Computational Fluid Dynamic Simulation of Liquid–Liquid Mixing in a Static Double-T-shaped Micromixer

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Abstract: The laminar flow structure and mixing performance of T-shaped and double-T-shaped micromixers with rectangular cross-section have been investigated using computational fluid dynamic (CFD) simulation. FLUENT software is used to evaluate the mixing efficiency. The numerical simulation results show that the presented double-T-micromixer is highly efficient over T-shaped micromixer. The performance of double-T-micromixer with and without static mixing elements (SME) is also investigated. The enhancement in mixing performance is thought to be caused by the generation of eddies and lateral velocity component when the mixture flows through these elements. Mixing efficiency as higher as 97% is reached within a mixing length of 320 μm downstream from the first T-junction with the enhancement of three SMEs.

Key words: micromixing; microfluidics; T-shaped micromixer; microfabrication; microreaction; microelectromechanical systems

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1 INTRODUCTION

The term of micromixers refers to mixers with characteristic length scales that are in a micrometer range. A tangible effect of such small dimension is that fluid properties become increasingly controlled by viscous forces rather than inertial forces[1]. On the other hand, reduction of micromixer dimensions leads to a large ratio of surface to volume, which increases heat and mass transfer efficiencies. Heat transfer efficiency allows for fast heating and cooling of reaction mixtures within the micromixers whereby reaction under isothermal conditions with exactly defined residence time can be carried out[2]. The reduction of micromixer dimensions also leads to small Reynolds number (*Re*) of flow, typically smaller than 100, so that flow is essentially laminar. Thus, mixing in micromixers is mainly driven by molecular diffusion with shorter residence time. Micromixers are broadly classified as active and passive types, based on mixing mechanism. In general, active micromixers require power input in order to affect mixing, while a passive one achieves mixing by driving fluids through channels with cleaved geometries.

Due to the simple fabrication technology of passive T-shaped micromixer (T-micromixer) and its easy implementation in a complex microfluidic system, mixing mechanisms of flow in this type of mixers were the focus of many investigations[3–15] (for more, see Mansur et al.[4]). Bökenkamp et al.[3] fabricated a T-micromixer with a 500 μm width that used turbulence as the mechanism for fast mixing between liquid samples. Gobby et al.[5] studied the mixing characteristics of two gases with different viscosities in a T-micromixer through computational fluid dynamic simulation. They reported that as aspect ratio increases, the effect of horizontal wall shear decreases, which leads to symmetrical velocity profiles achieved closer to the entrances of center channel and hence better mixing. Kockmann et al.[6] and Engler et al.[7] carried out numerical studies on mixing in a T-shaped and Y-shaped micromixers. They highlighted three regimes of flow in a mixing channel, namely strictly laminar flow, vortex flow and engulfing flow, depending on *Re* of flow in the mixing channel. Qian et al.[8] used a T-shaped micromixer to investigate the influences of channel cross-sectional dimensions and flow velocity on the gas and liquid slug length. Hoffmann et al.[9] carried out experiment on mixing characteristic in a T-shaped micromixer with rectangular cross-sections fabricated by using reactive ion etching technique. They reported that T-micromixer promotes the generation of vortex structures at low *Re* range without turbulence. They also reported that with higher *Re* the flow regime changes from the stratified flow (where both streams flow side by side in channels) to the engulfment flow. The intertwinement of both input streams leads to an enlarged interfacial surface area. Bothe et al.[10] studied

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the mixing characteristics in a T-micromixer using computational fluid dynamics and experiments. They reported that in the laminar flow regime only the engulfment flow with intertwinement of the input streams leads to efficient mixing by rolling-up the initially planar contact area.

