Numerical Simulation of Mixing Performance for A Design Three Dimensional Chaotic Micromixer

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ABSTRACT

Obtaining homogenization and thorough mixing of reagents or solutions is an essential process in microfluidic devices. However, mixing process in the micro scale level has extremely low efficiency due to purely diffusive mixing method. A three-dimension chaotic micromixer, Diagonal Ridge Micromixer(DRSRM)，is proposed in this paper. It has advantage for easy fabrication and integration based on conventional microfabrication techniques. We employed CFD simulation to investigate the mixing performance. Based on the results of numerical simulation, this DRSRM micromixer demonstrates outstanding mixing capability for normal and hard-to-mix fluids over the wide range of inlet velocity from 1.946×10^{-4}m/s to 2.919m/s and from 3.73×10^{-3}m/s to 3.73m/s, repectively. The chaotic advection can be induced to efficiently boost fluids mixing when inlet velocity is higher than the critical inlet velocity of 0.3892m/s and 1.946×10^{-2}m/s in the DRSRM with 2:1 and 1:1 width-depth ratios of inlet channel, respectively. When the inlet velocity is lower than the critical inlet velocity, the mixing performance is dominated by passive particle diffusion. Through absence of the chaotic advection, remarkable short mixing lengths can still obtained relying on impactful splitting-combination, stretching and torturing mixing mechanism in the DRSRM.

Keywords: Passive micromixer, Chaotic advection, Secondary flow, Vortex

1. INTRODUCTION

In the past decades, micromixer, one of the most important components in microfluidic devices, has demonstrated their capabilities in a wide application domain ranging from micro-total-analysis system (μTAS) or lab-on-chip (LOC) biotech devices to industrial applications in replacing traditional batch synthesis of a chemical to continuous reaction(Falk and Commenge, 2010)(Park et al. 2010). These devices require integration, automation, and miniaturization of liquid handling, sample processing and analysis to facilitate fast diagnostics, low cost, operation by minimally trained personnel, and low contamination risk (Chen et al. 2010). However, fluids in such small scale are difficult to be well mixed at short distance due to small Re numbers of 200 or less, where only a laminar flow is activated and thus high Péclet numbers is difficulty in applying conventional approaches used at the macrosacles(Gao et al. 2009) (Chen et al. 2011). In the absence of turbulent flow, viscosity inhibits the flow instability that makes fluids at the contact interface difficult to achieve advection effect to enhance the mixing. Under this condition, fluid mixing only relies on the effect of molecular diffusion. In a simple micromixer composed of smooth straight microchannel, diffusive mixing in microchannel requires more than several tens of centimeters to achieve acceptable mixing performance, which is unacceptable in a compact microfluidic devices.

Micromixers can be divided into active and passive micromixer according to the operating condition. Active micromixer introduces external energy, such as acoustic, thermal, electrokinetic, dielectrophoretic, and magneto, with complex control system to improve the mixing efficiency when fluids flowing through microchannels. Even though active micromixers can obviously speed up micromixing process, integrating and implanting the corresponding incentive components or circuits into the microfluidic devices would require complex production processes which would be difficult to achieve industrial production and contrary to the purpose of low cost and small size. On the other hand, the passive micromixer completely depends on the specially designed structure of microchannels to boost mixing efficiency. It has advantage of relatively simple fabrication, small size, low cost and easy operation. Lamination of interface and chaotic advection are two main types of mixing mechanisms in passive micromixer. Laminating micromixer adopts laminated injection, droplet injection or split-and-recombination mixing method (SRM) to exponentially increase contact interface while two or more fluids flowing continually in the microchannels. Otherwise, when the inertial force of a fluid flows against a structural disturbance in the microchannel, the secondary flow stretches and folds the contact interfaces to create chaotic advection which increases as the flow rate increase (Lee and S.Lee, 2008). Comparing to lamination, chaotic advection is a better method to increase fluid mixing efficiency through stretching, folding, bending and twisting fluids. Conventional design idea of chaotic mircomixer depends on implanting simply obstacles, such square block or cylinder, in channels. However, it requires the Re number to be greater than 200(Wong et al. 2004). To induce chaotic advection at low Re number, we need to introduce more complicate geometries, such as connected-groove(Yang et al. 2004), staggered herringbone bones (Kee et al 2008)(Choudhary et al. 2011), diamond-shaped obstructions(Bhagat et al. 2007), crosswise ridge and three dimension(3D) structure formed by the multilayers.

In this paper, we present a 3D micromixer that is based on coupling principle of splitting-recombination and chaotic advection. The diagonal ridges on the upper and bottom layer of the micromixer are used to stretch and rotate the flows. Thus, we refer to this design as DRSRM. In the appropriate inlet velocity, these ridges would help induce the chaotic advection to accelerate fluid mixing. Furthermore, the simply design allows it to be easily integrated into microfluidic system with standard microfabriation techniques. Numerical simulation is conducted to investigate the mixing performance of the micromixers.

