

Numerical study of the effect on mixing of the position of fluid stream interfaces in a rectangular microchannel

M. A. Ansari · Kwang-Yong Kim · Sun Min Kim

Received: 21 December 2009 / Accepted: 6 May 2010 / Published online: 19 May 2010
© Springer-Verlag 2010

Abstract A numerical study has been carried out to investigate the effect on mixing of the position of fluid stream interfaces in a rectangular microchannel. The velocity profile in a microchannel has a parabolic shape which shows maximum local velocity at the center of the channel and minimum velocity near the wall. This velocity profile governs the residence time of the fluid streams and hence effects on the mixing of fluid streams. Single and double interfaces of the fluid streams have been studied in rectangular microchannels for the range of Reynolds numbers ($0.1 \leq Re \leq 10$) where mixing is mainly governed by molecular diffusion. Significant variations in the mixing performance have been shown at various positions of the interfaces at different Reynolds number.

1 Introduction

Development of efficient micromixers and understanding the mechanism of the mixing of fluid samples has become a focus of research in the area of microfluidics. Attaining rapid mixing of liquids in a limited time is required for many microfluidic applications (Burns et al. 1998; Hashimoto et al. 2006; Lee et al. 2005). However, the flow in microchannels is predominantly laminar which makes it difficult to mix the fluid samples (Stone et al. 2004). In simple microchannels, fluid mixing is solely due to molecular diffusion, which is a very slow process, because the Reynolds number in microchannels is in the regime of

laminar flow due to small channel dimensions. Understanding the basic mechanism of mixing under different operating conditions is essential to enhance the mixing rate and develop new micromixers.

Micromixers can be broadly classified as active and passive micromixers (Nguyen and Wu 2005; Hessel et al. 2005). Passive micromixers utilize specially designed shapes of the channel to create the desired flow inducing mixing. The operation of the passive micromixer is easier and simpler because of no additional moving parts or energy sources. By contrast, active micromixers use external energy sources and are more efficient for mixing the fluid as compared to passive micromixers. However, active micromixers require a cumbersome fabrication process and hence are not cost effective as compared to passive micromixers.

The simplest design of a passive micromixer is T- or Y-shape in which the inlets join the main channel with T- or Y- shape branches. These micromixers are quite suitable to carry out basic fundamental studies to understand mixing at the microscale. Engler et al. (2004) performed numerical and experimental investigations on T-shape micromixers and distinguished three flow regimes, i.e. stratified laminar flow, vortex flow and engulfment flow. Bothe et al. (2006, 2008) numerically investigated on the same T-shape micromixer and found that only engulfment flow with intertwinement of the input fluid streams is efficient in mixing by rolling up the initial planar contact area between the fluids. Hoffmann et al. (2006) performed experimental investigations on T-shape micromixer with rectangular microchannel in the stratified and engulfment flow regimes. They reported that the flow promotes the formation of the vortex even at low Reynolds number and enhance mixing by the short diffusion lengths. In these flow regimes, the intertwinement of the two fluid streams increases the

M. A. Ansari · K.-Y. Kim · S. M. Kim (✉)
Department of Mechanical Engineering, Inha University,
253 Young Hyun-dong, Nam-gu, Incheon 402-751,
Republic of Korea
e-mail: sunmk@inha.ac.kr

interface area of the fluid along with reducing the diffusion lengths. Soleymani et al. (2008a, b) carried out numerical and experimental analyses on the flow and the mixing characteristics in a T-shape micromixer and reported the formation of vortices and its effect on mixing. The formation of the vortices is greatly dependent on Reynolds number and geometrical parameters. This study reports on the determination of identification number for the differentiation of flow regimes and its critical value at which transition from vortex flow to engulfment of flow. Adeosun and Lawal (2009) carried out numerical and experimental investigations on T-shape microchannel and characterized mixing performance using the concept of residence time of the fluid.

