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Computer Fluid Dynamics (CFD) Simulation on Mixing in T-Slit Shaped Micro-mixer

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ABSTRACT

Numerical simulations were performed to study the mixing performance of two miscible liquids within a T-slit shaped micro-mixer, comparing the cases where the two inlet fluids are ethanol-water (E-W) and glycerol-water (G-W). The parameter that involved in this simulation is the inlet velocity varies from 0.0001 m/s to 1 m/s and width is ranging from 0.01 cm to 0.04 cm. The T-slit shaped micro-mixer which having a micro-channel of the outlet slit was constructed, the effect of inlet velocity on mixing and also effect of width towards mixing intensity (IM) were investigated via COMSOL Multiphysics software. The IM values defines whether a good or bad mixing quality could be achieved for T-slit shaped micro-mixer. The simulation results show a good mixing quality is achieved at low inlet velocity where the IM value approaches to one otherwise approaching to zero for high velocity.

Keywords:
Mixing, microchannel, micro-mixer, mixing Intensity

1. Introduction

The importance of micro-scales devices in chemical engineering has increased significantly during last 10 years as it provides considerable potential benefits to process industries such as polymerization and crystallization. The large surface to volume ratio is an advantage for the micro-mixer in which significantly improved the mass and heat transfer, thus improving yield and selectivity than conventional mixer. The conversion and selectivity in the liquid phase depends on the effective mixing so the effective mixing is important in many miniaturized flow systems. Mixing two different fluids in a micro-mixer is one of the basic processes in microfluidics. The simplest design of micro-mixer are T and Y-shaped micro-mixer [1]. In recent years, several researchers have been studied extensively on the mixing performance in of Y-shaped [2] and T-shaped [3,4] by experimental and computer simulation as they are quite suitable to carry out fundamental studies to understand the mixing at microscale.

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An attractive methodology for investigating mixing performance in micro-mixer is numerical simulation by Computational Fluid Dynamic (CFD), since its objective is to solve the flow and basic equations that provide a qualitative prediction of the movement and characteristics of the fluid flow [5]. There are three fundamental of the CFD which are Newton's second laws, mass and energy conservation that used to control the physical of fluid flow [6]. In this work, the actual T-shaped have been modified in which the outlet channel become a slit channel. The present study are focuses on the comparison between the case where the two inlets fluids are ethanol-water (E-W) and glycerol-water (G-W) at different inlet velocity and width of the outlet channel. In order to do that, the CFD is used to solve the two dimensional model of T-slit shaped. The mixing intensity is evaluated at different inlet velocity and width of the outlet channel; the result is observed. The implications of this result on the mixing efficiency of T-slit shaped micro-mixer will be discussed in details.

2. Numerical Simulation

2.1 Geometry and boundary condition

The two dimensional (2D) model geometry was constructed in COMSOL Multiphysics software. The T-slit shaped geometry consist of two inlets and one outlet slit channel as in Figure 1. The inlet width was 0.05 cm and the length was 2 cm. The outlet length was 3 cm and width of the outlet varies from 0.01 to 0.04 cm. The dimension of T-slit shaped was shown in Figure 2. The software provides two types of meshing that can be used by user which is physics-controlled meshing and user-controlled meshing. Physics-controlled meshing sequence will build the mesh for the domain which adapted to the physics setting of the model while the user-controlled meshing build mesh based on the user input of size and element type [7] . In this work, physics-controlled meshing with finer size was chosen as gives the better for the physical simulation study. The computational work was done by using numerical solution into solving the Navier-Stokes Equation together with Convection-Diffusion Equations [8].

