfluidic channel, and the flow is laminar under normal conditions, especially for liquids. Therefore in a microchannel the mixing of binary or multicomponent fluid stream is difficult without the turbulence mixing mechanism, and the mixing due to pure molecular diffusion mechanism may take considerably long time. Meanwhile, mixing in lab-on-a-chip or µTAS (micro total analysis system) is responsible for preprocessing, sample dilution, or reactions between samples and reagents in particular ratios [22]. The initial concept of lab-on-a-chip, or “miniaturized total chemical analysis system,” has been accredited to Manz et al. [19], who proposed the use of integrated microfabricated devices for sample pretreatment, separation, and detection for chemical analysis. Now lab-on-a-chip is becoming an increasingly familiar term used to connote the miniaturization of chemical, biological and biochemical analyses, environmental chemical assays, electrochemistry, thermocapillary pumping, and electro-osmotic flow [1, 8, 9, 20, 32]. The ability to create structures and patterns on micro and smaller length scales has triggered a wide range of scientific investigation, as well as the development of many devices to transport and manipulate fluids and pattern surfaces. Recently studies on patterned surfaces [7, 12, 13, 14, 26] revealed interesting phenomena that can be exploited to control liquid motions in microfluidic devices.

Since Qian et al. [23] brought forth the simple lattice Boltzmann equation based on the single relaxation time model for collisions [2], the model has become the most popular, and been successfully applied to various complex physical processes, such as the interfacial dynamics and multiphase flows [10, 25], flows through porous media [3, 24], reaction-diffusion systems, and other complex systems. However, numerical simulation for microchannel about micro-devices is one of the recent new frontiers of computational fluid dynamics (CFD) and lattice Boltzmann method (LBM). Meanwhile, studying or simulating the multiphase fluids, multi-component fluids and phase transitions in micro- and nanochannel by LBM has increased significantly in recent years. Many of lattice Boltzmann models for multiphase fluids come forth that based on mean-field interaction, or two-component lattice gas model, or using the free-energy approach, or using the idea of level-set [10, 11, 27]. In 1998, Chen et al. [4], through the comparison with a macroscopic two-phase fluid flow model suggested by Nadiga and Zaleski [21], derived a lattice Boltzmann equation from the continuous Boltzmann Bhatnagar-Gross-Krook (BGK) equation with an external force term. Recently, Luo, and Luo and Girimaji [15, 16, 17] have rigorously obtained the LBM model for multicomponent fluids based on kinetic theory by Chapman-Enskog analysis. Verberg et al. [31] used a lattice Boltzmann model to carry out numerical study of the flow pattern of binary fluids confined between rough, chemically heterogeneous surfaces. chew et al. [6] presented a 3D lattice Boltzmann BGK model for simulation of microflows with heat transfer in a rectangular microchannel.

In this paper, we applied Lou and Girimaji’s model [15, 16, 17] to study the optimum surface pattern for binary fluids mixing in a microchannel. The surface is arranged alternatively with either hydrophilic and hydrophobic features. Our work is motivated by the golden mean phenomenon in science, mathematics and nature, and the objective is to investigate the effect of golden mean of micro mixing. In the following, Section II simply states binary-fluid mixing lattice Boltzmann model under the isothermal assumption suggested by Luo and Girimaji [15, 16, 17]. Section III presents the mixing boundary conditions of optimum surface pattern. In section IV, we design a T-type microchannel to enhance fluids mixing effectively. The T-type channel can combine two fluid streams, in which the streams are parallel to each other in the microchannel, and the alternating surface pattern enhances the mixing effectively. Then Section V gives the conclusion.

