Chapter

Computational Fluid Dynamics of Mixing Performance in Microchannel

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Abstract

In microchannel, fluid viscous effect becomes dominant, and the micro-flow typically falls in laminar regime. Mixing of fluid in the absence of turbulence is a slow molecular process as it is solely dependent on diffusion. Fast and complete mixing of relevant fluids is of crucial importance in many chemical engineering processes, thus computational fluid dynamics simulation on mixing in microchannel is the main topic in this chapter. The simulation was based on laminar flow and convective diffusion equation model. The factors affecting the mixing performance in microchannel was further simulated. The finding provides some insight of transport phenomena on mixing in microchannel.

Keywords: mixing, microchannel, laminar, diffusion, simulation

1. The microreactors and microchannel

Microreactor is more commonly known in the field of process intensification and microsystems technology that has attracted significant interest in several years. The channel of microreactor is known as microchannel due to the micro size, while under microreactor group, there are micro mixers which are designed for mixing purpose. Numerous plausible advantages of microreactors for the pharmaceutical and fine chemical industries have been realized, thanks to their excellent capability for mixing and for thermal exchanges which increase yields and selectivity of reactions [1–4].

Microreactors have two major advantages with respect to smaller physical size and the increase in numbers of units. Benefits from reduction of physical size became more apparent in chemical engineering aspects. The difference of physical properties between microreactors and conventional reactor such as temperature, concentration, density, or diffusional flux increase with decreasing of linear dimension [5, 6]. Consequently, the driving forces for heat transfer, mass transport increase when using the microreactors. Besides, a significant reduction in volume for microreactor as compared to conventional reactors lead to smaller hold up that increase process safety and improves selectivity due to shorter residence time [7, 8].

2. Fluidic and mixing environment

The smooth and constant fluid motion represents the laminar flow, whereas the vortices and flow fluctuation are properties of turbulent flow. These two types of flow are determined by using Reynolds number. Reynolds number (Re) measured the relative importance of viscous force and inertial forces. The Re is defined as

$$\mathrm{Re} = \frac{\rho \nu D_{\mathrm{h}}}{\mu} \tag{1}$$

where ρ and μ are the fluid density (kg/m^3) and viscosity (kg/m s), respectively; v is the velocity of the fluid (m/s) and D_h is the hydraulic diameter of the channel (m). Due to specific microstructuring technology employed to build microreactor, the channels of the microreactor have rectangular or trapezoidal cross section [9]. Thus, the hydraulic diameter D_h has to be properly defined. The hydraulic diameter of rectangular shapes is defined as [10]:

$$D_h = \frac{2wh}{(w+h)} \tag{2}$$

where w is the width and h is the height of the microchannel.

On the other hand, mixing is a physical process with a goal of achieving a uniform distribution of different components in a mixture, usually within a short period of time [7]. Conventionally, at a macroscale level, the decrease in the mixing path and increase in the contact surface are achieved by a turbulent flow. The segregation of the fluid into small domain occurred by the help of vortices and flow fluctuation [11].

The fluid entity is constantly subdivided into thinner layers by an induced circular motion of fluid compartments, the so-called eddies, and subsequent breaking into fragments. In a laminar regime, a similar breaking of fluid compartments cannot occur due to the high viscous forces. Instead, the fluid entity has to be continuously split and recombined, forming regularly sized fluid embodiments [7].

Due to small dimension of microreactor, the fluid in microreactor is considered as microfluidic. The mixing in microfluidic is achieved and improvised by the decrease of mixing path and increase of surface area. The designed microreactor that highlights reduction of mixing path increases the effect of diffusion and advection on the mixing [11].

