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Micro T- mixer: The effect of scaling factor and mixing angel

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Abstract:

Different phenomena observed in various experiments indicate that the flowing mechanisms of liquids in microchannels are still not understood clearly. Computational fluid dynamics (CFD) simulation was used to simulate liquid flow in a T-shaped micromixer whose structural dimensions and operating conditions were varying. The results show that, the formation of vortices in the mixing zone arises through the influence of a T-junction (changes flow direction and gives rise to a secondary flow). After the mixing zone, the flow is almost fully developed and mixing occurs by a molecular diffusion mechanism only. The results also show that the mixing angle had a significant effect on the T-mixer performance. This can be attributed to the fact that for the engulfment flow regime, there is an optimum T-angle at which the effect of sharp bend reaches a strength value. If liquids enter into inlets with the same velocities, the flow was symmetrical; otherwise, the symmetry was broken up. The asymmetrical inlet velocities help to promote mixing quality. To illustrate the differences of liquids flow between macro- and micro-scale, the mixer is scaled in proportion, and the simulation shows that the smaller the mixer, the better the mixing quality.

Keywords: micromixer, geometry scaling factor

1. Introduction

The term of micromixers refers to mixers with characteristic length scales that are in a micrometer range. A tangible effect of this 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 surface to volume ratio, 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 micromixers dimension also leads to small Reynolds number (*Re*), typically smaller than 100, so that flow is essentially laminar. Thus, mixing in micromixers is mainly driven by molecular diffusion with smaller residence time.

Micromixers are broadly classified as active and passive, based on the mixing mechanism. Each type has its specific mixing concepts, capacity, mixing speed, and operating conditions. In general, active micromixers require power input in order to affect mixing, while passive mixers primarily rely on the channel geometry to fold fluids to increase the interfacial area over which diffusion occurs [3,4].

Due to the simple fabrication technology of micro T-mixer and its easy implementation in a complex microfluidic system, micro T-mixers were the focus of many investigations. Najaf pour et al.[5] proposed T-junction passive micromixer with twisted design, they reported that, improvement in mixing implementation by increasing mixing index up to 172 percent. Mixing times in T- and V-shaped micromixers were obtained experimentally by using of fluorescence microscopy imaging, a mixing time of 1ms was achieved with the V-shaped micromixer[6]. Kockmann et al.[7] carried out computer simulations on mixing in T-shaped micromixers with both rectangular and trapezoidal cross-sections. The influence of asymmetrical flow conditions in mixer geometry and flow velocity was investigated. Johnson et al. [8] carried out numerical and experimental studies on mixing in T-shaped micromixer with slanted well. They found that the slanted well design was able to induce a high degree of lateral transport across the channel. Kockmann et al.[9] and Engler et al.[10] carried out numerical studies on mixing in a T-shaped and Y-shaped micromixers. They highlighted the three regimes of flow in the mixing channel, namely strictly laminar flow, vortex flow and engulfing flow depending on *Re* of flow in the mixing channel. Hoffmann et al.[11] carried out computer simulation and experimental work on mixing in T-shaped micromixers with trapezoidal cross-section. They found that, the mixing performance could be improved with engulfment flow. Mixing in T-shaped micromixer also has been characterized by using a blue dye and a colorless liquid [12] and it was found that for a T-shaped micromixer with a mixing channel having a hydraulic diameter of 67 µm, and the applied pressure drops of 0.55 MPa is sufficient to cause complete mixing within less than 1 ms.

The more recent works on mixing within T-shaped micromixer have been reported. Qian et al.[13] used micro T-mixer to investigate the influence of channel cross-sectional dimensions and flow velocity on the gas and liquid slug length. Hoffmann et al. [14] carried out experiment on mixing characteristic in a T-shaped micromixer with rectangular cross-sections fabricated by using reactive ion etching technique. Non-invasive measurement technique, micro laser-induced fluorescence (µ-LIF) and particle image velocimetry (µ-PIV) were used. They concluded that only the combination of µ-LIF and µ-PIV enables visualization of momentum and mass transfer inside micromixers. They also reported that T-shaped micromixer promotes the generation of vortex structures at low *Re* range without turbulence. 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.[15] studied the mixing characteristics in a T-shaped 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.