The basic T- or Y- shape micromixers generate interface of the fluid streams to be mixed over which mixing take place. These micromixers have been modified to generate multiple interfaces of the fluid streams using specially designed inlets. Wu and Nguyen (2005) carried out analytical studies and proposed two important parameters for T-mixer, i.e. Peclet number and mixing length. The model can be applied for multiple interfaces of fluid streams as well. Tafti et al. (2008) studied the effect of velocity profile and its variation in a microchannel on mixing. Yang and Liu (2008) carried out numerical simulation on the hydrodynamic behavior of Taylor dispersion to understand its theoretical background.

Most of the previous works on T- or Y- shape micromixers is directed towards analyzing mixing for a wide range of Reynolds numbers and finding various flow types. It is well known, that the mixing performance varies significantly with Reynolds number because mixing is mainly governed by the molecular diffusion of the fluids. At very low Reynolds number, the mixing is higher due to longer residence time of fluid. However, as the Reynolds number increases, mixing decreases due to decrease in the residence time of the fluid. The effect of convective flows starts to mix the fluid after a certain critical Reynolds number. So, exploring a way to increase mixing performance for the range of Reynolds numbers where low mixing is depicted is an interesting and important issue.

Abonnenc et al. (2009) studied mixing of two fluid flows in a microchannel, with one central laminar flow being sandwiched between two outer flows. The effects of the diffusion coefficient, flow rates and species concentration ratios were analyzed. The location of two interfaces was away from the center of the microchannel. The position of the interface of the fluid streams in the microchannel affects the mixing performance of the device. The work reported only at one position of the interface of the fluid streams away from the center of the channel.

From the above study, it has become obvious that the position of the interface of the fluids streams in a

microchannel affects mixing performance. The center position of the interface where the flow velocity is maximum value will show least mixing performance due to the low residence time of the fluid. Due to parabolic shape of the velocity profile, the mixing performance will keep on increasing as the interface positions shift towards the wall side. However, the position of the nearest interface to the wall does not look realistic due to no slip condition at the wall and the required mass flow rate of the fluids. In such situation, there will be a certain optimum position in the microchannel, where the mixing will be higher and can be practical for microfluidic applications. Some detailed study on the interface position in a microchannel need to be performed to investigate mixing performance at various positions in the microchannel for different Reynolds numbers. Such information will be helpful to design the channel with optimum location of the interface position for attaining effective mixing.

In this work, the effect on mixing of the position of fluid stream interfaces has been investigated for a range of the Reynolds numbers ($0.1 \leq Re \leq 10$) in which the diffusion mixing is dominant. Both single- and two-interface has been considered. In case of two-interface, each interface is equidistant from the wall of the rectangular channel. The result shows different mixing behavior for various locations of the interface in the channel.

2 Basic idea

The velocity profile of laminar flow in a rectangular channel has parabolic shape when the flow is fully developed as shown in Fig. 1. The velocity at the center of the channel is the highest and attains a value of zero at the wall to satisfy no slip boundary condition. There is gradual decrease in the local velocity of the fluid stream from the center to the wall. Due to the high local velocity of the fluid streams at the center, which causes short resident time, low mixing will be depicted when the interface of fluid streams lies at the center of the microchannel. In order to take the advantage of the velocity profile, the position of the interface can be located away from the center. This will provide longer resident time to the fluid streams for mixing in the regime of given Reynolds numbers ($0.1 \leq Re \leq 10$) in which the mixing is dominated by diffusion.