2. MICROMXIERS DESIGN

If possibility of reducing the mixing length, there must be transverse components of flow that stretch and fold volumes of fluid over the cross section of the channel(D.Stroock et al. 2002). Hence, fluids can more effectively mix in 3D micromixer due to prompting fluids to fold and rotate in the parallel and transverse directions better than planar or 2D micromixer. Combining advantages of the simple fabrication method of planar micromixer and relatively high mixing efficiency of 3D micromixer, the design DRSRM composes of two layers fabricating by the one simple pattern. As shown by Figure 1, the length of one unit in DRSRM is 310μm, the width and length of mixing chamber are 150μm and 200μm, respectively. And the widths of inlets and ridges are 50μm and 20μm, respectively. The micromixer is composed of the upper and lower layers. The depth of layer is designed as 25μm and 50μm. The ridges and layer have the same depths. Hence, both of these can be fabricated through one process.

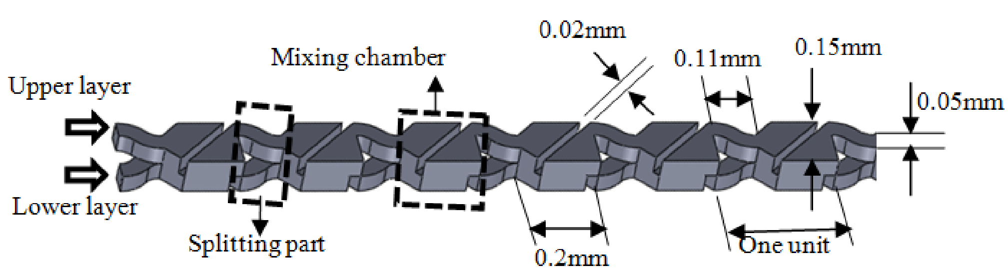

Figure 1 3D Structure of DRSRM

3. NUMERICAL ANALYSIS

The property of fluid in the microchannel is considered to be steady and incompressible. Ignoring the body force, the governing equations including the continuity equation, Navier-Stokes equation and species convection-diffusion equation can be described as:

$$\nabla \cdot V = 0 \tag{1}$$

$$\rho V \cdot \nabla V = -\nabla P + \mu \nabla^2 V \tag{2}$$

$$V \cdot \nabla C = D \nabla^2 C \tag{3}$$

where V is fluid velocity vector, ρ is the fluid density, P is the pressure, μ is the fluid dynamic viscosity, C is the species mass concentration and D is the diffusion coefficient of the species.

ANSYS Fluent is employed to solve equation (1) through (3). In the Fluent Solver, we choose pressure-based and time steady laminar flow without reaction mixing; set energy and species transport models on, in which set two fluid concentrations at 1 m/mol and 0 m/mol, respectively. In the boundary conditions, all inlets are set as velocity inlet, static pressure of outlet is chosen at 0 Pa, the wall is set as stationary wall and no slip shear condition. SIMPLIC scheme of solution method is assigned to calculate pressure velocity coupling. For obtaining more accurate result, the second order upwind of momentum and energy is brought to calculate with choosing PRESTO!.

To quantify the mixing performance of fluids, the following equation is employed:

$$\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(C_i - C_\infty)^2} \tag{4}$$

$$\sigma_{max} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(C_0 - C_\infty)^2} \tag{5}$$

$$M = 1 - \frac{\sigma}{\sigma_{max}} \tag{6}$$

The variance of the species in the micromixer is based on the concept of the intensity of segregation. Where σ is the coefficient of mass fraction at a cross sectional plane, N is the number of sample cells in the cross section, C_i is the mass fraction of sample cell i; C_∞ is optimal mass fraction which is 0.5 if the two fluids have the same amount in micromixer, σ_{max} is the maximum of, C_0 is original mass fraction that should be 1 or 0, M is the mixing index, its range from 0 which is no mixing to 1 for complete mixing.

4. SIMULATION RESULTS AND DISCUSSION

In the micromixer, since the streamlines of fluids in the micromixer are difficult to be visualized from both inlets, we separately show the streamlines that represent the fluid injecting into one inlet for a clear understanding of fluid flow in micromixer. As shown in Figure 2, one stream of fluid is injected into the inlet 1, and then it is expanded asymmetrically and distorted in the mixing chamber, as shown in Figure 2(a). Meanwhile, it not only flows through the upper layer but also transfer into the lower layer (Figure 2(b)). Due to the identical structure of upper and lower layers, the fluid flow has the same action but opposite direction in the lower layer. Coupling the above mass transfer of fluids in the mixing chamber, mixing process can be improvement because: first, extensive fluid area could bring lager interfacial area to promote mixing; second, the opposite action of fluids in the upper and lower could induce conflict at the confluent space helping to stretch and rotate fluids to increase contact interface. In the immediate flowing downstream, the partial mixing fluids are rearranged to split into upper and lower sub-flows passing though the two curved channels and flowing into next mixing chamber. This mixing process is repeated in each unit from converged flow to sub-flow.

