CHEMICAL ENGINEERING TRANSACTIONS

VOL. 56, 2017

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.aidic.it/cet

Guest Editors: Jiří Jaromír Klemeš, Peng Yen Liew, Wai Shin Ho, Jeng Shiun Lim

ISBN 978-88-95608-47-1; **ISSN** 2283-9216

DOI: 10.3303/CET1756014

Computational Fluid Dynamic Simulation of Mixing in Circular Cross Sectional Microchannel

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The application of process intensification has been catching up with the trend already observed in the chemical engineering area, where the use of microfluidic devices has already been elevated to production scale. Microreactor technology, an element of process intensification, offers potential benefits to the future of chemical engineering for its well-defined 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. Since mixing has a crucial impact on the overall performance of micro reaction processes, the need for measuring and comparing mixing performance have also increased. To exploit the resulting potential, the mixing behaviour of flow mixers on micro-scales need to be further investigated. In this work, three-dimensional Computational Fluid Dynamics (CFD) model with circular cross section micro channel has been developed instead of rectangular cross section done by other researchers as circular micro channel can withstand large pressure difference without undergoing any significant distortion where non-circular cannot. The CFD simulation was carried out using COMSOL Multiphysics 4.2a software to investigate the effects of "T" and "Y" micro channel configurations, inlet velocity and diffusion coefficient towards the mixing quality in the micro reactor. The results demonstrated that inlet velocity and diffusion coefficient has significant effects on mixing performance where low inlet velocity and high diffusion coefficient value resulted in better mixing performance. It was found that "Y"-shaped micro channel showed complete mixing at a shorter distance as compared to "T"-shaped micro channel and the minimum mixing length of micro channel needed for complete mixing is 20 mm.

1. Introduction

Research works on micro-scaled devices in chemical engineering have significantly increased as it provides considerable potential benefits to process industries (Song et al., 2006). The main benefit of micro reactor over the conventional reactors is the large area-to-volume ratio of micro reactors which considerably enhanced mass and heat transfer rates that offers better yield and selectivity (Hessel et al., 2005). This highlights the importance of understanding the concept of microfluidic environment and their applications in the context of mixing. There is an increase need for measuring and comparing mixing performance since mixing has a crucial impact on the overall performance of reaction in micro-vessel.

Due to the absence of turbulence in microfluidic devices, micro mixers mainly depend on the micro channel geometry for fluid mixing by folding fluids to increase the interfacial area over which diffusion occurs. Mixing in these devices is achieved solely based on diffusion between the two fluid streams, as there is no external force applied (Bhagat et al., 2007). Micro channel geometry plays important role for the mixing to take place faster within shorter distances.

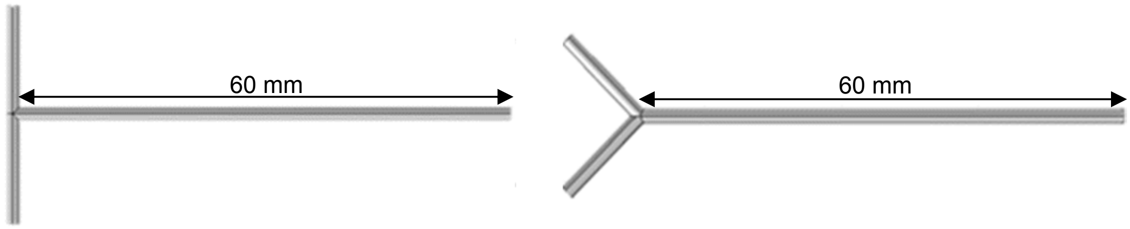
Several researchers have studied on the mixing performance of T-shaped (Zhendong et al., 2012) and Y-shaped (Shi et al., 2012) micro reactor with a rectangular cross section and other type of micro mixers via experimental and computer simulation approaches. Little information on simulation study was found with regards to T and Y-shaped micro reactor with circular cross section, which is the main interest in this work. Owing to this situation, this research took the opportunity to construct the geometry of the microreactor and analysis via Computational Fluid Dynamics (CFD) simulation. Investigation on the effect of microchannel

Please cite this article as: Rahim N.A.A., Azudin N.Y., Shukor S.R.A., 2017, Computational fluid dynamic simulation of mixing in circular cross sectional microchannel, Chemical Engineering Transactions, 56, 79-84 DOI:10.3303/CET1756014

configurations, inlet velocity and diffusion coefficient towards mixing of the two geometry configurations were also included in this study.