3 Physical model

Figure 2 shows the schematic diagram of the micromixer for both single and double interfaces of the fluid streams. For single-interface fluid streams, one side inlet channel joins the main channel, while for creating two interfaces,

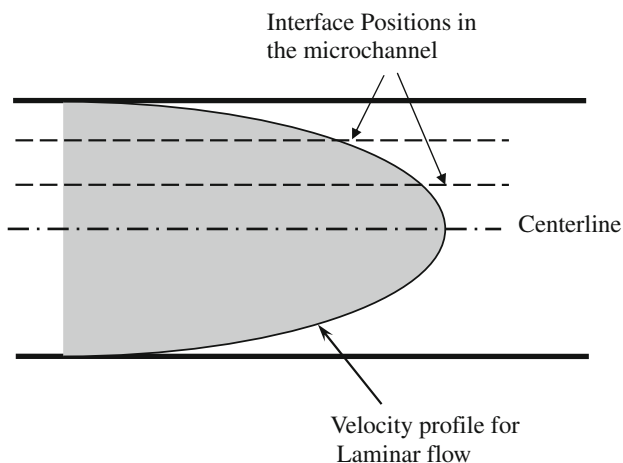


Fig. 1 Schematic drawing showing the position of the interface of the fluid streams in the microchannel. For laminar flow, the velocity profile is a parabolic shape, with maximum velocity at the center of the channel and zero velocity at the wall

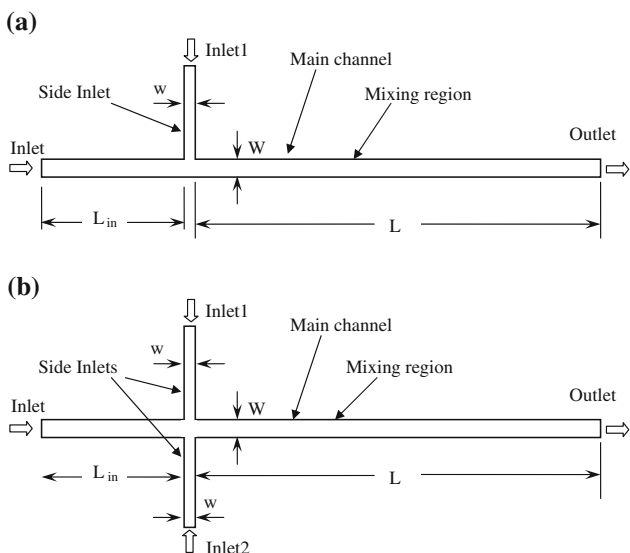


Fig. 2 Schematic of the model rectangular microchannels with **a** single interface **b** double interfaces. The side inlets are connected to the main channel at right angle. The width of the main channel is fixed at $W = 200 \mu\text{m}$, while the width of side inlet channels are varied ($50\text{--}200 \mu\text{m}$). In case of two-interface the width of both side inlets are equal

two side inlet channels has been considered. In both cases, the side inlet channels connect the main channel at right angle to the main channel.

The height of the inlet channels as well as main channel has been kept constant at $140 \mu\text{m}$. The width of the side inlet channels (w) has been varied from 50 to $200 \mu\text{m}$ and the width of the main channel (W) is fixed as $200 \mu\text{m}$. In case of two-interface fluid streams the width of both side

inlet channels are equal. The width of the main inlet channel is fixed and is equal to the width of the main channel. The length of the main mixing channel and inlet channel is fixed, $L = 5 \text{ mm}$, $L_{\text{in}} = 1.8 \text{ mm}$. In case of single-interface fluid streams, two separate fluid streams flows from the two inlets. While for two-interface fluid streams, one fluid stream is sandwiched between the two streams of the similar fluids entering from the side inlets. Both interfaces are equidistant from the wall of the rectangular channel. The distance of the interface of the fluid streams from the wall of the channel has been expressed by the ratio w/K , where w is the width of the side inlet channels and $K = w + W$ for single-interface and $K = 2w + W$ for two-interface.

4 Numerical model

The numerical analysis on mixing was carried out by solving the continuity equation (Eq. 1) and the Navier–Stokes equation (Eq. 2) using ANSYS CFX-11 solver. This flow field in the micromixer was considered steady and incompressible. The governing equations are as follows.