4.1 COMPARISON WITH SPLITTING-RECOMBINATION MICROMIXER (SRM)

In order to verify the accuracy of our simulation, we compared our SRM result with Fang's(Fang and Yang, 2009) SRM result by using the exact same geometry and fluid properties, in which viscosity is 8.55×10^{-4} kg/ms, diffusivity is 2×10^{-10} m^2/s, and the inlet velocity is 8.5×10^{-3} m/s. The inlet of SRM has a depth of 50μm and width of 100μm. The Re number is 1. Figure 3 shows good agreement between our result and Fang's result, which has been verified by the experimental results.

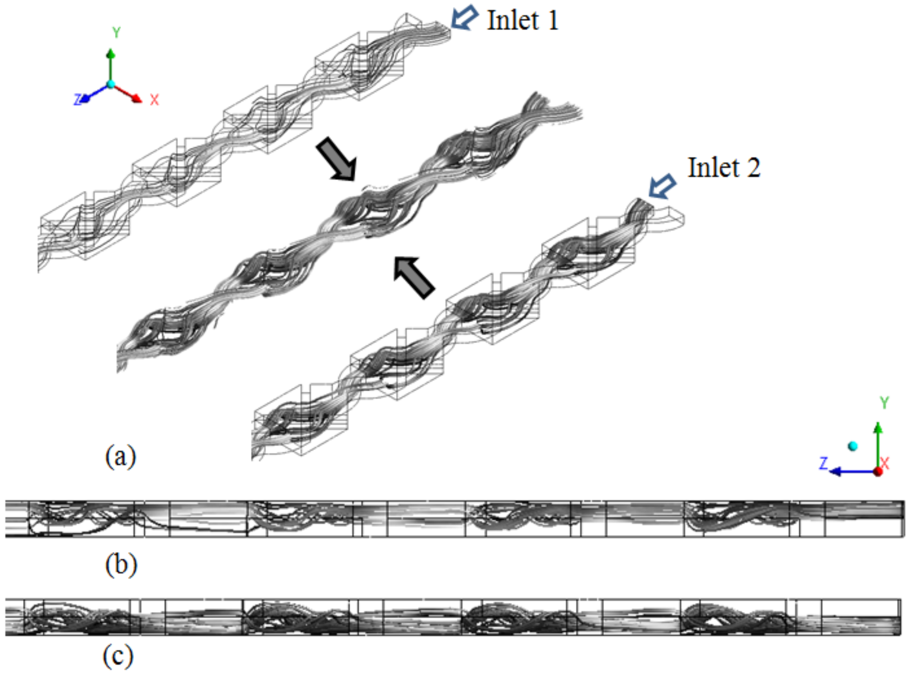

Figure 2 Streamline of the DRSRM, (a) separated streamline from inlet 1 and inlet 2, and coupling streamline without wireframe, (b) side view streamline from inlet 1, (c) side view streamline from inlet 2

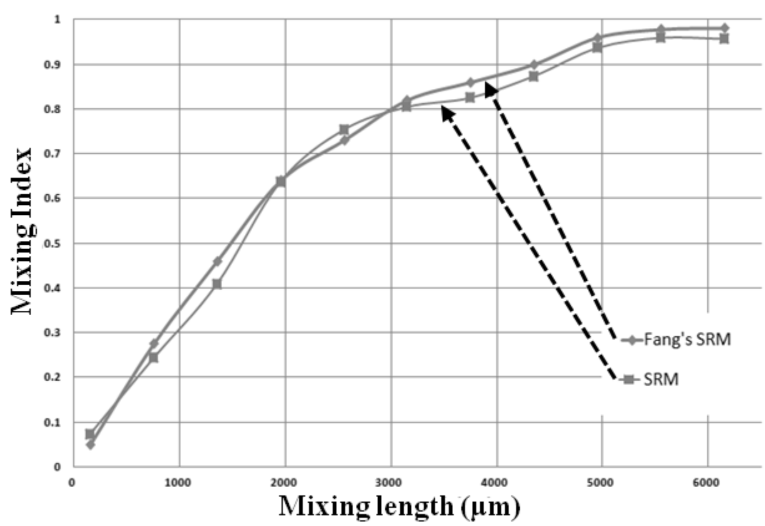

Figure 3 Compared simulation result with Fang's SRM

4.2 PARAMETERS FOR SIMULATION

Two fluids with different inlet velocities will be employed with the purpose of particularly investigating the mixing performance in DRSRM. The properties of both fluids are listed in Table 1. Reynolds number is an important parameter to determine the type of fluidic flow to be turbulent or laminar. Its equation can be defined as following:

$$Re = \frac{\rho V D_h}{\mu} \tag{7}$$

where V is mean velocity of the fluid, μ is the dynamic viscosity of the fluid, ρ is the density, D_h is characteristic linear dimension or the hydraulic diameter of the pipe or channel. In micromixer design, the cross section of microchannel is very small and the speed of fluid flow in the micrchannel is limited. Therefore, the Re number for fluids flow in microchannels is also small. The inlet velocities and corresponding Re numbers for each fluid are shown in

Table *2* and

Table 2 The Re numbers are from 0.01 to 150 which relate to velocities of normal fluid

Velocity(m/s)		**1.946×10^{-4}**	**1.946×10^{-3}**	**1.946×10^{-2}**	**0.1362**	**0.1926**	**0.3892**
Re	**25μm depth**	0.0067	0.067	0.67	4.67	6.67	13.3
	50μm depth	0.01	0.1	1	7	10	20
Velocity(m/s)		**0.9729**	**1.3621**	**1.946**	**2.335**	**2.919**	
Re	**25μm depth**	33.3	46.7	66.7	80	100	
	50μm depth	50	70	100	120	150	

Table 3.

Table 1 Fluid properties

	Density (kg/m^3)	**Viscosity (kg/ms)**	**Diffusivity (m^2/s)**
Normal Fluid	997	9.7×10^{-4}	3.6×10^{-10}
Hard-to-mix Fluid		0.186	9×10^{-13}

Table 2 The Re numbers are from 0.01 to 150 which relate to velocities of normal fluid

Velocity(m/s)		**1.946×10^{-4}**	**1.946×10^{-3}**	**1.946×10^{-2}**	**0.1362**	**0.1926**	**0.3892**
Re	**25μm depth**	0.0067	0.067	0.67	4.67	6.67	13.3
	50μm depth	0.01	0.1	1	7	10	20
Velocity(m/s)		**0.9729**	**1.3621**	**1.946**	**2.335**	**2.919**	
Re	**25μm depth**	33.3	46.7	66.7	80	100	
	50μm depth	50	70	100	120	150	

Table 3 The Re numbers are from 0.001 to 1 which relate to velocities of hard-to-mix fluid

Velocity(m/s)		**3.73×10^{-3}**	**3.73×10^{-2}**	**0.373**	**3.73**
Re	**25μm depth**	0.00067	0.0067	0.067	0.67

	50μm depth	0.001	0.01	0.1	1

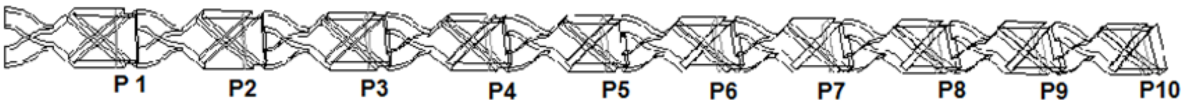

Figure 4 Ten cross sectional planes in DRSRM for mixing indexes calculation

4.3 MIXING SIMULATION FOR FLUID

In order to accurately characterize the mixing performance in the micromixers, 10 cross sectional planes (P1-P10) in the mixing chamber part are chosen to calculate the mixing index, as shown by the Figure 4. Around 900 mesh cells are contained in each cross sectional plane ensuring the accuracy of mixing index calculations.

4.3.1 SIMULATION RESULT OF 25MM-DEPTH-DRSRM AND 50MM-DEPTH-DRSRM

Figure 5 shows the relationship between the mixing lengths and mixing indexes under the different inlet velocities in the 25μm-depth-DRSRM micromixer. When the mixing index reaches to 90%, mixing performance of fluids is considered as complete mixing and the length is counted as the complete mixing length. Figure 7 shows the relationship between inlet velocity and complete mixing length. The curve of 25μm-depth-DRSRM micromixer can be divided into three regions which are shown in Figure 7:

I. The lengths of complete mixing increase from 500μm to 4000μm while the inlet velocities are increasing from 1.946×10^{-4}m/s to 0.3892 m/s. The length of 4000μm is longer than the total length of ten units of the micromixer that we design. Hence, the fluids cannot be completely mixed after flow through the micromixer at the inlet velocity of 0.3892m/s.
II. The complete mixing length quickly reduces to 1050μm with the inlet velocity increasing to 1.362m/s.
III. Between the inlet velocity of 1.362m/s and 2.919m/s; the complete mixing lengths keep constant as 1000μm.