2. Computational Fluid Dynamic Model

The model geometry was built in COMSOL Multiphysic 4.2a software (COMSOL, 2012). The T-shaped (Figure 1(a)) and Y-shaped (Figure 1(b)) geometry both consist of circular cross section micro channel with two inlets channels, each with a length of 15 mm and a diameter of 2 mm. The mixing channel is 60 mm long with the same diameter as the inlet channels. The software provides two option types of meshing that can be used by user which is physics-controlled meshing and user-controlled meshing. Physics-controlled meshing sequence will built the mesh for the domain which is adapted to the physics setting of the model. While the user-controlled meshing build the mesh based on the user input of size, element type and etc. (COMSOL, 2012). In this work, physics-controlled meshing with normal size was chosen as it suits the best for the physical setting of the simulation understudy. The numbers of mesh elements build for both geometries are shown in Table 1.
The computational work was done by using numerical solution into solving the Navier-Stokes Equation together with convection-diffusion equation (Baccar et al., 2009).



(a) (b)

Figure 1: Microreactor geometry: (a) T-shaped (b) Y-shaped

Table 1: Number of mesh elements

Mesh Element	T-shaped Channel	Y-shaped Channel
Tetrahedral	47,151	36,907
Pyramid	128	52
Prism	17,112	14,972
Triangular	8,860	7,724
Quadrilateral	96	96
Edge	1,020	948
Vertex	17	24
Total Elements	74,384	60,723

2.1 Numerical Solution

The flow of an incompressible Newtonian liquid in micro channels can generally be described by the Navier–Stokes equation and continuity equation as shown in Eq(1) and Eq(2) (Baccar et al., 2009).

$$\rho\frac{\partial v}{\partial t} + \rho(v \cdot \nabla)v - \eta\nabla v + \nabla p = 0 \quad (1)$$

$$\nabla \cdot v = 0 \quad (2)$$

where v, p, ρ and η represent the velocity vector, the pressure, the density of the fluid and the dynamic viscosity. The density and the viscosity data are those of water (ρ = 1,000 kg/m^3 and $\eta = 0.001$ 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 is assumed to be equal to zero. The channel wall is assumed to have a non-slip boundary condition. Mixing is achieved by diffusion of the species in the fluid. The species are diluted in the water, thus having material properties like water. The transfer equation with a reaction term is as shown below (Wong et al., 2004):

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

Where c, D, R and v represent the concentration of the species, diffusion coefficient, reaction rate and velocity vector. In this model, R = 0 because there is no reaction occurred. The species is introduced at different concentration from the range of 0 to 1 mol/m^3, where one species is at a concentration of 0 mol/m^3 on one of the input boundary while the other is at 1 mol/m^3. At the output boundary, the substance flows through the boundary by convection (Baccar et al., 2009).

3. Result and Discussion

Visualisation of mixing process in this work can be seen clearly by the plotted concentration profile of the species before and after the mixing process which represented by different colour gradient. In particular, blue and red colour represented the unmixed species while the mixed species represented by green colour. The cross sectional area view is arranged in ascending order of the inlet velocity from 10 µm/s to 1,000 µm/s and at diffusion coefficient, D, from 1.0 x 10^{-10} m^2/s to 1.0 x 10^{-8} m^2/s for comparison purposes.

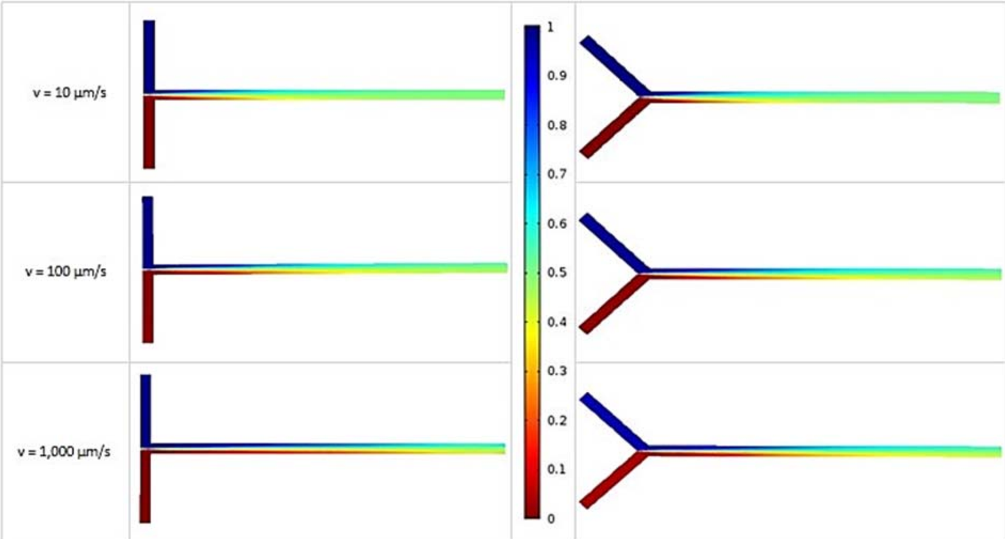


Figure 2: Concentration profile of T- and Y-shaped micro channel for various inlet velocities at D = 1.0 x 10^{-10} m^2/s