On top of that, mixing characterization is important to show how mixing performances in certain mixing process are described. Mixing performance of microreactor can be measured by evaluating the mixing quality as be done numerously in literatures [12–16]. A common definition of the mixing quality is based on Danckwerts' intensity of segregation [17] and is defined by

$$I_s = \frac{\sigma^2}{\sigma^2_{\max}} \tag{3}$$

where $\sigma^2_{\max}$ is the maximum possible variance (which is 0.5 for symmetrical boundary condition) and σ^2 is defined by

$$\sigma^2 = \frac{1}{|V|}\int_V (c - \bar{c})^2 dV \tag{4}$$

and also can be written as

$$\sigma^2 = \frac{1}{N} \sum (c - \bar{c})^2 \quad (5)$$

where $\bar{c}$ denotes the mean value of the concentration field c and N as the sampling point inside the cross section. Then, a measure for the intensity of mixing or the so-called mixing intensity can be deduced as

$$I_M = 1 - \sqrt{I_s} = 1 - \frac{\sigma}{\sigma_{\max}} \quad (6)$$

Since I_s is normalized, the quantity I_s reaches a value of 0 for a completely segregated system and a value of 1 for the homogeneously mixed case.

3. Simulation of mixing in microchannel

3.1 Geometric and meshing

Geometry is defined as the computational domain of the flow region where the governing equation of fluid flow, mass, and energy is applied with its boundary condition. The computational domain is different from physical domain as the physical domain is the real physical flow that might include the wall, etc. [19]. The geometry may result from measurement of the existing configuration or may come with a design study.

In this work, the geometry is chosen, aspired by the actual geometry domain (physical domain) which is depicted in **Figure 1** of the standard slit interdigital micro mixer (SSIMM) mixing element. The mixing element of the micro mixer consists of the corrugated wall of microchannels and discharge slit. Simulation of the complete geometry of this mixing element required large number of degree of freedom to be solved. This can only be achieved by large computational resources. However, due to the limitation of the computational resource, simplification of the geometry is preferred and required. Thus, to simplify the computational work, only the middle part of the mixing element structure domain was taken to represent the overall mixing element as shown in **Figure 2**.

The middle part was chosen based on strategies of the macro model approach of computational fluid dynamics in [9] that partitioned the reactor domain prior to simulation. It was noticed that the mixing element of the SSIMM has trapezoidal shape with two bifurcations and parallel microchannel that served as flow guide to avoid maldistribution of the fluid stream. A fluid maldistribution would induce unequal residence time in different channels, with undesired consequences for the product distribution in the micromixer [9]. However, this is not considered in this study as only the middle part of the mixing element is taken as computational fluid domain.

There are two inlets and an outlet assigned to this model geometry as in **Figure 2**. An additional geometry domain with a straight-line microchannel was built for the purpose of comparisons with the SSIMM mixing element. The geometry has the same dimension as the simplified corrugated microchannel domain. On the other hand, meshing is the process of generating mesh or grid cell overlaying the whole domain geometry. In CFD, the domain is required to be subdivided into a number of smaller, non-overlapping subdomains in order to solve the flow physics within the domain. COMSOL Multiphysics software chosen as the simulation platform in this work provides two option types of meshing that can be used by the user which are physics-controlled meshing and user-controlled meshing. Physics-controlled meshing sequence will build the mesh for the domain which is adapted to