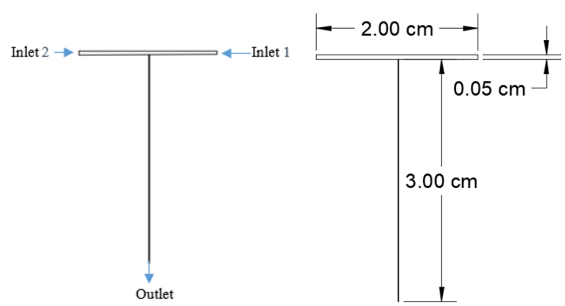

Fig.1. Boundary Condition of Computational Model (left) and dimension of T-slit Shaped Model (right)

2.2 Governing Equation

Consider two fluids converging into T-slit junctions. The two inlet stream have same temperature so that the heat of mixing has a negligible effect as assumed that the process is in isothermal. When a small velocity, a single phase of fluids can be often assumed incompressible which is density is constants. In general, the flow of an incompressible fluids under normal conditions which at 1 atm and 25 ^oC in micro channels can be described by the Navier-Stokes Equations [9] as shown in Eq (1) and Eq (2).

$$\rho \frac{\partial u}{\partial t} + \rho(u \cdot \nabla)u = \nabla \cdot [- PI + \mu(\nabla u + (\nabla u)^T)] + F \quad (1)$$

$$\rho\nabla \cdot u = 0 \quad (2)$$

where ρ is the density, u is the velocity vector, P is a pressure and F is the volume force vector. T is the absolute temperature. μ is the dynamic viscosity. The liquid is water at ambient conditions with the density, $\rho=1.0 \times 10^3$ kg/m^3 and viscosity, $\mu=1.0 \times 10^3$ Pas. The boundary conditions for both configurations are specified which the velocity profile is imposed at the inlet sections, the pressure outlet conditions assumed to be equal to zero are used for the outlets and no-slip boundary conditions are applied on the walls of the channels. For transport of diluted species, the diffusion flux was given by Fick's law depends on the diffusion coefficient. At highest diffusion coefficient, the diffusive flux was larger which lead to the fast and better mixing otherwise leads to the slow and bad mixing. Mixing is achieved by diffusion coefficient of the species in the fluid. The species are diluted in water, thus having material properties like water. The convection-diffusion equations for steady state flow, no-slip boundary conditions and incompresibble fluids as shown in Eq (3) [10].

$$\frac{\partial c}{\partial t} + u \nabla c = \nabla \cdot (D \nabla c) + R \quad (3)$$

where c is the concentration of the species, D represents the diffusion coefficient, u is the velocity vector and R is a reaction rate expression for the species where in this case it equal to zero since there is no chemical reaction involved. The initial concentrations were set as 0 and 1 for the two inlets respectively. At the outlet boundary, the substance flows through the boundary by convection [11].

2.3 Mixing Intensity

The mixing intensity or mixing efficiency is defined as a mixing index's status and the spatial profile along the flow of direction was used to determine whether a good or poor mixing quality that obtained from T-slit shaped micromixer. Mixing efficiency can be characterised by mixing intensity using the following equations [12–15]:

$$I_M = 1 - \sqrt{\frac{\partial^2}{\partial^2_{max}}} \quad (4)$$

$$\partial^2 = \frac{1}{N} \sum(C_i - \bar{C}_m)^2 \quad (5)$$

where I_M is the mixing intensity, ∂^2 is variance of the tracer concentration along the cross section of the mixing channel, $\partial_{max}{}^2$ is maximum variance of the mixture, N is the number of sampling points inside the cross section, C_i is mass fraction at sampling point i and $\bar{C}_m$ is optimal mixing mass fraction. Theoritically, the mixing intensity was represented by zero and one. The zero value indicates bad mixing and value of one shows good mixing.