2 Lattice Boltzmann model for binary mixtures
According to the kinetic theory of gas mixture, Luo and Girimaji [15, 16, 17] proposed the LBM with binary fluids. Similar to single component LBM equation, one can derive N simultaneous equations for a system of N species, therefore the Boltzmann equations for a binary species system are:

\[ \frac{\partial f_\alpha(x,t)}{\partial t} + \xi \cdot \nabla f_\alpha(x,t) + a_\alpha \cdot \nabla \cdot f_\alpha(x,t) = Q^{\alpha\alpha} + Q^{\alpha\beta}, \]

(1)

where \( f_\alpha \) is the probability distribution function, \( \xi \) is the particle velocity, \( \alpha \) and \( \beta \) represent the two species, \( Q^{\alpha\alpha} \) and \( Q^{\alpha\beta} \) are the collision term due to the interaction between two different species \( \alpha \) and \( \beta \), \( \alpha \neq \beta \). \( Q^{\alpha\alpha} \) and \( Q^{\alpha\beta} \) are the self-collision term. The lattice Boltzmann equation can be discretized as follows:

\[ f^{(n)}(x + e_\alpha \delta t, t + \delta t) - f^{(n)}(x, t) = J^{\alpha\alpha} + J^{\alpha\beta} = F^{\alpha\alpha} \delta_\alpha \delta_\beta \]

(2)

The self-collision term is derived similarly to single fluid LBM, and also adopts the BGK model. Under the isothermal assumption of the system, the cross-collision is derived a two-fluid theory. At the right-hand-side the terms of the collision equation are:

\[ J^{\alpha\beta} = -\frac{1}{\tau_\alpha} \left[ f^{(n)} - f^{(n)(0)} \right]. \]

(3)

In the right-hand-side of the collision equation (4), the first term represents the particle distribution function of the binary mixture, \( f^{(n)(0)} \) represent the single phase mixture at equilibrium, \( f^{(n)} \) represent the distribution function of the mixture at time \( n \) and \( n+1 \). \( f^{(n)(0)} \) represent the equilibrium distribution function of the mixture at time \( n \) and \( n+1 \). The equilibrium distribution function of the mixture is defined as follows:

\[ f^{(n)(0)} = \frac{1}{N} \sum_{\alpha} \frac{N^{\alpha}}{Z^{\alpha}(x,t)} \left[ f^{(n)}(x + e_\alpha \delta t, t + \delta t) \right] \]

(4)

1 Introduction

1.1 Reynolds number

The Reynolds number Re is a dimensionless number that describes the ratio of inertial force to viscous force and is a key parameter in fluid dynamics. It is defined as:

\[ Re = \frac{\rho u L}{\mu} \]

where \( \rho \) is the density, \( u \) is the velocity, \( L \) is the characteristic length, and \( \mu \) is the dynamic viscosity. For a typical microfluidic channel, the Reynolds number is usually very low, typically less than 10, indicating that the flow is laminar and not subject to turbulence.

1.2 Microfluidics

Microfluidics is a field that deals with fluids at microscale dimensions. It is used in various applications such as lab-on-a-chip devices, microfluidic sensors, and microfluidic reactors. In lab-on-a-chip devices, microfluidics is used to manipulate small volumes of fluids and to perform chemical and biological analyses.

2 Lattice Boltzmann model for binary mixtures

2.1 LBM for single fluid

The Lattice Boltzmann method (LBM) is a computational method used to simulate fluid flow. It is based on the Boltzmann equation, which describes the evolution of the distribution function of particles in a fluid. The LBM is a discrete version of the Boltzmann equation, which is solved on a lattice.

2.2 LBM for binary fluids

The LBM for binary fluids extends the single fluid model to include two different species. The collision term for binary fluids is given by:

\[ J^{\alpha\beta} = -\frac{1}{\tau_\alpha} \left[ f^{(n)} - f^{(n)(0)} \right]. \]

(4)

where \( f^{(n)} \) is the distribution function of the mixture at time \( n \) and \( f^{(n)(0)} \) is the equilibrium distribution function of the mixture at time \( n \) and \( n+1 \). The equilibrium distribution function of the mixture is defined as follows:

\[ f^{(n)(0)} = \frac{1}{N} \sum_{\alpha} \frac{N^{\alpha}}{Z^{\alpha}(x,t)} \left[ f^{(n)}(x + e_\alpha \delta t, t + \delta t) \right] \]

(5)

The equilibrium distribution function is obtained by solving the Boltzmann equation for a single phase mixture at equilibrium.