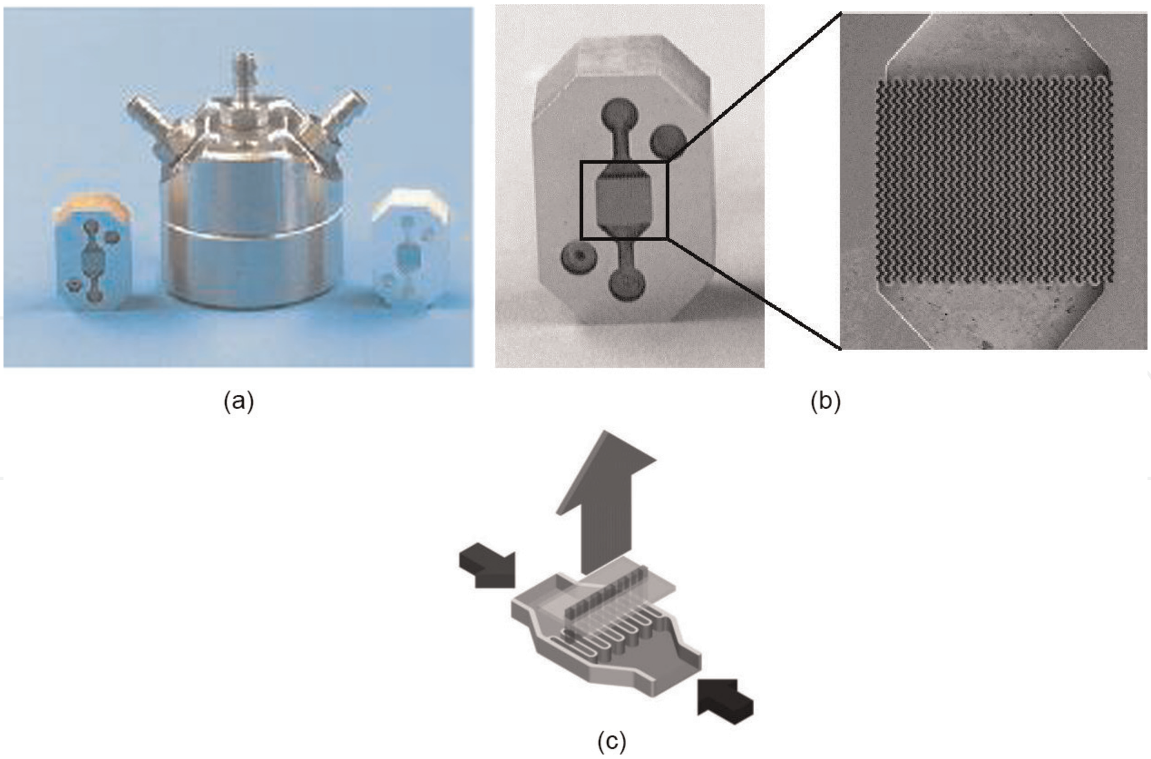

Figure 1.
(a) The photograph of SSIMM and (b) the mixing element; (c) the flow principle of SSIMM [18].

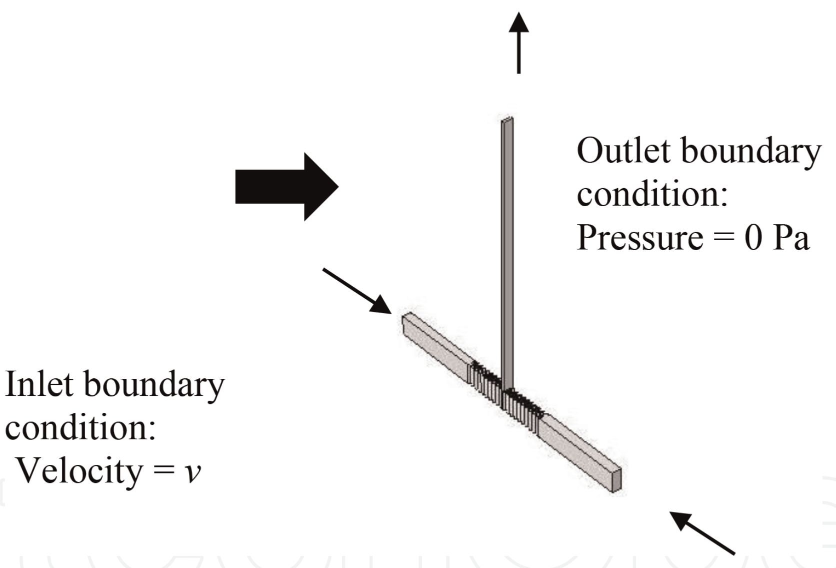

Figure 2.
Schematic diagram of the simulation system.

the physics setting of the model, while the user-controlled meshing builds the mesh based on the user input of size, element type, etc. [19, 20]. **Figures 3** and **4** are the meshed geometry domains with different types of the mesh element can be seen. The mesh element of corrugated microchannel has a high number at the shape of the corrugated section, while the straight microchannel has a high number at the entrance of the discharge slit.

3.2 Governing equation

Laminar flow interface is used to model and simulate fluid mechanics for laminar and incompressible fluids by using Navier-Stokes equation. Since the fluid flow is laminar flow in the microreactor, this interface is suitable to be implemented in this simulation work. The Navier-Stokes equation for incompressible flow is given as [20]:

$$\rho \frac{\partial v}{\partial t} + \rho(v \bullet \nabla)v = \nabla \bullet \left[-pI + \mu\left(\nabla v + (\nabla v)^T\right)\right] + F \\ \rho \nabla \bullet v = 0 \tag{7}$$

where v is velocity vector (SI unit: m/s); p is the pressure (SI unit: Pa); ρ is the density (SI unit: kg/m^3); F is the volume force vector (SI unit: N/m^3); μ is the dynamic viscosity (SI unit: Pa.s); and T is the absolute temperature (SI: K).