3. Results and Discussion

The concentration profile along the outlet slit channel and convergence region or mixing area for different inlet velocity has been visualized in Figure 2 (top) and Figure 2 (bottom). Difference in value of the species concentration supplies at two inlet boundaries, one with 1 mol/m^3 and the other with 0 mol/dm^3 species concentration. Both species concentrations are indicated by red and blue colours respectively. The complete mixing of both concentrations will result in 0.5 mol/dm^3 concentration of the species and indicated by the green colour as seen in Figure 2 (top) and Figure 2 (bottom). Both colour, blue and red is spread through the outlet slit channel and diffused into each other before absolutely turn into green colour as can be observed clearly in Figure 2 (a), (b). Initial observation showed that this concentration profile is about the same for all value of inlet velocity and diffusion coefficient. However, assessing the mixing intensity value at outlet slit provides a better and clearer observation on the effect of changing the inlet velocity and diffusion coefficient as can be seen in Figure 2 (top) and Figure 2 (bottom). There is not too much difference of concentration profile between the two cases due to it tend homogenize the mixture in micro-mixer. However, at the inlet velocity 0.01 m/s, there are differences between the both figures where in Figure 2 (top) (c), the green colour is obviously seen. However, in Figure 2 (bottom) (c), the orange colour is clearly spotted and little green colour is spotted. The concentration profile at the inlet of the T-slit shaped micro-mixer is same for the inlet velocity from 0.0001 m/s to 0.1 m/s but not inlet velocity 1 m/s, the concentration profile shows that the fluids start to mix to each other due to it induced with high inlet velocity. For inlet velocity of 0.0001 m/s, 0.001 m/s and 0.1 m/s, the concentration profile at the outlet slit channel for both diffusion coefficients are the same. In Figure 2 (top) (e), the concentration profile at the outlet slit channel shows clearly the bright red on the left side and the light blue colour on the right side. Even though, the inlet velocity for both Figure 2 (top) (e) and Figure 2 (bottom) (e) were same (1 m/s), but Figure 2 (bottom) (e) shows better mixing due to the colour on the left and right side of the outlet slit channel is more light. However, the inlet velocity 0.1 m/s and 1 m/s indicate the poor mixing for both cases since at the outlet slit channel have the blue and red colour which can be said the mixing is incomplete.

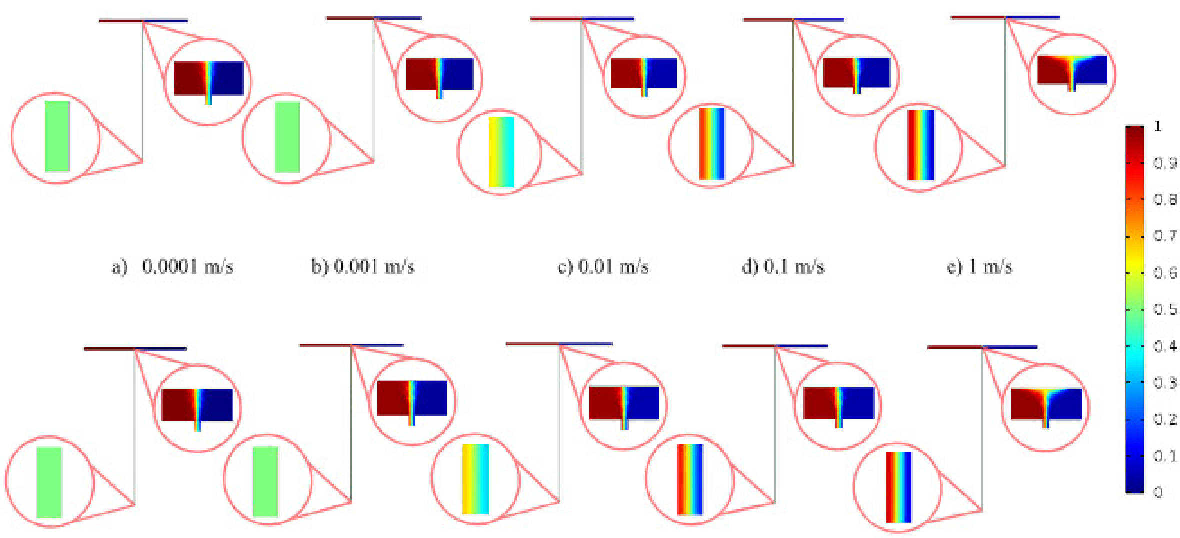

Fig. 2. Concentration Profile for Diffusion Coefficient of Ethanol and Water (top) and Glycerol and Water (bottom)