Comprehensive theoretical study concerning scaling-down effects in microscale reactors was also conducted. Goullet et al.[16] carried out numerical studies on mixing in T-shaped and Y-shaped micromixers with focus on the effect of pulsed flow and the channel geometry on mixing efficiency. Engler et al.[17] found numerically and experimentally that increasing number of vortices inside static T-shaped micromixers with rectangular cross-sections occurs even at low *Re* and these effects can be used to improve mixing quality. They also reported that *Re* is not a good identification for three different flow regimes (stratified, vortex and engulfment) and a new identification number for static T-mixers was proposed. T-shaped micromixer also has been investigated with regard to its applicability for nanoparticle precipitation. Experiments on the mixing influence using the iodide-iodate reaction system as well as barium sulfate nanoparticle precipitation were performed[18-22]. Zhao et al.[23] studied micromixing performance in T-shaped micrometers using fast parallel competing reactions (Villermaux-Dushman reaction) to study the effects of inlet and outlet dimensions, microchannel length, volumetric flow ratio on micromixing performance. Lin et al.[24] proposed a new T-shaped micromixer employed several J-shaped baffles in the tee 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 improved the mixing. Recently, Fu and Tsai [25] proposed active double-T-shaped micromixer, they reported that, the mixing efficiency can be as high as 95% within a mixing length of 1000µm downstream from the secondary T-junction when a100 V/cm driving electric field strength and a 2 Hz periodic switching frequency are applied.

To further understand of flow properties in the T-shaped micromixers, the computer simulations were carried out by using Fluent 6.2. A 3D solid model of the T-shaped micromixers was built with Gambit 2.2 (the preprocessor for Fluent 6.2). The influence of inlet velocity, mixing angle, and geometry scaling factor o the mixing quality has been studied.

2. Theory

2.1 Governing Equations

When you choose to solve conservation equations for chemical species, FLUENT$^{6.2}$ predicts the local mass fraction of each species, C_i, through the solution of a convection-diffusion equation for the *i*th species. This conservation equation takes the following general form:

$$\frac{\partial}{\partial t}\left(\rho C_i\right)+\nabla\cdot\left(\rho \mathbf{V} C_i\right)=-\nabla J_i+R_i+S_i \qquad (1)$$

where R_i is the net rate of production of species *i* by chemical reaction and S_i is the rate of creation by addition from the dispersed phase plus any user-defined sources. An equation of this form will be solved for N-1 species where N is the total number of fluid phase chemical species present in the system. Since the mass fraction of the species must sum to unity, the Nth mass fraction is determined as one minus the sum of the N-1 solved mass fractions. To minimize numerical error, the Nth species should be selected as that species with the overall largest mass fraction. J_i is the diffusion flux of species i, which arises due to concentration gradients. By default, FLUENT uses the dilute approximation, under which the diffusion flux can be written as

$$J_i=-\rho D_{i,m}\nabla C_i \qquad (2)$$

Here, $D_{i,m}$ is the diffusion coefficient for species *i* in the mixture. For certain laminar flows, the dilute approximation may not be acceptable, and full multicomponent diffusion is required. For two-component system, diffusion equation can be expressed as

$$\frac{\partial C_A}{\partial t}+(V\cdot\nabla V)C_A=D\nabla^2 C_A \qquad (3)$$

2.2 Mixing efficiency α

Dimensionless parameter α was defined with the maximum standard deviation to describe the mixing quality between species.

$$\alpha = 1 - \sqrt{\frac{\sigma_M^2}{\sigma_{\max}^2}} \tag{4}$$

$\sigma_{\max}^2$ is the maximum variance of the species, which is always equal to 0.5 under symmetrical inlet conditions. σ_M^2 is the mean square deviation of the concentration field as shown in Eq.(5),

$$\sigma_M^2 = \frac{1}{n}\sum_{i=1}^{n}(c_i - \overline{c}_M)^2 \tag{5}$$

In order to simplify the calculations, we chose the dimensionless concentration *c*, and then c_i is equal to 1 at one inlet and to 0 on the opposite side. $\overline{c}_M$ is the mean concentration distribution of the species *i* over *n* elements of the mesh in a certain cross section of the mixing channel.

$$\overline{c}_M = \frac{1}{n}\sum_{i=1}^{n} c_i \tag{6}$$

3. Simulation

3.1 Simulation Parameters

Commercial numerical tool FLUENT 6.2, uses a finite volume method (utilized by k-ω model) to calculate the flow and the diffusion inside the mixers. SIMPLE algorithm for pressure–velocity coupling and first order upwind for the computation of momentum, energy and species transport equations are employed in the simulations. When second-order upwind accuracy is desired, quantities at cell faces are computed using a multidimensional linear reconstruction approach. In this approach, higher-order accuracy is achieved at cell faces through a Taylor series expansion of the cell-centered solution about the cell center.