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

$$(\vec{V} \cdot \nabla) \vec{V} = \frac{\nabla P}{\rho} + \mu \nabla^2 \vec{V} \tag{2}$$

Water and ethanol were selected as the working fluids. The main reason for selecting water and ethanol is that there are a number of studies on mixing with these fluids (Chung and Shih 2008; Lin et al. 2007; Jeon et al. 2005; Wang et al. 2002). Second reason is that the physical properties, especially diffusivity, of these two fluids are quite suitable for carrying out numerical simulation for evaluating mixing. Fluids with low diffusivity will require longer computational time.

Structured grids for full domain of the micromixer were used to take advantage of simple geometry. The quality of the mesh was kept high near the zone where the interface of two fluid streams exists to increase the accuracy of analysis.

The inlets were assigned as normal velocity component while the outlet as zero static pressure. In case of single-interface fluid streams, main inlet was assigned 100% ethanol, while side inlet was assigned 100% water. For two-interface fluid streams, 100% water was assigned to both side inlets with 100% ethanol to the main inlet. Hence, the water stream flows along the side walls, with ethanol stream was sandwiched in between and two interfaces of the fluids were created. Walls were assigned with no slip boundary conditions. The properties of the water and ethanol were taken at 20°C (see Table 1) and the solutions

Table 1 Properties of fluids at 20°C

Fluid	Density (kg m ⁻³)	Viscosity (kg m ⁻¹ s ⁻¹)	Diffusivity (m ² s ⁻¹)
Water	9.998 × 10 ²	0.9 × 10 ⁻³	1.2 × 10 ⁻⁹
Ethanol	7.890 × 10 ²	1.2 × 10 ⁻³	1.2 × 10 ⁻⁹

were considered to have attained convergence when a root mean square (RMS) residual value reached 10⁻⁶.

Along with qualitative analysis on mixing, the performance of the micromixer was evaluated by quantitatively calculating the mixing index for various interface positions. Mixing was evaluated using a parameter called *mixing index*, defined as;

$$M = 1 - \sqrt{\frac{\sigma^2}{\sigma_{\max}^2}} \quad (3)$$

where σ is the variance of the mass fraction of the fluid component of the mixture, σ_{\max} is the maximum variance. Variance was calculated on a plane drawn perpendicular to the direction of the flow as follows.

$$\sigma = \sqrt{\frac{1}{N} \sum (c_i - \bar{c}_m)^2} \quad (4)$$

The value of the mass fraction was evaluated at N sampling points on the plane. c_i is the mass fraction at sampling point i , and \bar{c}_m is the optimal mixing mass fraction. The value of optimal mass fraction, \bar{c}_m is 0.5 for completely mixed mixtures of fluids. The total number of sampling points, N on the cross sectional plane was equal to 600.

5 Results and discussion

Numerical results for the effect on mixing of the interface positions in a rectangular microchannel are shown in Fig. 3 by the mass fraction distributions of ethanol along the channel. The distributions are drawn on xy -plane at the middle of the channel height for both single- ($Re = 0.5$) and two-interface ($Re = 1$) fluid streams at various positions of the interface of the fluid streams. Figure 3a shows the mass fraction distributions of ethanol for different positions of the interface in the single-interface channel for $Re = 0.5$. In cases, $w/K = 0.2$, the interface is near to the wall and the width of the interface is increasing along the channel length. The fluid component near the wall side of the interface gets mixed within a short distance. There is no more fluid left for mixing. Hence after a certain distance mixing becomes constant. As the interface position is shifted towards the center of the microchannel, the mixing rate decreases. However, the extent of mixing with change