3 Numerical results

3.1 Binary fluids in a microchannel

The LBM for binary fluids is used to simulate the mixing of two different species in a microchannel. The results show that the mixing is enhanced by the alternating surface pattern, which is consistent with the analytical results.

4 Conclusion

The LBM for binary fluids is a powerful tool for simulating mixing in microfluidic devices. The results show that the mixing is enhanced by the alternating surface pattern, which is consistent with the analytical results. Further studies are needed to understand the optimal surface pattern for different mixing conditions.
\[ J_{\alpha}^{eq} = -\frac{1}{\tau_D} \rho_s \frac{\sigma(\epsilon_{\alpha} - u)}{\rho \delta_c c_s^2} \left( (u_{\alpha} - u) \right), \quad (5) \]

\[ F^{eq}_{\alpha} = -w_\alpha \sigma_{\alpha} \frac{\epsilon_{\alpha} - u}{c_s^2}, \quad (6) \]

\( F^{eq}_{\alpha} \) represents the forcing term, \( \rho_s \) and \( \rho_c \), and \( u_\alpha \) and \( u \) are the mass densities and flow velocity for species \( \alpha \) and \( \gamma \), respectively. \( \alpha \) is the acceleration set. \( \rho \) and \( \omega \) are the density and velocity of the mixture fluid, which are defined as \( \rho = \rho_s + \rho_c \) and \( \omega = \omega_s + \omega_c \) respectively. In the binary fluid mixing model, the different viscosities of the two components are related to the \( \tau_D \) and \( \tau_c \), respectively. The cross-collision term determines how strong the diffusion effect is of the miscible or immiscible mixture, so the miscibility of the mixture can be adjusted easily by adjusting the collision coefficient \( \tau_D \). For simulating miscible mixtures, \( \tau_D \) should be less than 0.5. On the contrary, for simulating miscible mixtures, \( \tau_D \) should be more than 0.5. Therefore the viscosity and the diffusion of component fluid mixture are conveniently controlled by the clear physical insight. Zhu et al. [34] simulated miscible fluid mixtures successfully using LBM and found that the collision coefficient \( \tau_D \) has significant effect on the fluid mixtures. When \( \tau_D \) approaches 0.5, the obvious contact surface can be identified between the fluids.

The equilibrium distribution function \( f^{eq}_{\alpha}(0) \) is defined as

\[ f^{eq}_{\alpha}(0) = f^{eq}_{\alpha}(0) + \frac{1}{\epsilon_{\alpha}} \left[ (\epsilon_{\alpha} - u) \right], \quad (7) \]

\[ f^{eq}_{\alpha}(0) = w_{\alpha} \rho_{\alpha} \left[ \frac{\epsilon_{\alpha} + u}{c_s^2} + \frac{\epsilon_{\alpha} - u}{c_s^2} - u \cdot u \right], \quad (8) \]

For the \( DQ_2 \) model, \( \epsilon_{\alpha} \) is given by

\[ \epsilon_{\alpha} = \begin{cases} (0,0) & (\alpha = 0) \\ (0,0,1,0,1) & (\alpha = 1, \ldots, 4) \\ (1,0,0,1) & (\alpha = 0, \ldots, 5) \\ (1,0,0,1) & (\alpha = 0, \ldots, 8) \end{cases} \]

and \( w_0 = 4/9 \). \( w_{\alpha,2,3,4} = 1/9 \), \( w_{5,6,7,8} = 1/36 \).

3 Boundary conditions for the system

In this study, we simulate micro-channel fluid, in which the slip and no-slip boundary is used alternately. That means the concurrence of hydrophilic and hydrophobic wall, named composite boundary. The hydrophilic wall is bounce back and the other is specular reflection boundary [28, 29, 30, 33]. As shown in Figure 1, node A indicates the bounce back condition, the \( f_{s}, f_{s}, f_{s} \) are reflected to \( f_{s}, f_{s}, f_{s} \), respectively. Node C indicates the reflection condition, the \( f_{s}, f_{s}, f_{s} \) become \( f_{s}, f_{s}, f_{s} \), respectively. That means the angle of incidence is equal to the angle of reflection. This case is for perfect slip at the wall that no shear forces will be transmitted and their tangential momentum will be conserved. Node B is the joint node between hydrophilic and hydrophobic boundary conditions. The left side of node B is the bounce back boundary condition and the right side is the specular reflection boundary condition.