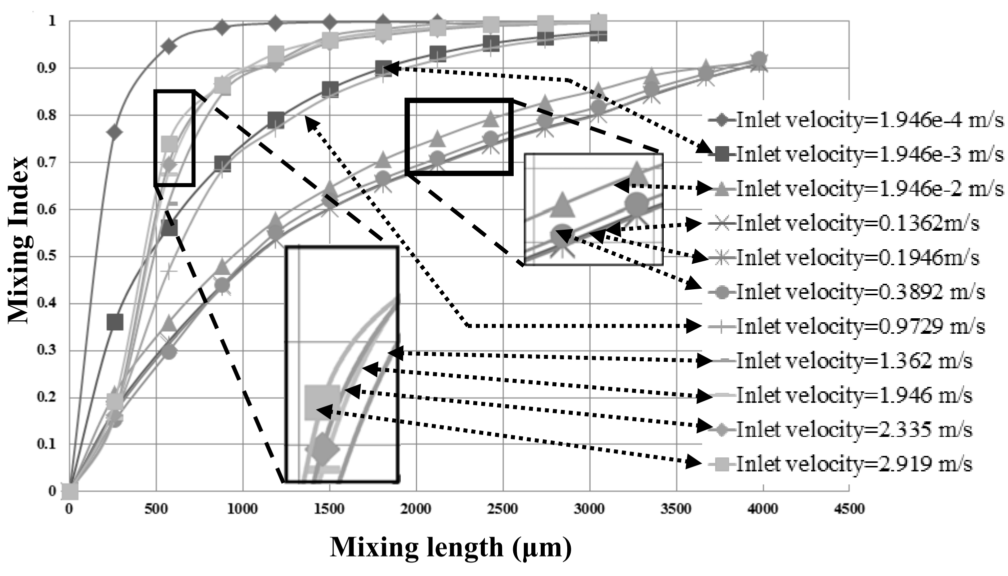

Figure 5 Mixing lengths versus mixing indexes in 25μm-depth-DRSRM using normal fluids

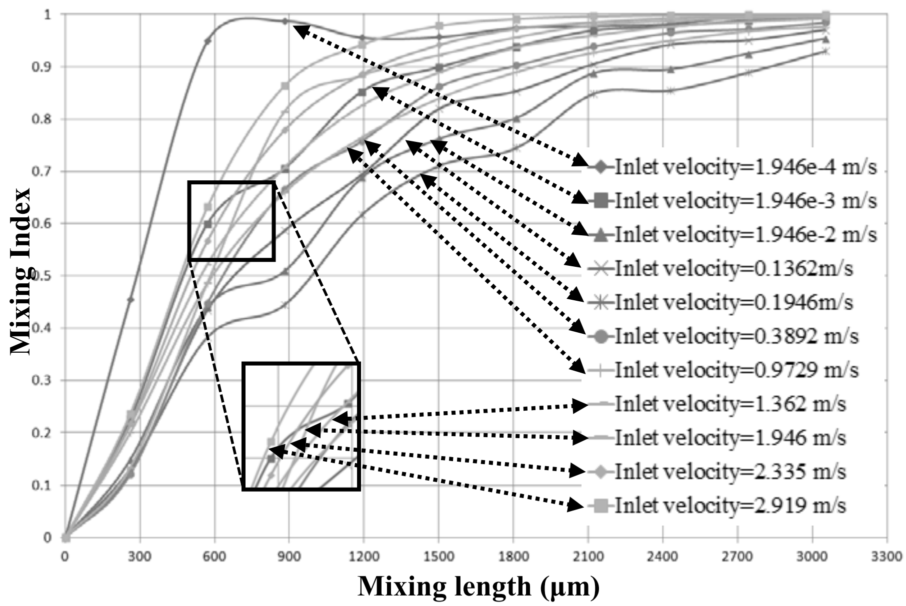

Figure 6 Mixing lengths versus mixing indexes in the 50µm-depth-DRSRM using normal fluids

The above results show that 25µm-depth-DRSRM can't achieve complete mixing fluids after passing through ten units of micromixer at some inlet velocities. Therefore, 50µm depth of DRSRM is simulated for further investigation the effect of the depth on the mixing performance.