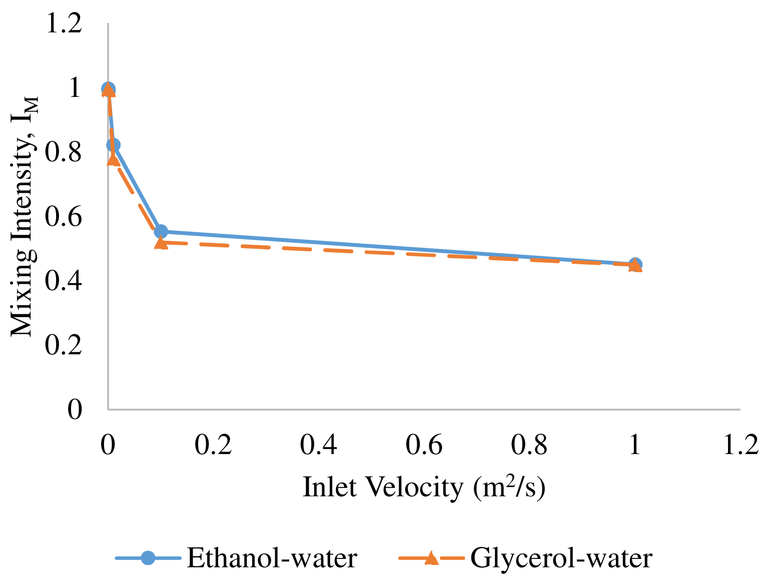

Fig. 3. Mixing Intensity at Different Inlet Velocity Based on Diffusion Coefficient

The mixing intensity at different inlet velocity for diffusion coefficient of E-W and G-W are shown in Figure 3. As can be seen, the trend is similar where the mixing intensity decrease as increasing the inlet velocity, demonstrating that the mixing performance decrease with increase of inlet velocity. Similar results were obtained by Cengel and Cimbala, [9]. However, at 0.0001 m/s of the inlet velocity, it gives the highest mixing intensity while at 1 m/s give the lowest mixing intensity. There are three point had an intermediate mixing intensity value which at inlet velocity 0.001 m/s, 0.01 m/s and 0.1 m/s. Thus, the lowest inlet velocity has sufficient time for molecule diffuse to each other, therefore, it provides good mixing quality as compared to other inlet velocity.

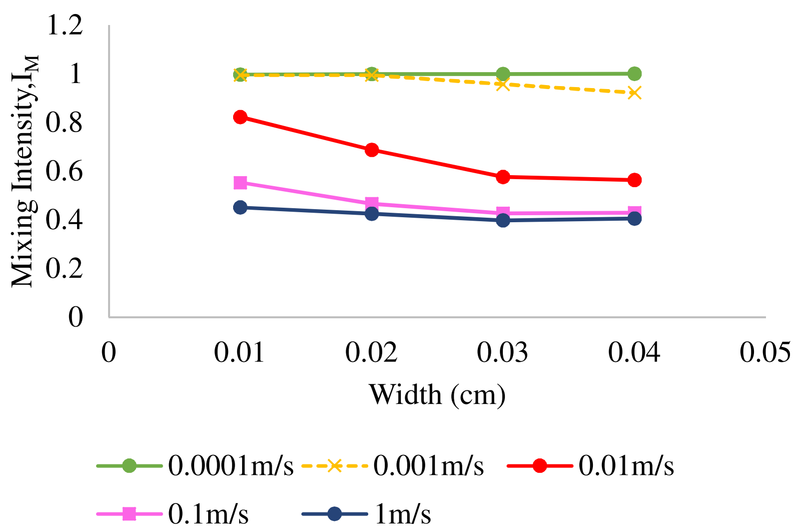

Fig. 4. Effect of Width on Mixing Intensity at Diffusion coefficient of Ethanol-Water