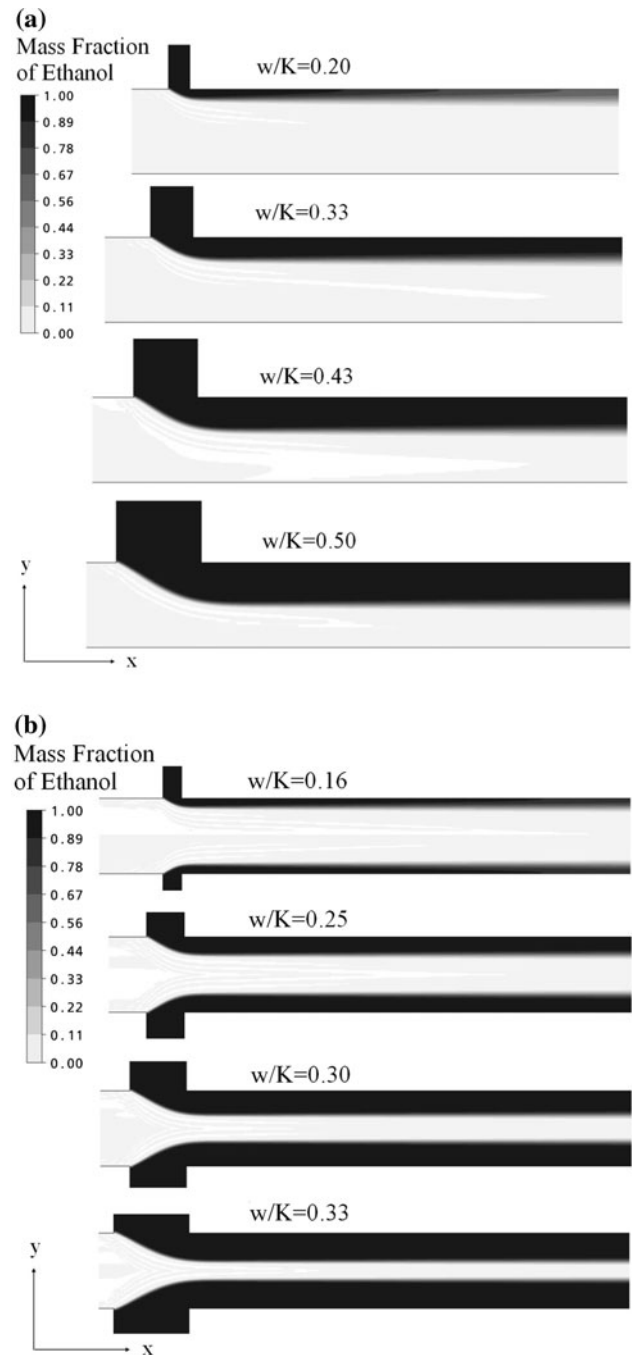
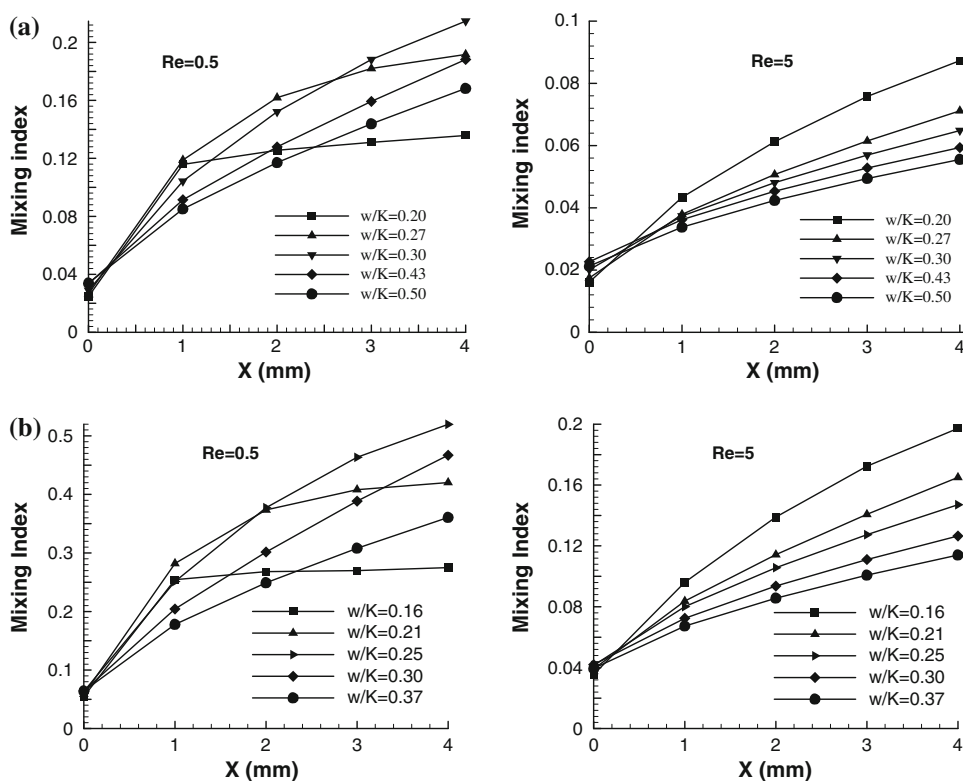