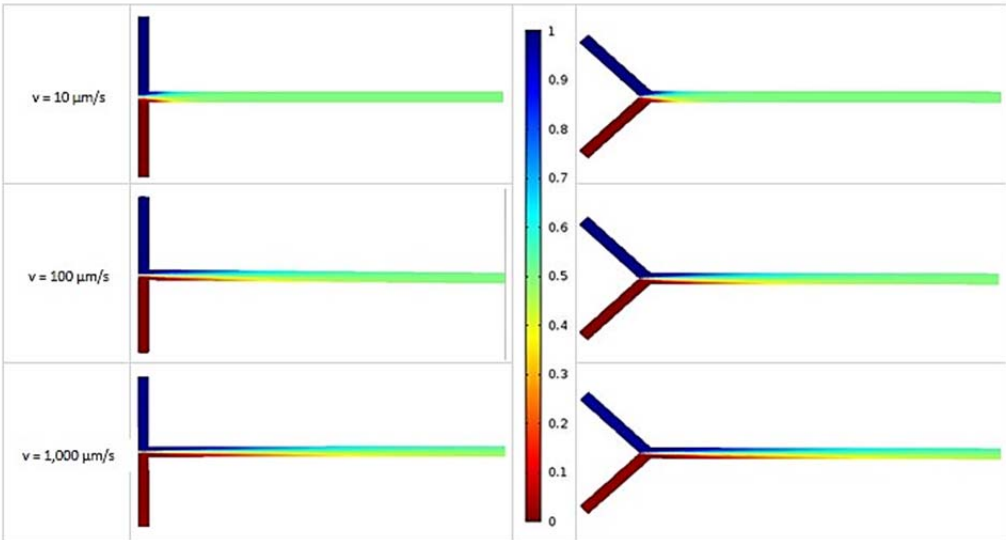


Figure 3: Concentration profile of T- and Y-shaped micro channel for various inlet velocities at D = 1.0 x 10^{-9} m^2/s

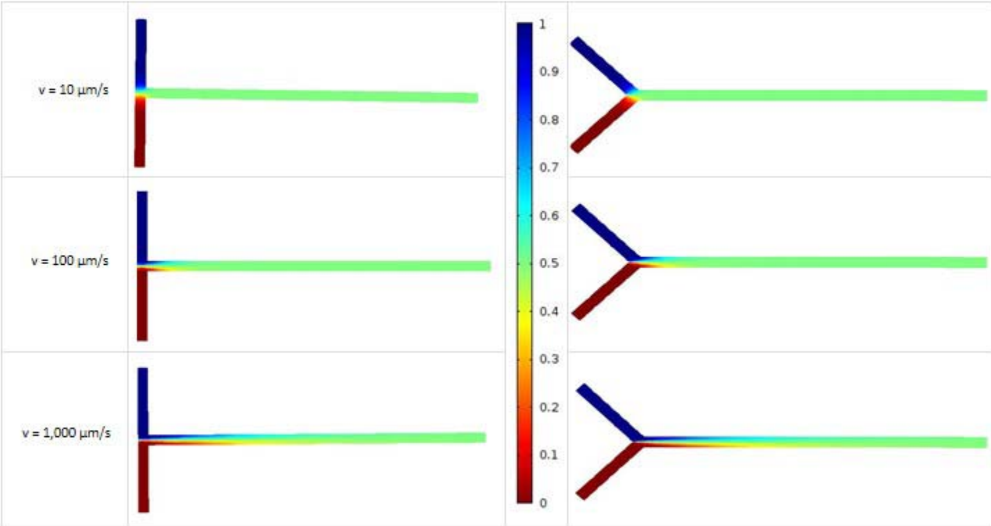


Figure 4: Concentration profile of T- and Y-shaped micro channel for various inlet velocities at D = 1.0 x 10^{-8} m^2/s

Figure 2 to Figure 4 show the concentration profile of T and Y-shaped micro channel for all the inlet velocities and diffusion coefficient studied in this work. The mixing start when the fluids with different concentration denoted as blue and red colour enters the mixing channel. For inlet velocity of 1,000 μm/s at diffusion coefficient of D = 1.0 x 10^{-10} m^2/s and D = 1.0 x 10^{-9} m^2/s as in Figure 2 and Figure 3, the mixing is incomplete as distinct of colour can be seen from entrance until the end of mixing channel. While at diffusion coefficient of D = 1.0 x 10^{-9} m^2/s and D = 1.0 x 10^{-8} m^2/s as in Figure 3 and Figure 4, a perfect split-up of the concentration is observed at the entrance for inlet velocity of 10 μm/s. The mixing process is completed. Both geometric domains have similar dimension but different configuration of micro channel. Complete mixing occurs much faster at low inlet velocity than at higher inlet velocity for the entire diffusion coefficient value tested.