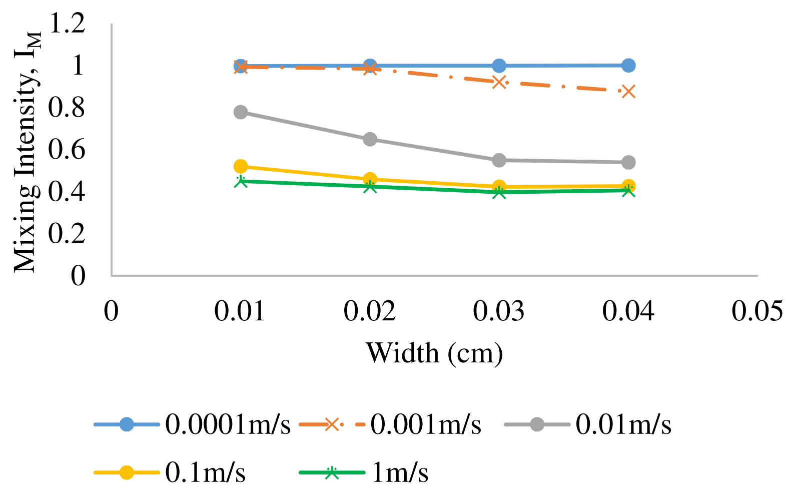

Fig. 5. Effect of Width on Mixing Intensity at Diffusion Coefficient of Glycerol-Water

The mixing intensity is observed for variation of outlet slit channel width from 0.01 cm to 0.04 cm with an increment of 0.01 cm. Simulation result for the effect of width of the outlet slit channel on mixing intensity at different inlet velocity for ethanol-water and glycerol-water are shown in Figure 4 and Figure 5. As indicated in both figures, the trends are about similar where the value of mixing intensity is decrease with increase the inlet velocity and widening the width. This have been proved by [3] that indicated widening the width of the outlet slit channel also weakens the mixing intensity. As can be seen in Figure 4 and 5, at 0.0001 m/s of inlet velocity does not have significant effect towards width and it indicated the highest mixing intensity due to the inlet velocity 0.0001 m/s have sufficient time to allow the molecule to diffuse. In both figures, the lines are about to overlaps to each other for inlet velocity 0.001 m/s at 0.02 cm of width and then the long dash dot line start to decrease at width 0.04 cm. For the inlet velocity 0.01 m/s, clearly shows that the mixing intensity is decrease with increasing width. At inlet velocity of 0.1 m/s and 1 m/s, the mixing intensity slowly decrease with enlargement of width. However, at width 0.01 cm, the highest mixing intensity could be achieved at the lowest inlet velocity which is 0.0001m/s and similar trend for other width.

4. Conclusion

It has been shown in this work how to characterize the mixing quality in micro-mixer via numerical simulation, CFD. The model of CFD simulation on mixing in T-slit shaped micro-mixer for fast mixing in laminar flow was constructed. The design of the micro-mixer has significantly affect the performance of the micro-mixer. In the micro-mixer, two liquids are force to be laminae. The effect of inlet velocity on mixing in T-slit shaped micro-mixer was studied where the mixing intensity decrease as increasing in the inlet velocity, demonstrating that the mixing performance decrease with increase of inlet velocity. The inlet velocity of 0.0001 m/s its indicated the highest mixing intensity compared to others inlet velocity. The effect of width towards mixing intensity was studied, where the most better inlet velocity 0.0001 m/s, which indicated the highest mixing intensity for all width in this simulation. Whereas, the inlet velocity 1 m/s, indicated the lowest mixing intensity at width 0.04 cm. For other velocity, the mixing intensity values is decrease with increase the inlet velocity and widening the width.

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