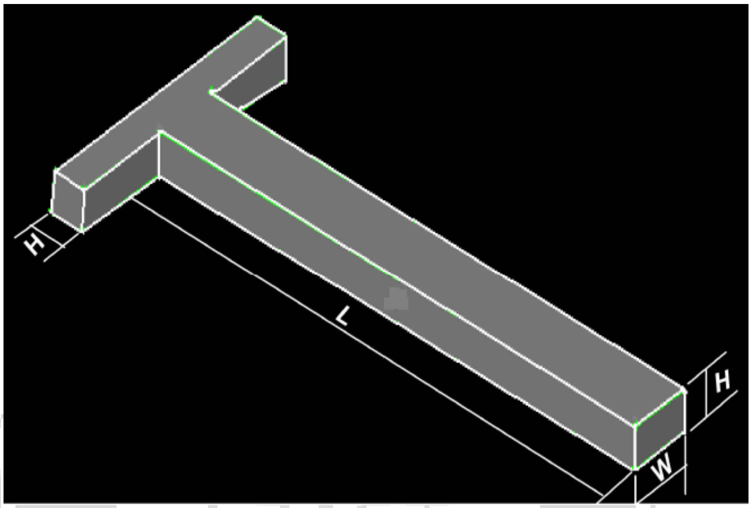

Figure.1 3D solid model of T-micromixer

A 3D solid model of the proposed mixers (Fig.1) was built and named in Gambit (the preprocessor for Fluent 6.2). The meshed structure was drawn as a hybrid structure, using cubic grids and tetrahedral meshes, with number of nodes in the range of 300,000-500,000 (Fig.2).

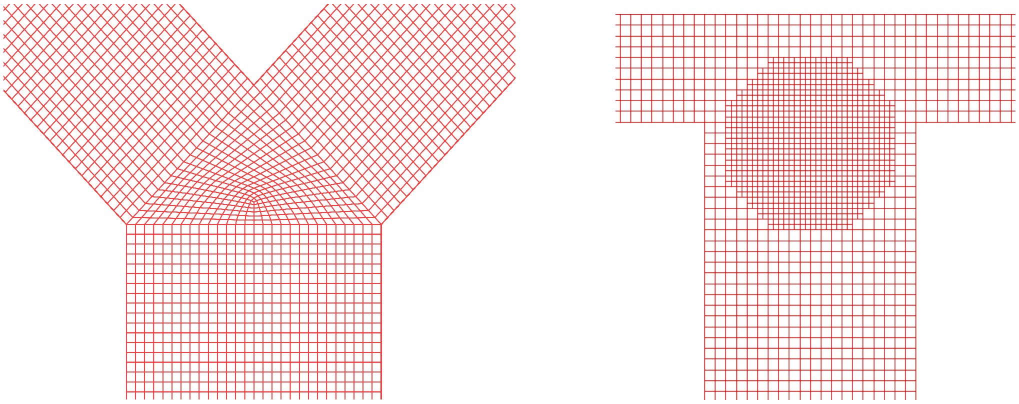

Figure 2 meshes structure

As grid elements we used rectangles for the channels and cubes for the mixing chamber where the inlet channels and the outlet channel meet. By using non-linear grids, adjacent grid elements never exceed a volume-to-volume ratio of 1.2 to avoid stability problems and to increase the accuracy of the numerical solution. The governing equations are solved sequentially by using the segregated solver (is the solution algorithm previously used by FLUENT). Because the governing equations are non-linear (and coupled), several iterations of the solution loop must be performed before a converged solution is obtained.

The model used considers the laminar mixing of species along a 3D section of microchannel, resulting from the contact between two similar fluids featuring the same viscosity and the same density. To establish this model, the following assumptions are proposed:

1) The variations of the concentration do not modify the viscosity and the density of the fluid (diluted solutions and no free convection);
2) The channel walls are assumed to be smooth (roughness);
3) The wall surface tension forces are neglected, and the medium is assumed continuous;
4) The effect of gravity is neglected (horizontal channels);
5) The flow field in the straight section downstream of the mixing channel and the upstream section of the inlet channels was considered to be laminar;
6) The steady state flow is established at the inlets;
7) The criterion for convergence is for the increment in each variable to fall below 1×10^{-5}; and
8) The liquids are assumed to be incompressible and their physical properties are identical to those for water at room temperature (see Table 2.1 below)

Table 2.1 Properties of used fluid

Properties	Symbol	Quantity
Molecular Weight	M.wt	18 kg·kgmol
Density	P	998.2 $\text{kg}\cdot\text{m}^{-3}$

Viscosity	M	0.001003 kg· m^{-1}·s^{-1}
CP	CP	4182 j·kg^{-1}· K^{-1}
Diffusivity	D_{AB}	2 × 10^{-9} m^2· s^{-1}
Droplet surface tension	Γ	0.0719404 N·m^{-1}
Thermal conductivity	κ	0.6 W·m^{-1}·K^{-1}

In the used model, the mixing process occurring at micromixers is investigated by solving the momentum and mass transport equations in two steps. First, the Navier-Stokes equation and the continuity equation are solved in the case of an incompressible fluid in a horizontal channel. Finally, the distribution of the species concentration is obtained by solving the diffusion convection equation.