The outflow boundary condition is applied at the outlet and the velocity boundary condition is applied at the inlet. The inlet boundary conditions for binary fluid model can be derived according to the methods of Chen et al. [5], Maier et al. [18], and Zou et al. [34]:

\[ f_1 = f_1 + \left( f_1^{eq} - f_{1}^{eq} \right), \quad (10a) \]

\[ f_2 = f_2 - \left( f_2^{eq} + f_{2}^{eq} \right), \quad (10b) \]

\[ f_1 = f_1 + \frac{1}{2} \left( f_{1}^{eq} - f_2^{eq} \right), \quad (10c) \]

\[ \rho_{\alpha} = f_{\alpha} + f_{\alpha} + 2 \left( f_{\alpha} + f_{\alpha} + f_{\alpha} \right) \frac{1}{1 - U_r}. \quad (10d) \]

4 Results and Discussion

In this study we use two-dimensional binary-fluid lattice Boltzmann model to examine the effect of boundary pattern on the mixing behavior of two partially immiscible fluids, A and B, which pass through a T-type microchannel as shown in Figure 2. The width of the mixing microchannel is \( h_1 \) and the length of the main channel is \( L \). The ratio of the width \( h_1 \) to the length \( L \) is 1.20. Figure 2 shows the schematic view of the micro channel. The \( h_1 \) denotes the length of the hydrophilic boundary and \( h_1 \) indicates the length of the hydrophilic boundary. The inlet velocity profile is parabolic and the maximum velocity is the same (i.e., \( U_{max} = 0.01 \)) for the two fluids at their entrance, respectively. The collision coefficient, \( \tau_D \), of the binary-fluid mixing lattice Boltzmann model is defined as 0.49999 for simulating immiscible fluids mixing, and the viscosities of the two different species fluids are 1.5 and 1.5001, respectively. These parameters can satisfy the immiscible requirement and make an obvious contact surface between fluids.

The viscosity of the species is equal to \( c_s^2 (\tau - 1/2) \mu_0 \), and the Re is defined as \( Re = (U/L)/\nu \). The gravity force constant is zero.
Figure 3 shows the comparison of streamlines and density contours between no-slip boundary and composite boundary conditions. It indicates clearly that the combined surface pattern can enhance the mixing behavior significantly. For no-slip boundary condition, the streamlines and density contours are typically stratified, indicating the diffusion is dominant in the micro channel. When the surface is patterned by hydrophilic and hydrophobic boundaries, the flow is obviously oscillating which would enhance the mixing definitely.

The physics of the enhancement of the mixing by surface pattern is to perturb the flow by fluctuating boundary conditions, therefore the length of the surface pattern and the width of the entrance would affect the mixing greatly. To investigate the effect of pattern parameters on the mixing behavior, we define $\beta = h_1/h_2$. Figure 4 shows the visualized species density contours at $\beta = 1.6$ with different ratio of hydrophilic length to entrance width, $h_2/h_3$. The $h_2/h_1$ has significant influence on the mixing behavior, when the $h_2/h_1$ is 0.5, the mixing effect is very weak; with increasing $h_2/h_1$ to 1.6 and 2.0, the mixing effect becomes significant. The most likely explanation of this phenomenon is that the perturbation from the boundary needs enough space to develop. If the frequency of the perturbation from the boundary is too high, i.e., if the length of the surface pattern is too short, then the mixing would be suppressed; if the frequency of the perturbation from the boundary is too low, the mixing would be certainly weak. This would provide us a hint there should exist an optimum spacing ratio for the micro mixing.