Clever geometry with the presence of additional parts such as a sharp bend slanted wall, obstacles, or a junction, can lead to discontinuity of fluid flow. When a liquid flows through a sharp bend, the change in flow direction gives rise to a secondary flow field perpendicular to the flow of the liquid. This lateral flow field could be used to improve mixing performance in a micromixer where mixing by turbulence is not feasible. Lin et al.[11] proposed a new T-micromixer with several J-shaped baffles as additional parts in the mixing channel to enhance mixing experimentally and numerically. The simulated and experimental results revealed that the J-shaped baffles result in lateral convection in the main channel, thus improves the mixing. Johnson et al.[12] and Goullet et al.[13] carried out numerical and experimental studies on mixing in a T-micromixer with slanted walls. They found that the slanted walls of mixer with such design was able to induce a high degree of lateral transport across the channel. Since mixing with this design occurs by lateral transport, and is not limited by diffusion. Mixing efficiency of 80% has been reported at the mixing length of 443 μm and velocity of 0.81 cm/s, whereas with the absence of slanted walls, a channel with 2300 μm is needed to achieve the same mixing efficiency at the same flow rate. Recently, Fu et al.[14] proposed active double-T-shaped micromixer (DT-micromixer). They reported that the mixing efficiency can be as high as 95% within a mixing length of 1000 μm downstream from the secondary T-junction when a 100 V/cm driving electric field strength and a 2 Hz periodic switching frequency are applied.

The above literature review shows that the fundamentals of transport phenomena in passive T-micromixers are still unclear, making it difficult to predict the performance of these mixers precisely and quantitatively. The difficulty in rapid mixing of liquid streams results from the fact that the system is often restricted to the laminar flow regimes. Detailed examination onto the underlying vortex phenomena is often missing, especially that of the local process inside of these vortex mixers is often not accomplished. This gives the motivation to study these phenomena in more detail. Comparing the types of T-micromixers described above, static type micromixers with the presence of additional parts have the highest potential in fulfilling the needs for complete mixing within short mixing length.

The objective of this research work is to investigate mass transfer enhancement in microchannels. The approach that will be used to bring about mass transfer enhancement is the “swirling action of eddies, lateral velocity component in the flow, and splitting the inlet streams into substreams”. For this aim, three geometrical configurations will be used, the first one is the standard T-micromixer and the second one DT-micromixer[14], whereas the third one (DT-micromixer with static mixing elements) is proposed here for the first time. For this theoretical mixing study, computational fluid dynamic (CFD) modeling and simulation tools provided by commercial software packages of FLUENT$^{6.2}$ in conjunction with Gambit are used to solve the three-dimensional flow and mass transfer equations in the proposed geometrical configurations. The predictions of this work can be served as basic reference for future experimental study.

2 THEORY

2.1 Basic Equations

The assumptions of continuous medium and none of slip boundary conditions were adopted. When the impact of gravity was neglected and no other source item existed, the steady flow of an incompressible Newtonian liquid in microchannels can generally be described by Naive−Stokes equation and continuity equation as shown in Eqs.(1) and (2), respectively. The distribution of species concentration is governed by the diffusion convective equation [Eq.(3)].

$$\rho\frac{\partial \boldsymbol{V}}{\partial t}+\rho\boldsymbol{V}\cdot\nabla\boldsymbol{V}=-\nabla p+\mu\nabla^2\boldsymbol{V}, \tag{1}$$

$$\nabla\cdot\boldsymbol{V}=0, \tag{2}$$

$$\frac{\partial c}{\partial t}+\overline{V}\cdot\nabla c=D\nabla^2 c, \tag{3}$$

where $\boldsymbol{V}$ is the velocity vector, t time, ρ density of the fluid, p pressure, μ viscosity of the fluid, c, concentration of the species, and D molecular diffusion coefficient of the species. The macro-fluid dynamics in the channel is characterized by Re number, Re:

$$Re=\rho u d_{\mathrm{h}}/\mu, \tag{4}$$

where u is mean velocity, and d_{h} hydraulic diameter, which is a computed value that depends on the cross-sectional geometry of channel .

