Computational Fluid Dynamics (CFD) Simulation on Mixing in T-Shaped Micromixer

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Abstract: Computational Fluid Dynamics (CFD) simulation used to analyse the fluid mixing in micromixer. There are two cases of miscible liquids that involved within T-shaped micromixer which are ethanol-water and glycerol-water. The T-shaped micromixer consist of micro channel with two inlets channels and one outlet channel was constructed by using AutoCAD software. The effect of inlet velocity and width size toward mixing intensity were investigated. The mixing intensity values determine either good or bad mixing quality could be achieved. In this simulation, at low inlet velocity indicates good mixing quality as the mixing intensity value approaching to one. Whereas the effect of width size on mixing intensity are almost similar throughout simulated width sizes. Mixing intensity for the two cases of diffusion coefficient showed similar trend for different inlet velocity and width size of mixing channel.

1. Introduction
The application of process intensification already observed in the chemical engineering area where use of microfluidic devices has been elevated to production scale. Microreactor technology is an element of process intensifications that provides potential benefits to future of chemical engineering. Due to its high specific interfacial area available for heat and mass transfer resulting in higher transfer rates and enhances safety due to its low hold-ups. In relation to the time scale of chemical kinetics, diffusive transport in micro devices is faster than in conventional mixers [1]. Mixing has a crucial impact on the overall performance of micro reaction processes, the need for measuring and comparing mixing also increased. In general, mixing is the process of thoroughly combining different materials to produce a homogenous product. Due to the scale dimension which mixing takes place, mixing can be classified as micromixing, mesomixing and macromixing [2].
Microscale mixing is most importance as ability to rapidly mix samples at microscale is vital to the successful implementation of microfluidic system. In most microfluidic devices, mixing occurs between inlet streams that must be dispersed to remove concentrations gradients within mixing chamber. Microreactor can be defined as chemical reactors of extremely small dimensions that usually have a sandwich-like structured which consist a number of layer with micromachined channel (20 – 400 µm). Therefore, microstructured devices offer greatly enhanced mixing and heating capabilities compared to batch process which is leading to improved product profiles and higher yield. The simplest design of micro-mixer are T and Y-shaped micro-mixer [3]. In recent years, several researchers have been studied extensively on the mixing performance in of Y-shaped [4] and T-shaped [5], [6] by experimental and computer simulation as they are quite suitable to carry out fundamental studies to understand the mixing at microscale.

Therefore, the aim of this project is to study mixing in T-shaped micromixer by using Computational Fluid Dynamics (CFD) analysis by investigate the parameter that affect the mixing. The effect of inlet velocity and width size on the mixing in T-shaped micro-mixer for the two cases of miscible liquid which are ethanol-water and glycerol-water are simulated.

2. Methodology
The T-shaped micromixer geometry consists of micro channel with two inlets channels with a length of 2 cm and diameter of 0.05 cm. The mixing channel is 3 cm long with same diameter as the inlet channels. The dimensions of this model geometry is shown in figure 1(a) and the boundary condition of the micromixer is shown in figure 1(b).

![Figure 1](image)

Figure 1. (a) Dimensions T-shaped micromixer, (b) Boundary Condition of T-shaped micromixer

For this simulation, fluid flow and chemical species transport physic interfaces was chosen. Fluid flow interface consist of laminar flow which is used to compute velocity and pressure fields for flow of single phase fluid in laminar flow regime [7], [8]. The physics interface supports incompressible flows and compressible flows at low March numbers (typically less than 0.3). The equation solved by laminar flow interface are Navier-Stokes equation, (1) for conservation of momentum and continuity equation, (2) for conservation of mass [9], [10].

\[
\rho \frac{\partial \mathbf{v}}{\partial t} + \rho (\mathbf{v} \cdot \nabla) \mathbf{v} - \nabla p + \nabla \cdot \mathbf{f} = 0
\]

(1)
Where \(\mathbf{v}, p, \rho\) and \(\eta\) represent velocity vector, pressure, density of the fluid and the dynamic viscosity. The density and the viscosity data are water which \(\rho = 1000 \text{ kg/m}^3\) and \(\eta = 0.001 \text{ Pa.s}\). The driving force for the fluid to flow through the mixing channel to the outlet is the applied inlet velocity boundary conditions on the inputs while the pressure boundary condition at the outlet is assumed to be equal to zero. The channel wall assumed as a non-slip boundary condition. In this simulation, inlet velocity is varying at 0.0001 m/s, 0.001 m/s, 0.01 m/s, 0.1 m/s and 1 m/s. While the chemical species transport of diluted species interface is used to compute concentration field of dilute solute in solvent. The driving force for transport can be diffusion by Fick’s Law \([7],[8]\). The convective diffusion equation with a reaction term as shown in (3).

\[
\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = \nabla \cdot (D \nabla c) + R
\]  

(3)

Where \(c, D, R\) and \(\mathbf{v}\) represent concentration of the species, diffusion coefficient, reaction rate and velocity vector. Reaction rate, \(R\) equal to zero because there is no reaction occurred. Different concentration was introduced to species where one species at concentration of 0 mol/m\(^3\) on the input boundary while the other one at 1 mol/m\(^3\). At the output boundary, the substances flows through the boundary by convection \([9]\). Diffusion coefficient are set in this simulation at \(1.24 \times 10^{-9} \text{ m}^2/\text{s}\) and \(9.4 \times 10^{-10} \text{ m}^2/\text{s}\) respectively for ethanol-water and glycerol-water case.

