



Increment of mixing quality of Newtonian and non-Newtonian fluids using T-shape passive micromixer: numerical simulation

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Abstract

In this paper, a T-shape microchannel containing a mixing unit inserted in the straight main channel is designed to increase the mixing quality by geometrical changings in the mixing unit. Governing equations on flow field and concentration field have been discretized and solved using finite element method. Obtained numerical results were validated by comparing the numerical data reported in literature which show acceptable agreement. A MQ parameter based on the concentration variation of the mixture is employed to evaluate the mixing quality in the micromixer. The PI factor is also represented to check the increment in mixing quality with reference to hydraulic parameters. The effect of the number of mixing unit periods and curvature of the obstacles located in mixing unit on the MQ and PI factors have been investigated. The numerical results indicate that the type II gives better PI, so it has been chosen as the main case for the rest of study. On the other hand, the number of mixing unit periods was increased up to 25 for the type II. The results show that the best mixing quality (85.8%) has been obtained when 25-period mixing unit has been used. Also, noticeable mixing quality (81.2%) has been achieved for blood as working fluid using the proposed micromixer which could make it suitable for all chemical systems.

List of symbols

C	Concentration (mol/m ³)
D	Diffusion coefficient (m ² /s)
J	Mass flux (kg/m ² s)
MQ	Mixing quality
N	Power law index
P	Pressure (Pa)
PI	Performance index
ΔP	Pressure difference (Pa)
V	Velocity (m/s)

Greek symbols

$\dot{\gamma}$	Shear rate (1/s)
λ	Relaxation time (s)
μ	Dynamic viscosity (Pa s)
μ_0	Zero shear-rate viscosity (Pa s)
μ_∞	Infinite shear-rate viscosity (Pa s)
ρ	Density (kg/m ³)

σ Variation of the concentration in mixture (mol/m³)

Subscripts

i	i th species of the mixture
$mean$	Mean value
max	Maximum value

1 Introduction

Microfluidics is a science that deals with micro-dimensional systems; microfluidic systems are built-up into circuits known as microfluidic chips. Many researchers have widely studied this technology as an assistant of chemical and biological fields (Samuel and George 2003; Stone and Kim 2001).

Microfluidics has lots of applications in DNA sequencing diagnostics, drug delivery, micro-reactors, fuel cells, and Lab-On-a-Chip (LOC) (Samuel and George 2003; Stone and Kim 2001; Kröger 2006; Tsui et al. 2008). In microdimension; flow is influenced by the Capillary Effect; also, effects of surface forces are more dominant than volume forces. Because of the Low Reynolds Flow (Laminar Flow) effects in microchannels, it is difficult to achieve a complete mixing in microsystems. Many techniques have been proposed by previous researchers to

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enhance the mixing quality in microchannels (Lee et al. 2011; Nguyen and Wu 2005). Micromixers generally fall into two categories: passive and active. Passive micromixers use geometries modifications method to mix two fluids. Herringbone type wall (Somashekar et al. 2009), inserting obstacle(s) into the microchannel (Chen and Cho 2007), bends in the channel geometry (Liu et al. 2000), recessed grooves in the channel wall (Stroock et al. 2002) and using vortex generators along the channel (Ortega-Casanova 2016; Hsiao et al. 2014; Kim et al. 2011) are some examples of passive techniques. In return, active micromixers take advantage of an external energy source like electrical (Oddy et al. 2001), Pulsing of inlet flow (Goulet et al. 2006), electro-magnetic (Bau et al. 2001) and ultrasonic vibratory fields (Liu et al. 2003) to mix fluids. Also, combined passive and active method was also studied in literatures (Chen and Cho 2008; Lim et al. 2010).

Mao and Xu (2009) examined a 3D T-shape micromixer using CFD for three different Reynolds number, Strouhal number, and pulsing inlet velocity.

Miranda et al. (2010) investigated a 2D micromixer with pulsing inlet flows. The best mixing achieved when two inlet flows were anti-phase and number of the obstacles in the middle of channel outlet were a lot.