The density and the viscosity data are those of water (ρ = 1 × 10^3 kg/m^3 and μ = 1 × 10^{-3} Pa s).

The driving force for the fluid to flow through the mixing slot 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. Meanwhile, the chamber wall is assumed to have a nonslip boundary condition. Mixing is obtained by diffusion of various species in the fluid. The species are diluted in the water, thus having material properties like water. The transfer equation is then taken as the convection-diffusion equation with a reaction term as shown below [20]:

$$\frac{\partial c}{\partial t} + \nu \bullet \nabla c = \nabla \bullet (D \nabla c) + R \tag{8}$$

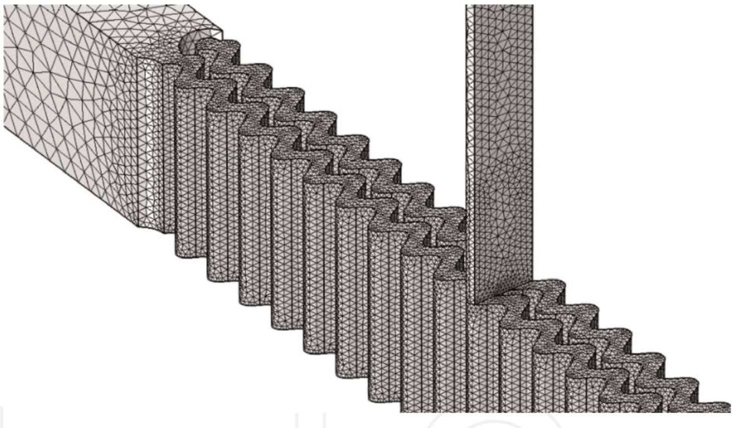

Figure 3.
The meshing for corrugated microchannel.

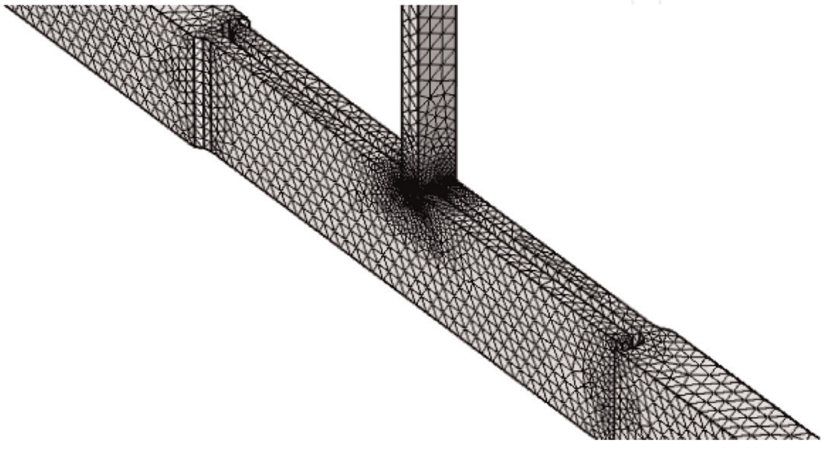

Figure 4.
The meshing for straight microchannel.

where c is the concentration of the species (SI unit: mol/m^3); D is the diffusion coefficient (SI unit: m^2/s); R is a reaction rate expression for the species (SI unit: mol/(m^{3}s)); and v is velocity vector (SI unit: m/s).

In this model, $R = 0$, because there is no reaction occurred. The species is introduced at different concentration from the range of 0–1 mol/m^3 where one species is at a concentration of 1 mol/m^3 on one of the input boundaries, while the other is at zero concentration. At the output boundary, the substance flows through the boundary by convection [21].