Fig. 3 Mass fraction distribution on xy -plane at various locations in the rectangular microchannel; **a** single-interface fluid streams, $Re = 0.5$, $K = w + W$, **b** two-interface fluid streams, $Re = 1$, $K = 2w + W$

of interface position cannot be clearly distinguished by the mass fraction distribution. The effect was more clear and distinguishable, when it was analyzed with mixing index (presented in later section). The contour plot for $w/K = 0.50$ is for the interface located at the center of the microchannel. The other results correspond for different

Fig. 4 Mixing index distribution along channel axial length for different interface positions $Re = 0.5$ and 5 ; **a** single- and **b** two-interface fluid streams



interface positions which are away from the center of the microchannel.

Figure 3b shows the mass fraction distributions of ethanol for different positions of the interface in the two-interface channel for $Re = 1$. The flow rate from the inlets was adjusted to maintain constant Reynolds number in the main channel. The widths of the two sub inlets were same for each case and hence both interfaces of the fluid streams are at same distance from the center of the microchannel. The distribution of mass fraction at the interface is similar to the results presented in Fig. 3a. The only main difference is the rate of broadening of the interface of the fluids streams. The rate of interface broadening along the channel length is at $Re = 1.0$ is slow as compared to $Re = 0.5$ (Fig. 3a). This is mainly due to longer residence time of the fluids streams to mix. The inertia of incoming fluid streams is also not strong enough to distort interface of the fluid streams. Hence, the area of interface is also constant and is almost undisturbed by the fluid flow. Each fluid stream follows its own side in the channel and thin and straight interface can be clearly visualized in the results.

Mixing index distribution along the channel length for different positions of the interface in the microchannel at two Reynolds numbers ($Re = 0.5, 5$) are shown in Fig. 4. The quantitative results correspond to the results of the contour plots at the same conditions presented in Fig. 3. Significant variations in the mixing performance are shown

at various positions of interface. The mixing index is gradually increasing along the channel length at all positions of the interface. In case of single-interface, $w/K = 0.50$ corresponds to the situation when the interface lies at the center of the rectangular channel (see Fig. 4a). As the interface position is shifted towards the wall, mixing rate is increasing. This is due to the shortest residence time of fluid stream located at the center of the channel. This residence time gradually increases as the interface position is shifted towards the wall. At $Re = 0.5$ and $w/K = 0.20$, the mixing rate is very high till $x = 1.0$ mm, then it becomes almost constant by the end of the microchannel. For $w/K = 0.27$, mixing rate is also high till $x = 1.0$ mm, then slows down. For $w/K = 0.20$, the quantity of one fluid on wall side of the interface is less as compared to $w/K = 0.27$, which mixes earlier and get consumed within a certain distance in the microchannel. For $w/K = 0.30$, mixing rate is lower than the above two cases, but finally at the end of the channel mixing is higher. For any given Reynolds number, lowest mixing is depicted for the interface location at the center of the microchannel. The mixing increases as the interface position is shifted away from the center towards the wall. Similar behavior is shown for two-interface channel (see Fig. 4b). For two-interface case, at $Re = 1$, mixing index is increasing along the channel length at all interface positions. For $w/K = 0.16$, interface is near to the wall and shows similar mixing