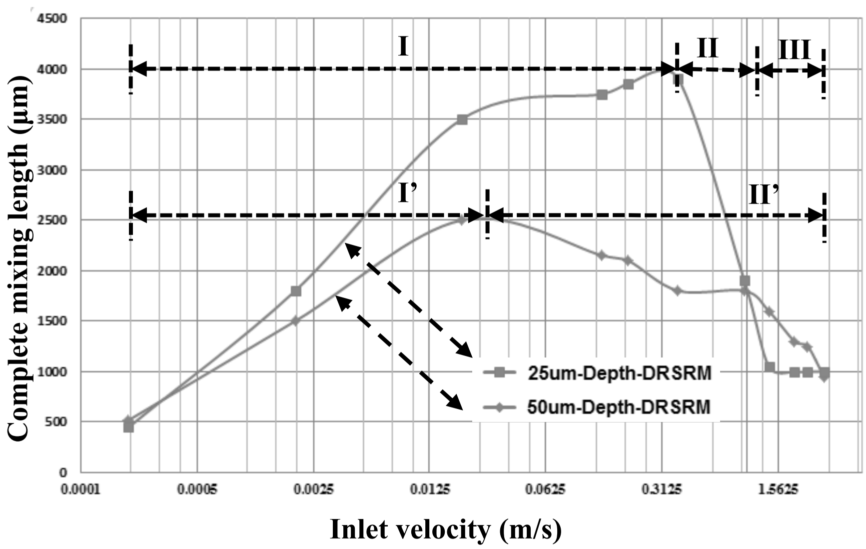

Figure 7 Complete mixing lengths versus different velocities in the two depths of DRSRM using normal fluids

Figure **6** shows mixing lengths versus mixing indexes at different inlet velocities in the 50µm-depth-DRSRM with Fluid 1. The curve of the complete mixing lengths versus different inlet velocities is shown by Figure 7. Two regions of curve are described as following:

I'. While the inlet velocity is increasing from 1.946×10^{-4}m/s to 1.946×10^{-2}m/s, the corresponding complete mixing length also increases. The shortest complete mixing length is 500µm at the inlet velocity of 1.946×10^{-4}m/s.

II'. The complete mixing lengths gradually decrease with inlet velocities increasing from 1.946×10^{-2}m/s to 2.919m/s. The longest complete mixing length is 2500μm when inlet velocity is 1.946×10^{-2}m/s.

Comparing to the results of the 25μm-depth-DRSRM, the better mixing process can be achieved in the 50μm-depth-DRSRM due to the shorter complete mixing lengths are demanded in the range from 1.946×10^{-4}m/s to 0.9729m/s; however, longer complete mixing lengths are demanded in the range from 1.362 to 2.335m/s. At the inlet velocity of 2.919m/s, both DRSRMs are has the similar complete mixing lengths. The critical inlet velocity of 50μm-depth-DRSRM is 1.946×10^{-2}m/s which is much lower than the 0.3892m/s in the 25μm-depth-DRSRM. Therefore, we can consider that the ratio 1:1of width and depth can reduce the critical inlet velocity for readily inducing chaotic advection than ratio 2:1 for our design structure.

4.3.2 VELOCITY CURL

To investigate the mixing phenomenon of each region, vectors of velocity curl in a cross sectional plane at different injection inlet velocities are shown in Figure 8. Upper and lower cross ridges in DRSRM are expected to generate secondary flow or vortex, which can create chaotic advection even under the low Re number. At the velocity of 1.946×10^{-4}m/s, the vortex exists in the middle of the vector of velocity curl in the plane, as shown in Figure 8(a). This situation almost doesn't change even through the inlet velocity increases to 0.3892m/s. Only one vortex in the middle is not efficient enough to reduce the complete mixing length, which is the reason that longer complete mixing length is required as inlet velocity increases in the region I of Figure 7. As shown in Figure 8(b), two vortexes appear on the top right and bottom left when inlet velocity increases to 0.9729m/s, which further rotates and enhances contact interface between fluids. Hence, the complete mixing drastically decrease to 1900μm. While inlet velocity increases to 1.3621m/s (Figure 8 (c)), two vortexes occupy larger space in the plane than them at the inlet velocity of 0.9729m/s, which indicates more chaotic advection is generated and the complete mixing length further decreases to 1050μm. At the inlet velocities of 1.3621m/s and 2.919m/s, the vectors of velocity curl are similar to each other (Figure 8 (d)), therefore, its complete mixing lengths remain unchanged. From these results, it is concluded that: two vortexes appear in the plane obviously boost the mixing efficiency; if without impactful chaotic advection which induce by higher inlet velocity, the better mixing performance can be obtained at the lower inlet with generating the longer diffusion time. Hence, 0.3892m/s is regarded as critical inlet velocity, which is an important parameter for micromxier. When inlet velocity is less than critical one, the fluids mixing mainly depend on passive particle diffusion. But, over the critical inlet velocity, chaotic advection is induced to boost mixing process.