2.2 Characterization of the Degree of Mixing

Dimensionless parameter α was defined with the maximum standard deviation to describe the mixing quality between species along a cross section:

$$\alpha = 1 - \sqrt{\sigma_{\mathrm{M}}^2 / \sigma_{\max}^2}, \quad (5)$$

where $\sigma_{\max}^2$ is the maximum variance of the species and σ_{M}^2 the mean square deviation of concentration field:

$$\sigma_{\mathrm{M}}^2 = \frac{1}{n}\sum_{i=1}^{n}(c_i - \bar{c}_{\mathrm{M}})^2, \quad (6)$$

where $\bar{c}_{\mathrm{M}}$ is the mean concentration distribution of the species i over n elements of the mesh in a certain cross section of the mixing channel:

$$\bar{c}_{\mathrm{M}} = \frac{1}{n}\sum_{i=1}^{n} c_i. \quad (7)$$

3 SIMULATION

To further understand the flow field in the micromixer, CFD simulations of mixing in T-micromixer and DT-micromixer with and without static mixing element was carried out by using Fluent software. A 3D solid model of the two mixers were built using Gambit, the preprocessor for Fluent. The dimensions of the two solid models are illustrated in Fig.1. The solid model of the T-micromixer was made up of 304000, whereas the DT-micromixer was made up of 676775 brick elements. Two species (A) and (B) are assumed to be incompressible and their physical properties are identical to those of water at 20 ℃. Species (A) was specified to enter the DT-micromixer from the first right inlet and second left inlet while species (B) was specified to enter from the first left inlet and second right inlet.

In all simulations, the SIMPLEC algorithm for pressure–velocity coupling and second order upwind for the computation of Navier–Stokes and diffusion–convection equations were employed. Steady laminar flow model was selected to simulate the flow of liquid in the three types of micromixer (T-, DT-, and DT-micromixer with SMEs) without slip boundary condition set at the walls of microchannels, and applied pressure of 0.2 MPa is set at the inlets to the micromixer. The numerical simulation was done with a kinematic viscosity of η at 858×10^{-7} $\mathrm{m^2/s}$ and a diffusion coefficient of D at 2×10^{-9} $\mathrm{m^2/s}$, which are typical values for an aqueous solution at room temperature.

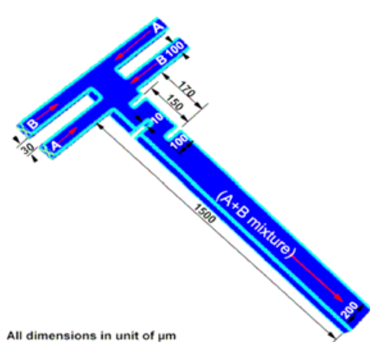

Fig.1 Passive double-T-shaped micromixer with 3 static mixing elements

4 RESULTS AND DISCUSSION

4.1 Effect of Geometrical Setup

Most micromixers used for mixing of liquids are based on the principle of producing thin liquid lamellae typically in the range of a few to several tens of micrometers and guiding them in contact through a flow-through-chamber[12]. Splitting the inlet streams into n substreams lead to increase of the contact surface between the two fluids, causing diffusion to occur faster. Based on this concept, T- and DT-micromixers (without SMEs) were fabricated to study the effect of geometry on the number of contact area between mixed fluids. Fig.2 clearly demonstrates that the number of effective contact areas between the two sample fluids increases from 1 to 3 for the T-micromixer and DT-micromixer.