Bottausci et al. (2004) designed a micromixer that contained a main channel and three secondary channels that were perpendicular to main channel. The secondary channels disturbed the main flow by exerting a pulsing pressure. Their results showed that the secondary channels increased mixing significantly.

Kim et al. (2009) reached 97.3% mixing quality as a result of simultaneous use of pumping and mixing for two identical flow patterns in which the Peclet number is 7338.

Karthikeyan et al. (2017) have modelled a passive micromixer with two inlets and one outlet with obstacles in various shapes and sizes to find out the effect of mixing on fluids with very low diffusivity.

Baheri Islami and Khezerloo (2017) studied a numerical research on the mixing of non-Newtonian power-law fluids in curved micromixers. They examined the effects of grooves inserted in the micromixers' bottom wall and geometrical parameters such as angle and depth of the grooves on mixing efficiency. They showed that the grooves improved the mixing efficiency but had no significant effect on dimensionless pressure drop.

Das et al. (2017) have done a numerical and experimental research on fluids mixing in straight and serpentine microchannels. They showed that in serpentine microchannel, a beneficial mixing could be achieved in almost all the flow conditions whereas in straight channel that is achievable only in 0.001 m/s velocity. They experimentally achieved the mixing efficiency of 95.5, 70.20, and 48.54% for straight channel at inlet velocities of 0.001,

0.007 and 0.0167 (m/s) respectively. They also showed in serpentine microchannel, the mixing efficiency has been achieved around 97, 95, and 65% at inlet velocities of 0.007, 0.0167 and 0.03 (m/s), respectively.

Fang et al. (2012) presented a numerical and experimental study of a passive micromixer consisting of a main T-shape channel and a mixing unit is imbedded in it. The mixing unit increased the mixing efficiency by means of oblique obstacles which caused to fold and stretch the mixing fluids when passing through them. Also, they showed that by increasing the number of the mixing unit up to 28, a near uniform mixing is achievable at the micromixer outlet. Also, Ortega-Casanova (2017) has completed the study of Fang et al. (2012) by optimizing the obstacles angle as the input parameter while the outlet parameters were the pumping power to run the fluids at the desired Reynolds number, the mixing efficiency and the mixing energy cost. Since Fang et al. (2012) and Ortega-Casanova (2017) did not study the curvature effects of used obstacles, so that will be examined in this study as the input parameter to obtain the mixing quality and PI factor of the micromixer. Governing equations on flow field and concentration field have been discretized and solved using finite element method. Obtained numerical results were validated with the numerical data reported in the literature which show acceptable agreement.

The rest of this study is arranged as follows. In Sect. 2 the computational description will be more detailed together with the channel geometry. Section 3 introduces the governing equations together with the corresponding boundary conditions. In Sect. 4 the obtained results will be presented and discussed. Finally, in Sect. 5 the conclusions will be presented.

2 Computational description

In present work it is assumed that the microchannel is two-dimensional (2D), since the channel depth is much larger than its width. The schematic of the T-shape micromixer is illustrated in Fig. 1. The micromixer contains a main T-shape microchannel with (one period) mixing unit located in it. The fluid with concentration value of 1 [mol/m³] flows into the microchannel from upper inlet and the fluid with zero value flows into the channel from lower inlet. Curved oblique obstacles inside the mixing unit cause to fold and stretch the flow field repeatedly, which enhance the convective acceleration effects and result in high mixing quality. The mixed fluids after crossing the mixing unit flow out from the microchannel outlet. The working fluid properties is as the same properties as water at room temperature.

Fig. 1 **a** Schematic of n-period micromixer, **b** sketch of the geometary for one-period mixing unit micromixer and **c** magnified and detailed sketch of mixing unit. **d–g** the mixing unit with different obstacles configuration for type I, II, III and IV, respectively