To further study the effect of the surface pattern on mixing behavior, Figure 5 shows the visualized species density contour at $h_2/h_3 = 1.0$ with different ratio of hydrophobic to hydrophilic length, $\beta$. Similar to Figure 4, when $\beta$ is lower, the mixing is weaker; with increasing $\beta$, the mixing behavior is apparently enhanced.

To quantify the mixing behavior, we use the oscillating velocity ratio between y-direction velocity root-mean-square value and inlet velocity ($U_{y,RMS}/U_{in-mean}$) to express the fluid mixing intensity. The velocity root-mean-square is defined

$$U_{y,RMS} = \sqrt{\frac{\sum (U_y - \bar{U}_y)^2}{n}}$$ (11)

Figure 6 shows the variation of the oscillating velocity ratio ($U_{y,RMS}/U_{in-mean}$) along the centerline of the channel with different surface pattern parameters. Generally, when $h_2/h_1 < 1.0$, the oscillating velocity ratio is quite low, indicating a weak mixing behavior. With $h_2/h_1 = 1.0 - 1.6$, the oscillating velocity ratio reaches its maximum; when further increasing $h_2/h_1$ to 2.0, the oscillating velocity ratio decreases apparently. This indicates that $h_2/h_1 = 1.0 - 1.6$ is the optimum ratio.
The ratio between hydrophobic and hydrophilic length, $\beta$, is also crucial to the micro mixing behavior. When $h_2/h_3 = 1.0$, i.e., the hydrophilic length is the same as the entrance width, the oscillating velocity ratio reaches the maximum at $\beta = 1.6$. It is interesting to note, with increasing $h_3/h_1$, the maximum oscillating velocity ratio occurs at lower surface pattern ratio $\beta$. For example, when $h_2/h_3 = 1.5$ and $1.6$, the optimum $\beta$ is around 1.2. The ratio between hydrophobic and hydrophilic length, $\beta = h_1/h_2$, at different ratio of no-slip length to entrance width, $h_2/h_1$

From the discussion of Figure 6, it seems that the golden mean (1.618) plays some role in micro mixing enhancement. To further evaluate the effect of this optimum number, the effect of hydrophobic length is also studied. Figure 7 shows the variation of the oscillating velocity ratio ($U_{y-RMS}/U_{mean}$) along the centerline of the micro channel with $\beta$ at different ratio of hydrophobic length to entrance width. It is surprising to note, when the ratio of hydrophobic length to entrance width is 1.6, $h_1/h_3 = 1.6$, the velocity oscillation reaches its maximum within a quite wide range of $\beta (= 1.0 - 1.6)$. At other $h_1/h_3$ ratio, the oscillating velocity is either lower or reaches the maximum within a very narrow band of $\beta$. For example, at $h_1/h_3 = 2.0$, the oscillating velocity reaches its maximum at only $\beta = 1.3$; at $h_1/h_3 \leq 1.0$, the oscillating velocity becomes apparently lower. This indicates that the golden mean number 1.618 is the optimum surface pattern parameter in micro mixing. The most likely explanation of this amazing phenomenon is that the slip perturbation on the wall can be delivered to the middle within just $1.6h_3$ if the slip section is shorter, the perturbation can not be developed fully; if the slip section is longer, then the perturbation from both sides would interact and suppress each other.

5 Conclusion

The binary fluid mixing in a microchannel is numerically studied using lattice Boltzmann method. To enhance the micro mixing, the surface pattern is designed as alternatively hydrophobic and hydrophilic conditions. The simulation results lead to the following conclusions:

1. The composite boundary conditions can enhance the micro mixing effectively. The entrance width, the hydrophobic and hydrophilic length together with their ratios has significant influence on the micro mixing.
2. There exist the optimum ratios between the hydrophilic length and the entrance width, i.e., when this ratio, $h_2/h_3 = 1.0 - 1.6$, the oscillation velocity ratio can reach its maximum value.
3. The golden mean number is the optimum ratio between hydrophobic length and entrance width, in which the micro mixing can be enhanced significantly.
4. The ratio between hydrophobic and hydrophilic length, $\beta$, is also crucial, the optimum ratio $\beta$ may vary with different $h_2/h_3$.

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References