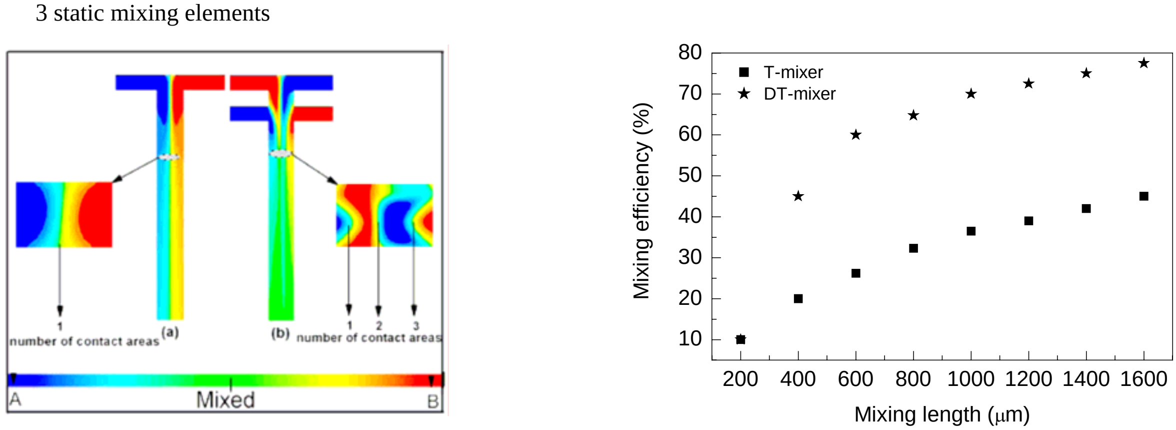

Fig.2 Number of effective contact areas between the two sample fluids (left) and mixing efficiency over the length of mixing channel (right) (Re=219, p=0.2 MPa)

Due to its larger contact area, the DT-micromixer provides the best mixing efficiency than T-micromixer. The simulation results of T-micromixer are quite close to the experimental and numerical results reported by Wong et al.[15] and Kockmann et al.[6] respectively, whereas further experimental study is needed for DT-micromixer.

4.2 Effect of Velocity Ratio ($\check{R}$)

The velocity of inlet streams has a major influence on the performance of microfluidic mixer, because it is a measure of residence time of the fluid flow in mixing channel. Several simulations were carried out on DT-micromixer (A) by varying the ratio of inlet velocities ($\check{R}$). Here, we defined $\check{R}$ as the ratio between the inlet velocities at the two inlet channels of the second T-junction (V_{J2}) and the velocities of fluid flow at the two inlet channels of the first T-junction (V_{J1}), $\check{R}=V_{J2}/V_{J1}$.

The results are presented in Fig.3, which indicates that the mixing efficiency of the two streams in the DT-micromixer is too sensitive to the variation of $\check{R}$. In this study, the velocity of 7 m/s is selected at the two inlet channels of first T-junction. Fig.3 also shows that at strictly low and high $\check{R}$, DT-micromixer works in the same as T-micromixer with the maximum mixing efficiency not more than 46%. But for the range of $\check{R}$ from 0.3 to 0.4, significant increase of mixing performance is observed at the out let of mixing channel. Mixing efficiency reaches as high as 78% at 0.4 of $\check{R}$.

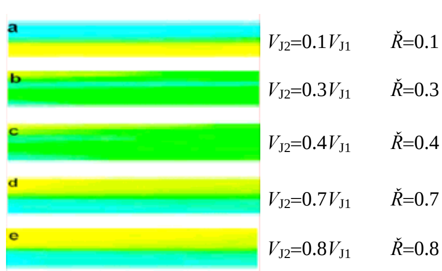

Fig.3 Contours of mass fractions at different $\check{R}$ values for DT-micromixer (without SME, *Re*=219, *p*=0.2 MPa)

4.3 Effect of Static Mixing Elements

Viscous forces and pressure gradients with a low moment of inertia govern the fluid flow in a micromixer. The result is a truly laminar, turbulence-free flow with *Re* in the order of 100. When the walls of micro-channel are incorporated with static mixing elements (SMEs), the separation of boundary layer occurs. Fig.4(a) shows that in the absence of static mixing elements the flow is laminar and mixing takes place entirely in molecular diffusion, so complete mixing cannot be achieved as distinct concentration difference can be observed at the end of mixing channel (see Table 1).

The introduction of SMEs results in significant improvement in mixing performance and mixture uniformity. This can be clearly seen in Fig.4(b), the concentration of the species is more uniform just after the two liquids flows past the third mixing element. The results of the simulations show that the mixing efficiency as high as 97% within a mixing length of 320 μm downstream from the first T-junction is achieved when three SMEs are introduced to the walls of mixing channel of DT-mixer (B) [see Fig.4(b) and Table 1].