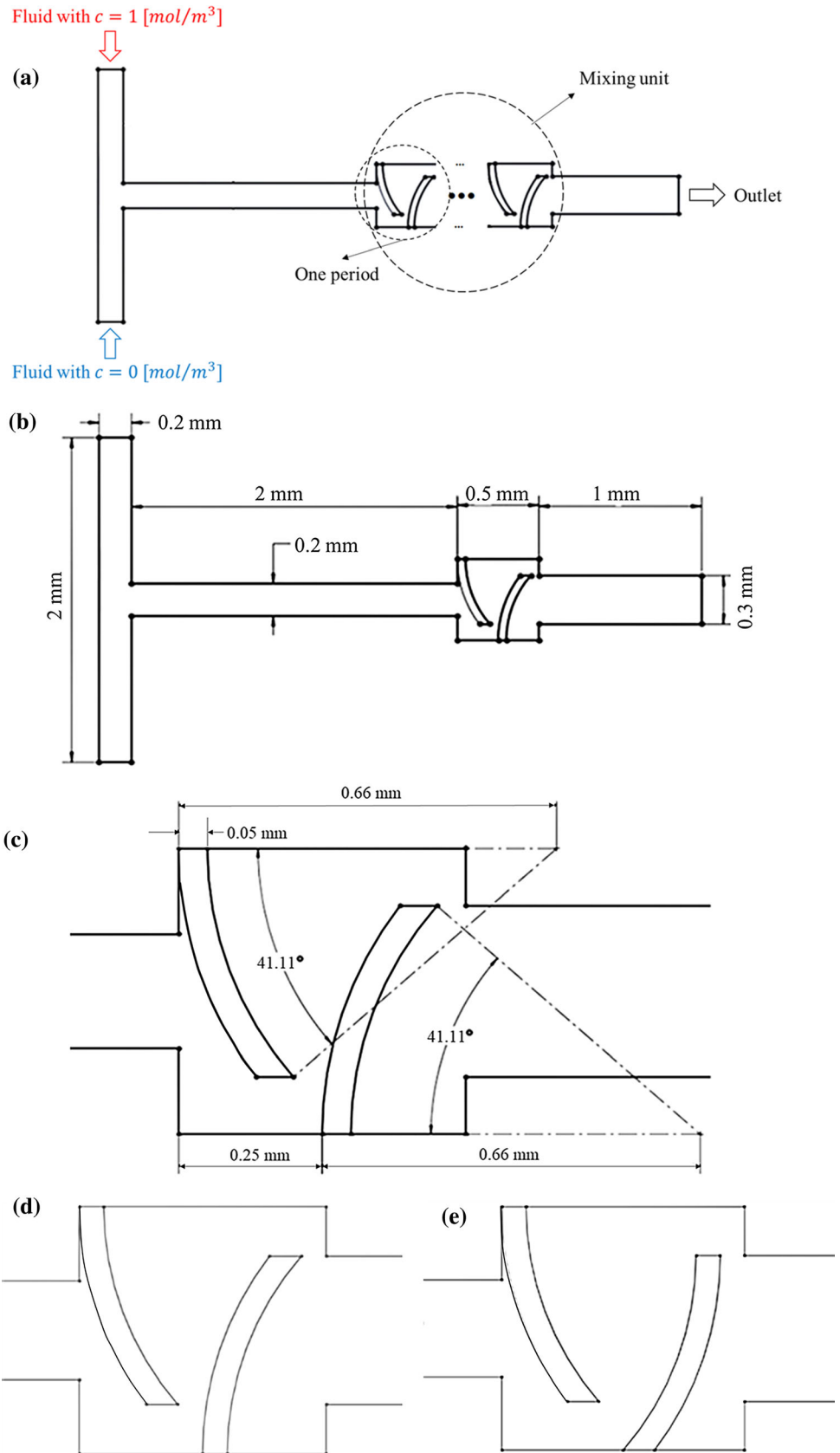
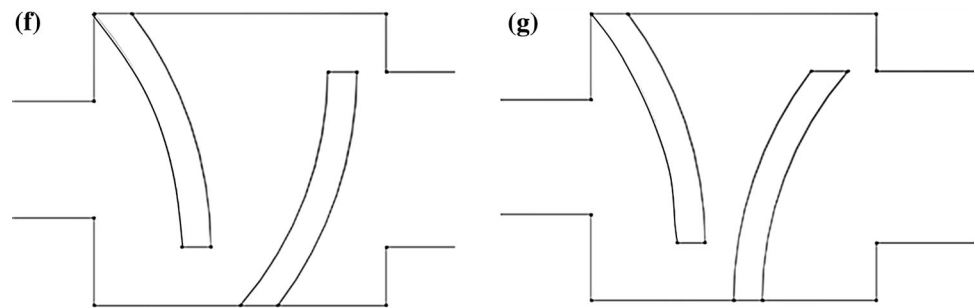


Fig. 1 continued



3 Governing equations

A steady state model is set up to simulate the flow field and concentration field in the system described above.