3.2 Color Analysis

Initially, when the micromixer is filled with red and blue, it indicates that there are two kinds of solutions with scalar values of 1 and 0, respectively. When these solutions come into contact with each other as an interface, the color changes to green, indicating a scalar value of 0.5; and color gradation, as illustrated in the color legend, which is due to the diffusion of the scalar values. Green stripes in the designed channel structure show the contour of a 0.5 scalar value as an interface. The cross-sectional views of the channel structure show the distribution of the scalar values in accordance with the color legend.

3.3 Simulation results

3.3.1 The effect of Mixing Angle

Mixing angle is defined here as half of the angle at which the two inlet channels meet (Fig.3). Numerical simulations of liquid mixing in a T-mixer with several of mixing angles ranging from 30 to 140◦ were carried out. Results for different mixing angles are shown in Table 2. The results show that the mixing angle had a significant effect on the T-mixer performance. The mixing efficiency was increased when an angle of the range of 90 to 100◦ was used.

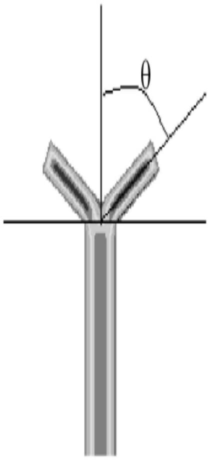

Figure 3 Sketch diagram shows the mixing angle θ

Furthermore, pressure drop along the mixing channel increased with the mixing angle. This can be attributed to the fact that for the engulfment flow regime, there is an optimum T-angle at which the effect of sharp bend reaches a strength value. It is wildly known that poor mixing occurs in the single-perpendicular inlet intersection (mixing angle =45°) where one of the inlet fluid doses not has to travel around any bends (see Fig. 4).

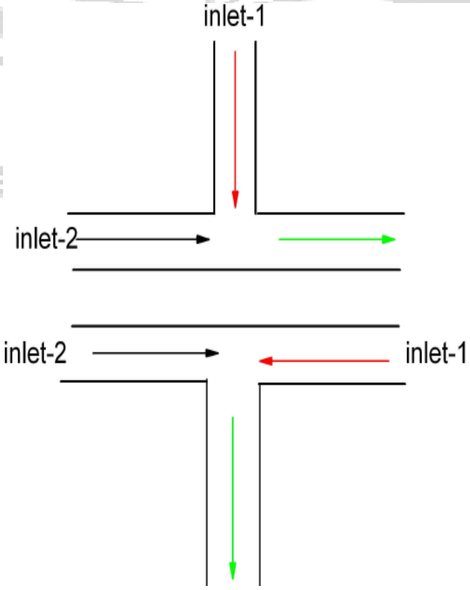

Figure 4 the direction of fluid flow. One of the inlet fluid doses not has to travel around any bends, θ=45°(*above*), and the two fluids has travel around bends of T-junction, θ=90° (*below*)

Table 2 Simulation results for different mixing angles

Mixing Angle	Mixing Efficiency	Pressure drop (MPa)
30°	0.172	0.55
45°	0.233	0.63
70°	0.273	0.69
90° (T-mixer)	0.688	0.78
100° (-90°)	0.593	0.79
120° (-60°)	0.539	0.83
150° (-30°)	0.507	0.88

3.3.2 The effect of Scaling Factor λ

To quantify the effect of scaling, a geometrical scaling factor, **λ**, is introduced. **λ** was defined by $\lambda = d'_H / d_H$, where d_H and d'_H is the hydraulic diameter before and after scaling respectively. According to Fick's low, $t_D = d^2/D$, d is the characteristic length of diffusion, usually, it can be replaced by d_H. Upon that $t_D = d_H{}^2/D$ and $t_D' = \lambda \cdot t_D$, which shows that the diffusion time shrank quickly if the geometric dimensions are reduced by a scaling factor λ**.** It was also known that Schmitt number $Sh = k_c \cdot d_H/D$ = constant, i. e., the smaller the d_H, the more the mass transfer coefficient. Figure 5 conforms this principle. A high mixing efficiency of the two liquids is achieved when d_H is reduced from 200 to 20 µm.