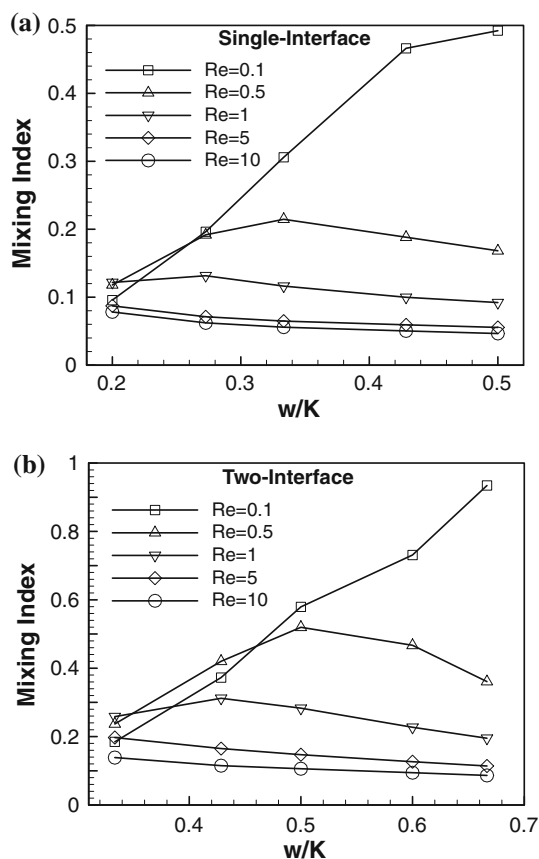


Fig. 5 Mixing index at different positions of the interface in the microchannel

behavior with the result of single-interface case. For $w/K = 0.37$, the interface is away from the center and shows lowest mixing performance.

The mixing performances of different interface positions and various Reynolds numbers are shown in Fig. 5. It shows the mixing index at the end of the microchannel ($x = 4$ mm) for different interface positions of the fluid streams for $Re = 0.1, 0.5, 1, 5$, and 10 in both single- and two-interface microchannels. At $Re = 0.5$ and 1 , mixing increases gradually as the position of interface is shifted towards the center and starts decreasing after attaining a peak value. At $Re = 0.1$, the fluid has very long residence time and shows highest mixing when the fluid interface is located at the center of the microchannel. In this case, there is sufficient fluid on both side of the interface for mixing and hence shows higher mixing. However, at $Re = 10$, there is not so much effect of the position of the interface on mixing. Mixing is almost constant for all positions of the interface. This is likely due to quite short residence time of the fluid in the microchannel. In contrary, significant variation is shown at Reynolds numbers lower than 10 . Hence, positions of interface can be kept in mind while designing a micromixer operating in the above mentioned range of Reynolds numbers.

6 Conclusion

Numerical analysis has been carried out to investigate the effect on mixing of the position of the fluid stream interfaces in a rectangular microchannel. Both single- and two-interface fluid streams have been considered for study at various Reynolds numbers. The Reynolds numbers lie in the range where mixing is mainly governed by the molecular diffusion of the fluids. Significant variation in mixing behavior is depicted for various positions of the interface in microchannel at various Reynolds numbers. The effect of position of the interface in the channel on mixing is more at low Reynolds number ($<Re = 10$), but less at higher Reynolds number ($>Re = 10$).

Acknowledgments This work was financially supported by INHA University Research Grant.