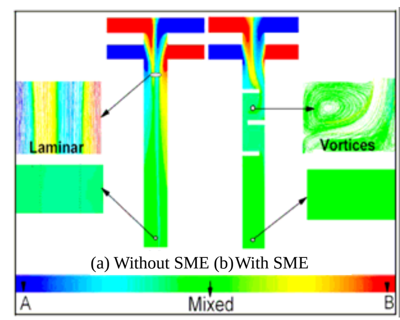

Fig.4 Mass fraction contours of a species in DT-micromixer [d_h=20 μm, V=7 m/s, p=0.2 MPa, $\check{R}$=0.4]

Table 1 The effect of SMEs on mixing efficiency and pressure drop at the mixing length of 320 μm from the first T-junction

Mixer type	Number of SMEs	Δp 1) ($\times 10^3$ MPa)	*Re*	Mixing efficiency (%)
T-mixer	0	0.78	219	23
DT-mixer (A)	0	1.26	217	56
DT-mixer (B)	3	9.96	165	97

Note: 1) Pressure drop.

The improvement in mixing performance of DT-micromixer (B) can be attributed to the following reasons: (1) The change of flow direction, which gives rise to a secondary flow field perpendicular to the liquid flow. (2) The separation of boundary layers, which can give rise to the generation of vortices. Vortices tend to break the stream up into layers, and each layer curls in a different manner. These breaking and curling actions lead to increased contact area and reduced molecular diffusion distance between the molecules of the two liquids in a mixing process.

Pressure drop across mixing channel results in energy dissipation through the formation of eddies. A relatively large energy input is needed for the deflection of the flow into the mixing channel and building up the vortex structure. The pressure drop values for the three designs of micromixer, at mixing length of 320 μm downstream from the first T-junction, are shown in Table 1. A strong increase in the pressure drop was observed in DT-mixer with SMEs, which originates from the bending of the streamlines and generation of the vortices around these static mixing elements.

High flow velocity in the region around the static mixing elements results in the so-called engulfment flow (Fig.5). Some fluid from one side reaches beyond the centerline of the micro-channel to engulf the fluid from the other side, disturbs the slow moving molecules in the boundary layer and sweeps them to the bulk of the flow. As a result, a higher mixing efficiency acting in cross directions, i.e., perpendicular to the axial direction, can be obtained. Unfortunately, the introduction of static mixing elements in a flow channel can lead to a reduction in the mean flow velocity in the channel. The mean flow velocities of 8.25 and 10.83 m/s are reported for DT-micromixer with and without SMEs respectively. It is very important that the introduction of these elements should not cause significant reduction in flow velocity.

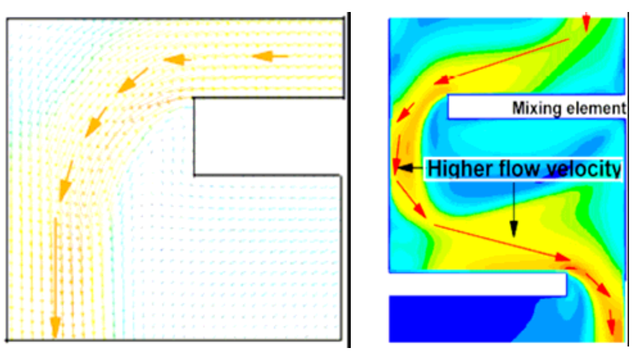

Fig.5 The velocity vector plot (left) and contour plot (right) showing the rotational flow of liquid caused by the static mixing elements (*Re*=165, *p*=0.2 MPa, $\check{R}$=0.4)

5 CONCLUSIONS

The flow behavior in T- and DT-micromixers has been investigated under asymmetrical conditions. Simulation results show that DT-micromixer provides the best mixing efficiency than T-micromixer. The numerical simulations of mixing in a DT-micromixer with static mixing elements incorporated in mixing channel show that significant improvement in mixing performance can be achieved, compared with a micromixer without them. The generation of vortices by static mixing elements improves the speed of mixing, as the former result in the increase of contact area between the liquid species and at the same time a reduction in the molecular diffusion distance to achieve mixing. The improved mixing is achieved at the expense of faster increase of pressure drop.

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