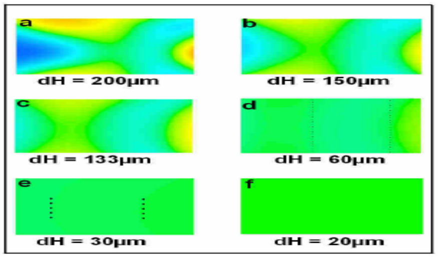

Figure 5 The effect of hydraulic diameter in mixing efficiency of T-mixer

3.4 The Effects of Asymmetrical Velocities

In an engineering problem the inlet flow conditions are often not symmetrical, i.e. different flow velocities of the components are given. Figure 6 shows the effect of asymmetrical conditions of flow velocity in performance of T-micromixer. At low symmetrical velocity both inlet streams run parallel through the mixing channel and the planar contact area remains unchanged (Fig. 6a). Whereas at asymmetrical velocity, the configuration of the streams line gets changed and the two vortex pairs get intertwined (Fig. 6b-d); which leads to a roll-up of regions with different concentrations. As a consequence, the specific contact area is enlarged, which is characteristic for the engulfment regime and an essential requirement for efficient diffusive mixing with reduced time needed for diffusive dissipation of gradients.

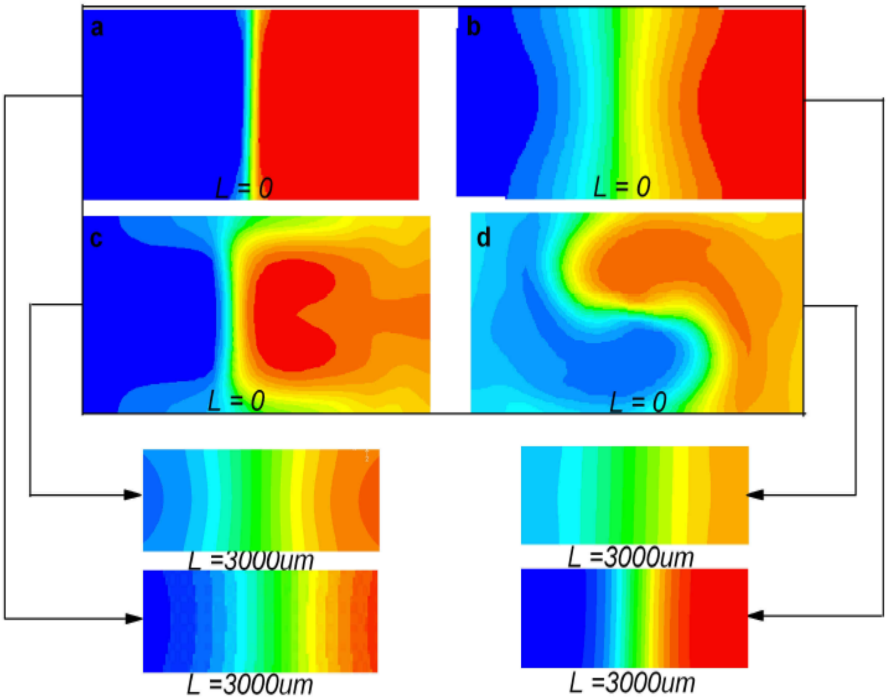

Figure 6 Effects of velocity on flow patterns and interface configurations behind entrance of mixing channel (L=0) and at its end (L=3000µm): (a) $V_1= V_2=$ 0.01m/s, (b) $V_1= V_2=$1m/s, (c) $V_1=$ 3.5m/s, $V_2=$2m/s and (d) $V_1=$7m/s, $V_2=$ 5.5m/s

Conclusion

The development of microfluidic systems has been progressing rapidly in recent years. Nevertheless, microfluidics is still considered a very young field of research.

The flow and mass transfer processes in the T-shaped micromixers have been investigated. Detailed studies of the effect of mixing angle, scaling factor and asymmetrical velocities were carried out using CFD software (FLUENT). Simulation results show that significant improvement in mixing performance of T-shaped micromixer can be achieved at small scaling factor and asymmetrical velocities. Mixing angle also had a significant effect on the T-mixer performance, this can be attributed to the fact that for the engulfment flow regime. There is an optimum T-angle at which the effect of sharp bend reaches a strength value.

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