References

- Abonnenc M, Josserand J, Girault HH (2009) Sandwich mixer–reactor: influence of the diffusion coefficient and flow rate ratios. *Lab Chip* 9:440–448
- Adeosun JT, Lawal A (2009) Numerical and experimental studies of mixing characteristics in a T-junction microchannel using residence-time distribution. *Chem Eng Sci* 64:2422–2432
- Bothe D, Sternich C, Warnecke HJ (2006) Fluid mixing in a T-shaped micro-mixer. *Chem Eng Sci* 61:2950–2958
- Bothe D, Sternich C, Warnecke HJ (2008) Computation of scales and quality of mixing in a T-shaped microreactor. *Comput Chem Eng* 32:108–114
- Burns MA, Johnson BN, Brahmamandra SN, Handique K, Webster JR, Krishnan M, Sammarco TS, Man PM, Jones D, Heldsinger D, Mastrangelo CH, Burke DT (1998) An integrated nanoliter DNA analysis device. *Science* 282:484–487
- Chung CK, Shih TR (2008) Effect of geometry on fluid mixing of the rhombic micromixers. *Microfluid Nanofluid* 4:419–425
- Engler M, Kockmann N, Kiefer T, Woias P (2004) Numerical and experimental investigations on liquid mixing in static micromixers. *Chem Eng J* 101:315–322
- Hashimoto M, Barany F, Soper SA (2006) Polymerase chain reaction/ligase detection reaction/hybridization assays using flow-through microfluidic devices for the detection of low-abundant DNA point mutations. *Biosens Bioelectron* 21:1915–1923
- Hessel V, Lowe H, Schonfeld F (2005) Micromixers—a review on passive and active mixing principles. *Chem Eng Sci* 60:2479–2501
- Hoffmann M, Schluter M, Rabiger N (2006) Experimental investigation of liquid–liquid mixing in T-shaped micro-mixers using μ -LIF and μ -PIV. *Chem Eng Sci* 61:2968–2976
- Jeon MK, Kim JH, Noh J, Kim SH, Park HG, Woo SI (2005) Design and characterization of a passive recycle micromixer. *J Micro-mech Microeng* 15:346–350
- Lee CY, Lee GB, Lin JL, Huang FC, Liao CS (2005) Integrated microfluidic systems for cell lysis, mixing/pumping and DNA amplification. *J Micromech Microeng* 15:1215–1223
- Lin YC, Chung YC, Wu CY (2007) Mixing enhancement of the passive microfluidic mixer with J-shaped baffles in the tee channel. *Biomed Microdev* 9:215–221
- Nguyen NT, Wu ZG (2005) Micromixers—a review. *J Micromech Microeng* 15:R1–R16

- Soleymani A, Kolehmainen E, Turunen I (2008a) Numerical and experimental investigations of liquid mixing in T-type micromixers. *Chem Eng J* 135:S219–S228
- Soleymani A, Yousefi H, Turunen I (2008b) Dimensionless number for identification of flow patterns inside a T-micromixer. *Chem Eng Sci* 63:5291–5297
- Stone HA, Stroock AD, Ajdari A (2004) Engineering flows in small devices: microfluidics toward a lab-on-a-chip. *Annu Rev Fluid Mech* 36:381–411
- Tafti EY, Kumar R, Cho HJ (2008) Effect of laminar velocity profile variation on mixing in microfluidic devices: the sigma micromixer. *Appl Phys Lett* 93:143054
- Wang HZ, Iovenitti P, Harvey E, Masood S (2002) Optimizing layout of obstacles for enhanced mixing in microchannels. *Smart Mater Struct* 11:662–667
- Wu ZG, Nguyen NT (2005) Convective–diffusive transport in parallel lamination micromixers. *Microfluid Nanofluid* 1:208–217
- Yang Y, Liu J (2008) Numerical simulation on Taylor dispersion enabled micromixture. *Forsch Ing* 72:93–100