3.3 Velocity and concentration profile visualization

As mentioned earlier, there are two physics interface models that were solved in this work which are laminar flow (LF) and transport of diluted species (TDS). The LF interface model considers the fluid flow of the system with inlet velocity ranging from 1 to 10,000 μm/s chosen as input parameter. The LF interface model is solved independently. However, the TDS interface model is solved by obtaining a data of velocity field from the solution of the LF interface model. This is the reason why both physics interface models are used together. **Figures 5** and **6** show the velocity profile from the top view (XY view) of the geometric configuration comprised of corrugated and straight microchannel, respectively. The color gradient shows the maximum velocity of the microchannel at the middle of the channel which can be

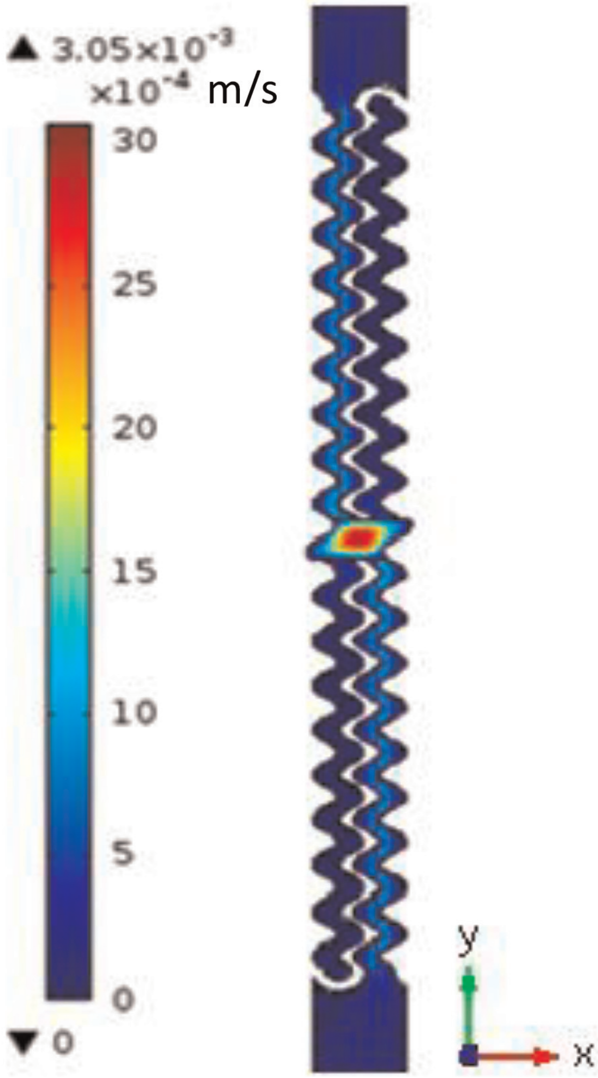

Figure 5.
Velocity profile of corrugated microchannel from XY-axis view.

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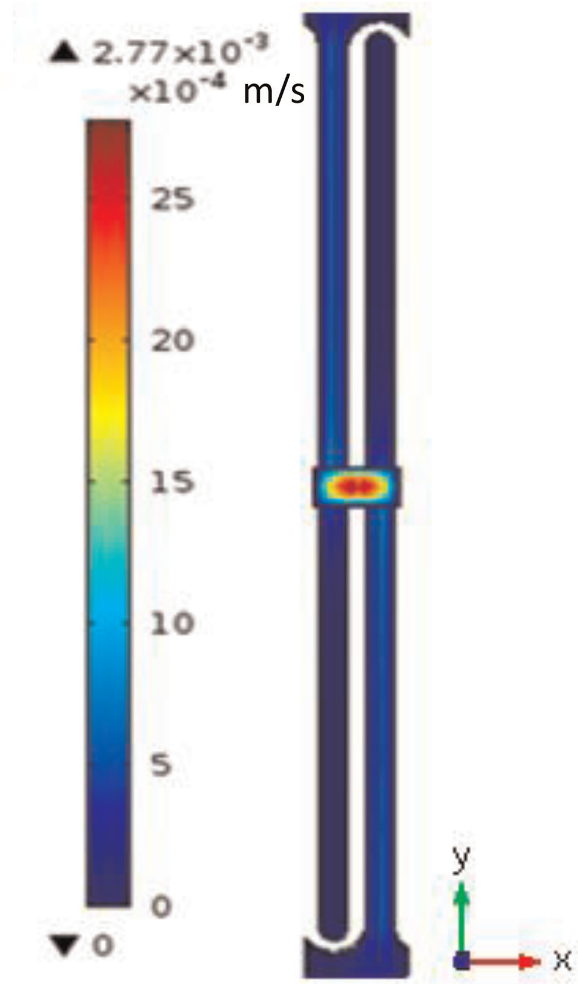

Figure 6.
Velocity profile of straight microchannel from XY-axis view.

seen in red color, while the blue color represents the low velocity value which is at the domain wall. This phenomenon indicates laminar parabolic flow where the velocity varies parabolically across the discharge slit with the maximum velocity at the center.