The concentration in mixing of micromixer is used to calculate mixing intensity by using (4) and (5). Thus, the result of mixing intensity indicates whether good or bad mixing quality obtained from T-shaped micromixer. \(I_M\) is described in (4) \([11]\).

\[
I_M = 1 - \frac{\partial^2}{\sqrt{\partial^2_{max}}}
\]

(4)

Where \(\partial^2_{max}\) is maximum variance of mixture and \(\partial^2\) is variance of tracer concentration along cross section of the mixing channel defined by (5):

\[
\partial^2 = \frac{1}{N} \sum (c_i - \bar{c}_m)^2
\]

(5)

Where \(N, c_i\) and \(\bar{c}_m\) represent number of sampling points inside cross section, mass fraction at sampling point I and optimal mixing mass fraction which equal to 0.5.

3. Result and Discussion

The concentration profile was illustrated in figure 2 for both diffusion coefficients at different inlet velocity which ranging from 0.0001 m/s to 1 m/s. Red colour and blue colour indicates that there are two species involved. Green colour indicates the complete mixing which results in 0.5 mol/cm\(^3\) concentration of the species. Red and blue colour were spread towards T-shaped micromixer before it turns into green colour that can be observed at inlet velocity of 0.0001 m/s and 0.001 m/s. This indicate complete mixing occurred at these inlet velocities. At inlet velocity of 0.01 to 1 m/s for both diffusion coefficient poor mixing occurred as the mixing channel contain red and blue colour.
Mixing is examined by evaluation of mixing performance parameter known as mixing intensity. Mixing intensity is evaluated by using (4) which indicates either good or bad mixing quality in the range of 0 to 1. The mixing quality at 0 indicates bad mixing quality while at 1 indicates good mixing quality. The effect of three parameters which are inlet velocity, different width size of outlet channel and diffusion coefficient are investigated towards mixing intensity.
Figure 3 shown the mixing intensity against inlet velocity for both cases of miscible liquid. The inlet velocity is varying at 0.0001 m/s, 0.001 m/s, 0.01 m/s, 0.1 m/s and 1 m/s and simulated with different diffusion coefficient which are $1.24 \times 10^{-9} \text{m}^2/\text{s}$, ethanol-water and $9.4 \times 10^{-10} \text{m}^2/\text{s}$, glycerol-water. As can be seen, the trend for both lines are similar which are mixing intensity decreasing as the inlet velocity increase agreed with the result had been obtained by [12]. The highest mixing intensity for both cases EW and GW are at inlet velocity of 0.0001 m/s whereas, the lowest mixing intensity at inlet velocity of 1 m/s. Early deduction can be as at lowest inlet velocity, the species having sufficient time for molecular diffuse through mixing channel for complete mixing.

![Figure 4: Mixing Intensity at Different Width Size for ethanol-water (EW)](image)

Figure 4 shows the mixing intensity against width size at different inlet velocity. The width size of mixing channel on T-shaped micromixer are varies from 0.025 cm to 0.1 cm. The effect of width size on mixing intensity is insignificant at lowest inlet velocity as the line show constant value and remain at value approaching 1. However, at higher inlet velocities simulated, the width size starts show some effect. At inlet velocity 0.001 m/s and 0.01 m/s, the lines show similar trend as the mixing intensity are reducing as the width is widening as reported by Liu Zhendong (2012) [5], broadening the width of mixing channel weakens the intensity of mixing. Whereas the mixing intensity for 0.1 m/s and 1 m/s inlet velocity shows almost similar value as the line overlap except for lower width size of 0.025 cm. The same result can be predicted for glycerol-water (GW) case as previously discussed, the effect of diffusion coefficient on mixing intensity is insignificant that might due to the small differences between both diffusivity values.
Figure 5. Mixing Intensity against Mixing Length at different inlet velocity

Figure 5 shows the mixing intensity against mixing length at different inlet velocity for ethanol-water case. As discussed previously, at lowest inlet velocity of 0.0001 m/s, complete mixing is achieved as the mixing intensity value approaching 1 and it happen at mixing length about 0.5 cm. The mixing length here represents the position of mixing channel with total length of 3 cm and the mixing intensity is evaluated at every 0.5 cm. The mixing length can be defined as the length required for the complete mixing occurred. At inlet velocity of 0.001 m/s, the mixing is almost complete as the mixing intensity approaching 1 at the end of mixing channel. Whereas, the mixing is incomplete for the rest of inlet velocity 0.01 m/s to 1 m/s simulated. Thus, it can be predicted that poor mixing quality resulted from higher inlet velocity regardless the mixing length as the mixing intensity shown constant value throughout the mixing channel.

4. Conclusion

In this research, the effect of inlet velocity and width size of mixing channel on mixing in T-shaped micromixer was investigated whereby the inlet velocity is varying at 0.0001 m/s, 0.001 m/s, 0.01 m/s, 0.1 m/s and 1 m/s was chosen. The concentration profile showed that complete mixing occurred only at inlet velocity 0.0001 m/s while the other inlet velocity showed mixing is not complete. The highest mixing intensity result at inlet velocity 0.0001 m/s while the lowest mixing intensity at inlet velocity 1 m/s. Therefore, it can be concluded that mixing intensity increase due to decreasing in inlet velocity. Meanwhile, for the effect of width size on mixing, the mixing intensity decrease as width of mixing channel widening for all inlet velocity except for inlet velocity of 0.0001 m/s. The T-shaped micromixer has sufficient length for complete mixing which is 3 cm at lower inlet velocity. As a conclusion, low inlet velocity shown better mixing quality regardless the width size and length of mixing channel of the T-shaped micromixer.
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