As can be seen in Figure 4, for T and Y-shaped micro channels, at lowest inlet velocity, the colour intensity shows the concentration is already diluted before it reached the mixing chamber entrance. The concentration profiles provide information of the mixing process inside the micro channel whether it is complete or incomplete. Further detail explanation about the difference of mixing performance between the domains demands new parameter to be evaluated. One of the parameter that can be used is the mixing quality in several cross sections.

The evaluation of mixing quality is to determine which micro channel has better mixing quality through visualisation of the colour gradient at five cross sections at the lowest inlet velocity which is 10 μm/s. Concentration of 0.5 mol/m^3 which represented by green colour indicates complete mixing at that particular cross section. For T and Y-shaped micro channel, the distances of cross section evaluated are at 0, 1, 20, 40, and 60 mm along the mixing channel. To get clear visual comparison between both micro channel configuration, all the cross sections at inlet velocity of 10 μm/s are summarised in Table 2.

Table 2 shows the summary of cross sections visualisation at inlet velocity of 10 μm/s and at all diffusion coefficients. It can be clearly seen that the cross section colour of Y-shaped micro channel at 1 mm and 20 mm at diffusion coefficient of D = 1.0 x 10^{-8} m^2/s and D = 1.0 x 10^{-10} m^2/s, are more intense than the cross section colour of T-shaped micro channel of the same diffusion coefficient. Thorough examination of the cross section visualisation show that Y-shaped micro channel have greater mixing quality at highest diffusion coefficient than T-shaped micro channel even though the trend of mixing quality of both micro channel more or less similar to each other which is also being agreed by Shi et al. (2012).

Table 2: Summary of cross section visualisation at inlet velocity of 10 µm/s

Inlet Velocity (µm/s)	Diffusion Coefficient, D (m²/s)	Shape	Distance of cross section along the mixing channel (mm)				
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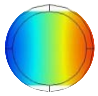
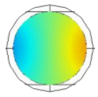
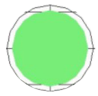
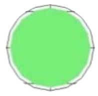
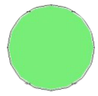
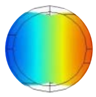
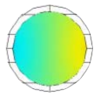
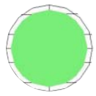
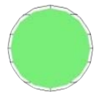
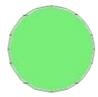
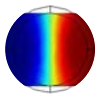
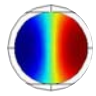
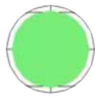
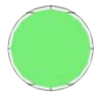
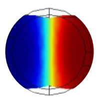
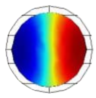
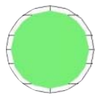
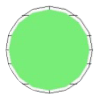
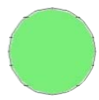
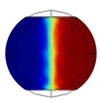
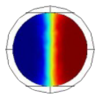
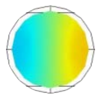
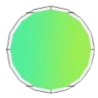
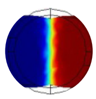
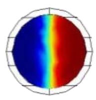
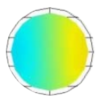
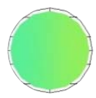
10	1.0×10^{-8}	T					
		Y					
	1.0×10^{-9}	T					
		Y					
	1.0×10^{-10}	T					
		Y					

4. Conclusion

T and Y-shaped geometry configurations with circular cross section were developed. A study of mixing simulation of the model geometries was conducted using a three-dimensional Computational Fluid Dynamics simulation via COMSOL Multiphysic software. Analysis was carried out to investigate the effect of the changes of inlet velocity and diffusion coefficient toward mixing quality over both micro channel configurations. The resulted simulations of both micro channel configurations were compared.

At lowest velocity (10 µm/s), the mixing length of micro channel needed is 20 mm while at lowest diffusion coefficient (1.0×10^{-10} m^2/s), 60 mm is needed to achieve complete mixing. The micro channel needs shorter mixing length if low inlet velocity is used, while longer mixing length is needed when lower diffusion coefficient is used.

The simulation shows that inlet velocity has significant effect on the mixing quality where it can be concluded that the lower the inlet velocity, the better the mixing quality. In order to shorten the mixing length, higher value of diffusion coefficient needs to be used. Careful observation on the mixing quality profiles of both geometry configurations shows that Y-shaped micro channel has better mixing quality than T-shaped micro channel at the same parameter.

Acknowledgements

This study has been supported by Fundamental Research Grants Scheme (FRGS-PJKIMIA/6071255).

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