Visualization of mixing process in this work can be seen clearly by the plotted concentration profile of the species in which the different color gradients represent the species before and after the mixing process. In particular, the unmixed species is represented by blue and red colors, and the green color represented the mixed one.

Figures 7 and **8** shows the concentration profile of the corrugated and straight microchannel respectively for all the inlet velocities studied in this work. Both geometric domains have similar dimension of length and width but different configuration of microchannel. The mixing starts when the fluids with different concentrations denoted as blue and red enter the discharge slit. A clear separation of the

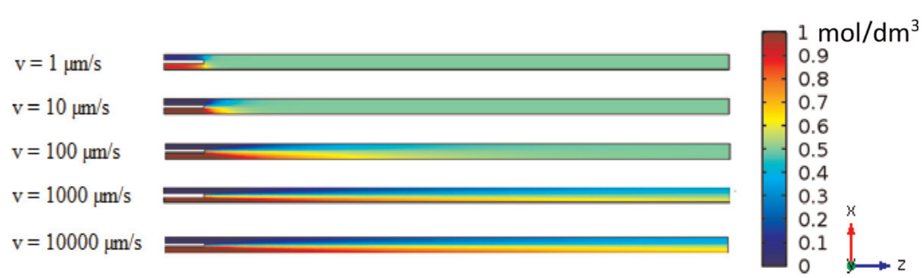

Figure 7.
Concentration profile of corrugated microchannel for various inlet velocities.

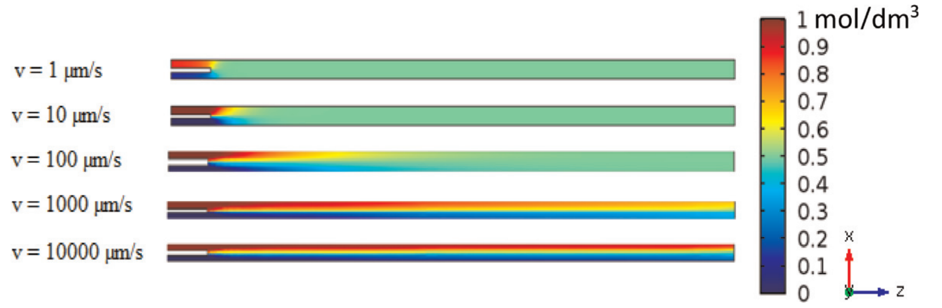

Figure 8.
Concentration profile of straight microchannel for various inlet velocity.

concentration is observed at the entrance, but this diminishes toward the end of the discharge slit for inlet velocity equal to 100 μm/s. Thus the mixing process is completed. For inlet velocity lower than 100 μm/s, the mixing completely occurred instantaneously as the fluids enter the discharge slit. For inlet velocity higher than 100 μm/s, the mixing is not complete as distinct color can be seen from the entrance until the end of discharge slit.

In short, complete mixing occurred at low inlet velocity, and the mixing is incomplete at higher inlet velocity of 100 μm/s for both configurations of microchannel.

3.4 Mixing intensity evaluation

As mentioned in previous section, the Danckwerts segregation intensity or the so-called mixing intensity is defined with the mean square deviation of the concentration profile of the component *i* in a cross section of the discharge slit. The segregation intensity can be transformed to a value between 0 (completely segregated) and 1 (completely mixed) [22].

In this work, to determine the mixing quality with respect to discharge slit length, the value of mixing intensity is evaluated at every 100 μm of discharge slit position starting from 300 μm where the fluid starts to mix until 4300 μm which is the end of discharge slit. The mixing intensity value against the discharge slit position for both corrugated and straight microchannels at inlet velocity of 10,000 μm/s is plotted in **Figure 9**. The mixing intensity of corrugated microchannel is higher than the mixing intensity of straight microchannel.