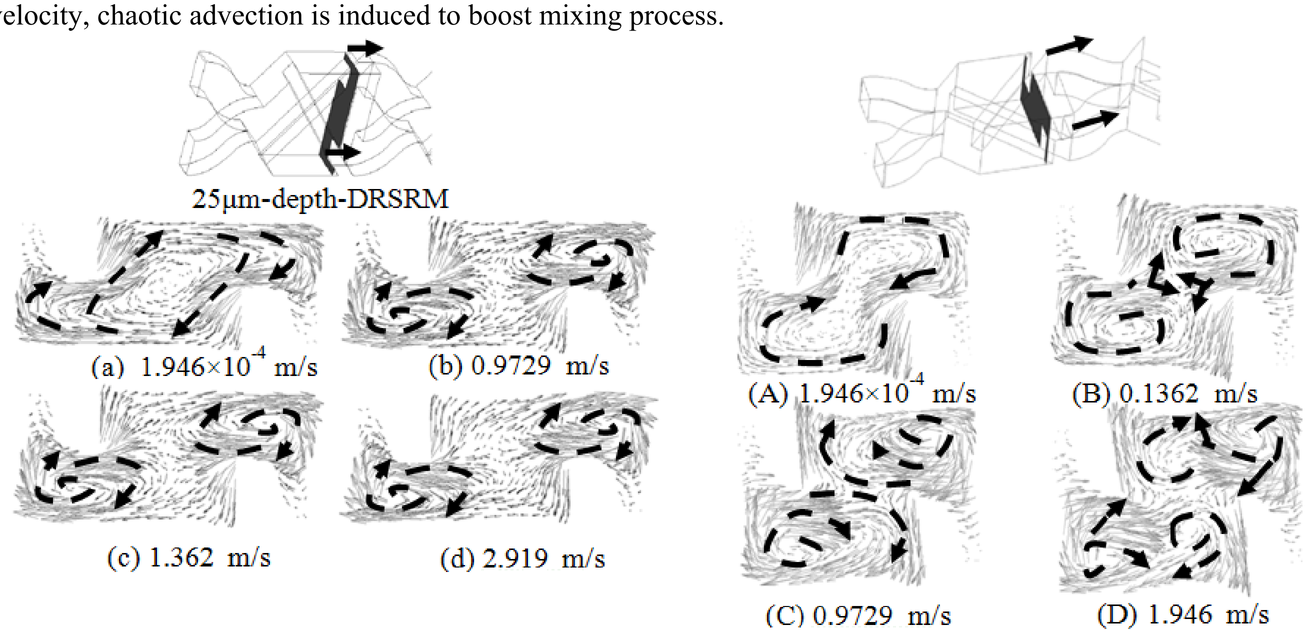

Figure 8 Vectors of velocity curl in cross sectional plane for different velocities in DRSRM

50μm-depth-DRSRM also has the vortexes at different inlet velocities as 25μm-depth-DRSRM. At the inlet velocity from 1.946×10^{-4}m/s to 1.94E-2m/s (Figure 8 (A)), two obscure conjunction vortexes have no capability to prompt mixing process efficiently, thus the complete mixing lengths rise when the inlet velocity increases in this range. Then, two conjunctive vortexes slowly change to totally separate powerful vortexes with the inlet velocity increasing to 0.1362m/s (Figure 8 (B)). Hence, the complete mixing lengths decrease when inlet velocity is higher than1.946×10^{-2}m/s, as shown by the region II' of curve of 50μm-depth-DRSRM in Figure 7. Two vortexes change to four vortexes as inlet velocity increases from 0.9729m/s to 1.946m/s (Figure 8 (C,D)). These four vortexes constantly expand at the higher inlet velocity. Therefore, the complete mixing length keeps decreasing.

4.4 MIXING SIMULATION FOR HARD-TO-MIX FLUIDS

Hard-to-mix fluid is difficult to mix well because it has higher viscosity and the corresponding molecular diffusivity is three orders of magnitude smaller than normal fluid. The viscous force, which is generated by the viscosity, is the main internal force of fluidic flow to impede mixing efficiency because it constantly drains eddy energy and limits the population of vortex. Thus, for improving mixing performance of the high-viscosity fluids, more external energy is required to force flow stretch and rotation to boost mixing efficiency. Increasing inlet velocity is a way to generate more external energy, but it is difficult to impose high inlet velocity in the micromixer due to exponential growth of corresponding inlet pressure is required. High inlet pressure can break the hardware and reduce the lifetime of the micromixer. Moreover, it is well known that high-viscosity fluid requires higher inlet velocity than low-viscosity fluid to achieve same Re number flow in the same dimension of micromixer. Therefore, only 4 inlet velocities from 3.73×10^{-3}m/s to 3.73m/s as shown in Table 3 can generate meaningful results for hard-to-mix fluids. As shown in Figure 9, in the 25μm-depth-DRSRM, the same complete mixing lengths, 4000μm, are obtained at various inlet velocities. In the 50μm-depth-DRSRM, the complete mixing length is 1500μm at the inlet velocity of 3.73E-3m/s; in the range of inlet velocities from 3.73×10^{-2}m/s to 3.37m/s, the complete mixing lengths are all around 2800μm. Thus, we can consider that critical inlet velocity should be higher than 3.73m/s. Through without the chaotic advection, the design micromxiers, relying on impactful splitting-combination, stretching and torturing mixing mechanism, can still obtain such remarkable short mixing lengths which are much more efficiency than the traditional micromixers and other micromixers were mentioned above.