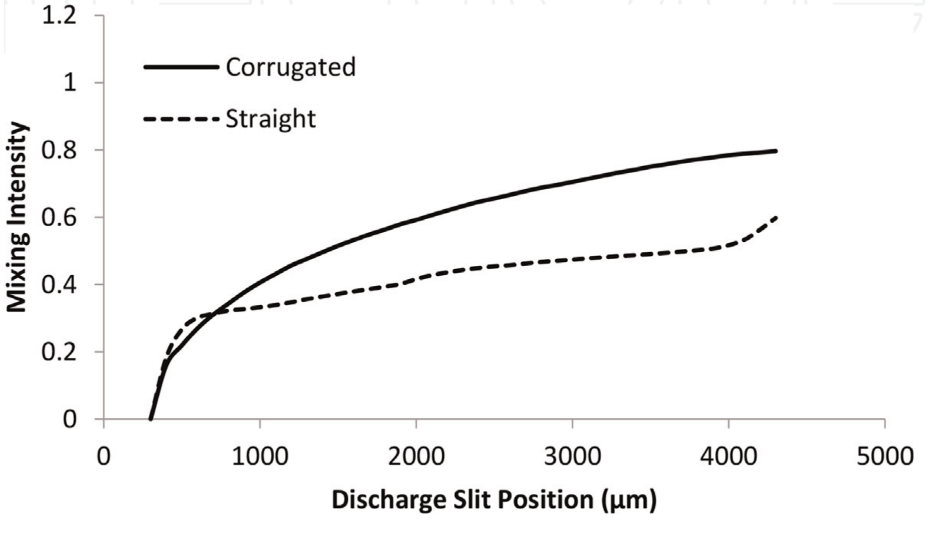

Figure 9.
Comparison of mixing intensity between geometric configuration at inlet velocity of 10,000 μm/s.

As compared to concentration profiles, the mixing intensity profile gave information of mixing quality with respect to discharge slit position. The discharge slit position can represent the mixing length. These mean that complete mixing occurred at different mixing length. The mixing profile shows the difference of mixing intensity profile among the microchannel configurations. The corrugated microchannel has gradually increased the profile of mixing intensity from the entrance toward the end of the discharge slit. This might be due to the corrugated shape of the microchannel which serves to form multi-lamination of fluid that gives even distribution of concentration which then results in a smooth mixing intensity profile. This might prove that the concept of multi-lamination of fluid as the purpose of microreactor is designed in such way.

4. Conclusions

This chapter discussed a study of mixing simulation in microchannel. An analysis is carried out to investigate the effect of the changes of inlet velocity toward mixing intensity over the two different microchannel configurations. The simulation results show the visualization of velocity and concentration profiles along the microchannel. A laminar parabolic flow of velocity profile is observed for two microchannel configurations simulated. The concentration profile gave visualization on the mixing process that occurred in the microchannel. Evaluation of the mixing intensity value represents the mixing performance of the geometry structure. It also gave information on the mixing length requirement to achieve complete mixing. The microchannel needs longer discharge slit to achieve complete mixing if high inlet velocity is used. The result showed that inlet velocity has significant effects on the mixing performance which is represented by the mixing intensity in this study. The higher the inlet velocity, the lower the mixing quality. Careful observation on the mixing intensity profiles among geometry configurations shows different trends of mixing intensity between the corrugated and straight microchannels.

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Appendices and nomenclature

c	concentration (mol/dm^3)
D	diffusion coefficient (m^2/s)
D_h	hydraulic diameter (m)
F	volume force vector (N/m^3)
p	pressure (Pa)
L	length (m)
w	width (m)
h	height (m)
R	reaction (mol/(m^{3}s))
T	absolute temperature (K)
v	velocity (m/s)
μ	dynamic viscosity (Pa.s)

ρ	density (kg/m^3)
V	volume (m^3)
λ	molecular diameter (m)
D	characteristic dimension (m)
σ	variance
σ_{max}	maximum variance
N	number of sampling point
I_S	intensity of segregation
I_M	mixing intensity
Re	Reynolds number

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