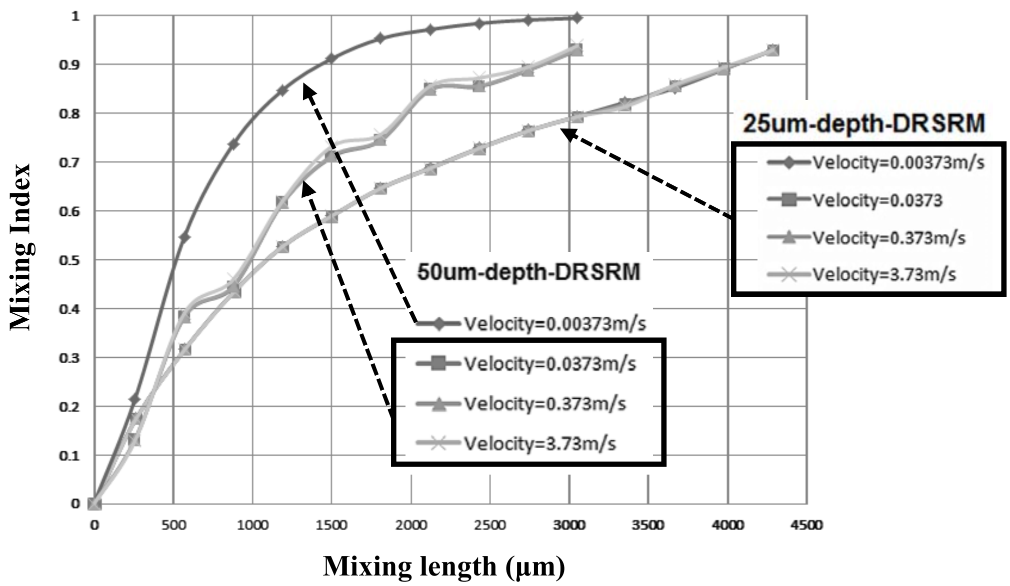

Figure 9 Mixing lengths versus mixing indexes in both depths of DRSRM using hard-to-mix fluids

5. CONCLUSIONS

DRSRM, with two different depths (25μm and 50μm) and two different fluids (viscosity is 9.7×10^{-4} kg/ms and 0.186 kg/ms) are simulated to investigate the mixing performance under the different inlet velocities, which include eleven different velocities from 1.946×10^{-4}m/s to 2.919m/s set for the normal fluid and four different velocities from 3.73×10^{-3}m/s to 3.73m/s set for hard-to-mix fluid. DRSRM can be easily fabricated and integrated into microfluidic devices, and can quickly obtain complete mixing over the wide range of velocity and properties of fluids. The chaotic advection can be induced to efficiently boost fluids mixing when inlet velocity is higher than the critical inlet velocity of 0.3892m/s and 1.946×10^{-2}m/s in the DRSRM with 2:1 and 1:1 width-depth ratios of inlet channel, respectively. When the inlet velocity is lower than the critical inlet velocity, the mixing performance is dominated by passive particle diffusion.

In contrast to the mixing results of the normal fluids, the complete mixing lengths of the hard-to-mix fluids are minor change at wide range of inlet velocity. In the In 25μm-depth-DRSRM, the complete mixing lengths always keep around 4000μm. In the 50μm-depth-DRSRM, the shortest complete mixing length is 1500μm at the lowest inlet velocity of 3.73×10^{-3}m/s, and then it increases to 2800μm and unchanged at the inlet velocity from 3.73×10^{-2}m/s to 3.373m/s. Solely relying on impactful splitting-combination, stretching and torturing mixing mechanism, the design micromxiers can still obtain such remarkable short mixing lengths even through absence of the chaotic advection.

Generally, the design DRSRM micromixer indicates outstanding mixing capability for normal or hard-to-mix fluids. The critical inlet velocity can be decided through changing the width-depth ratio of inlet channel. Based on the DRSRM, the chaotic advection can be induced when inlet velocity over the critical inlet velocity of 0.3892m/s and 1.946×10^{-2}m/s at width-depth ratio of 2:1 and 1:1, respectively. Therefore, engineers can adopt different width-depth ratio or inlet velocity to fulfill their mixing performance demands.

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