3.1 Flow field

In this section the flow field governing equations and the associated boundary conditions have been described.

3.1.1 Governing equations

The flow field is governed by continuity and Navier–Stokes equations which are presented in Eqs. (1) and (2):

$$\vec{\nabla} \cdot \vec{V} = 0 \quad (1)$$

$$\rho \left[\left(\vec{V} \cdot \vec{\nabla} \right) \vec{V} \right] = -\nabla P + \mu \nabla^2 \vec{V} \quad (2)$$

where ρ is the fluid density (kg/m^3), \vec{V} denotes the velocity vector (m/s), P is the pressure (Pa) and μ refers to the dynamic viscosity (Pa s). For Newtonian fluids, value of μ (the dynamic viscosity) is constant. But most of the biological systems deal with non-Newtonian fluids with variable μ . The dynamic viscosity of blood as a non-Newtonian fluid (which widely is used in biological applications) is a function of the shear rate ($\dot{\gamma}$) as follow:

$$\mu = \mu(\dot{\gamma}) \quad (3)$$

There are various models for evaluate the μ in non-Newtonian fluids, such as power-law model, Casson model and Carreau–Yasuda model (Shamloo et al. 2016). According to the Carreau–Yasuda model, the dynamic viscosity expresses as follow:

$$\mu = \mu_{\infty} + (\mu_0 - \mu_{\infty}) \left[1 + (\lambda \dot{\gamma})^2 \right]^{\frac{n-1}{2}} \quad (4)$$

where λ is the relaxation time constant, μ_0 is zero shear-rate viscosity, μ_{∞} is infinite shear-rate viscosity, and n is the power law index.

3.1.2 Boundary conditions

It is assumed that velocity at the inlets is uniform with value of 0.04 (m/s). No normal stress boundary condition is exerted at the outlet of the channel. Also, no-slip velocity boundary condition is applied on all walls.

3.2 Concentration field

In this section the concentration field governing equations and the associated boundary conditions are given.

3.2.1 Governing equations

An advection–diffusion-type equation is solved for the concentration field as follows:

$$\nabla \cdot \vec{j}_i = 0 \quad (5)$$

where j_i is the flux of the i th species and j is the mass flux,

$$\vec{j}_i = -D_i \nabla C_i + \vec{V} C_i \quad (6)$$

where V and C are the flow velocity and concentration, respectively. D denotes the diffusion coefficient, which is considered as 1×10^{-11} (m^2/s).

3.2.2 Boundary conditions

It is assumed zero concentration at lower inlet, and we have 1 (mol/m^3) concentration value at upper inlet. Furthermore, the convection in the outlet is dominant, and no flux boundary condition is considered on all other boundaries.

3.3 Mixing quality (MQ)

Mixing quality factor (MQ) can be expressed mathematically as:

$$MQ = 1 - \sqrt{\frac{\sigma_{mean}^2}{\sigma_{max}^2}} \quad (7)$$

$$\sigma_{mean}^2 = \int (C_i - C_{mean})^2 dy \quad (8)$$

This integral is applied to grid points of the outlet of the channel. C_i is the mass fraction at point i , and C_{mean} is the average concentration. σ_{max} equals to the maximum variation of the concentration in the mixture. According to above equations, the value of 0% for MQ indicates no mixing, whereas the value of 100% means complete mixing.

3.4 Performance index (PI)

The hydraulic performance index is defined as the ratio of the mixing quality to the dimensionless pressure drop. This parameter is used to compare different passive techniques and enables a comparison of two different methods. The performance index (PI) is defined as:

$$PI = \frac{MQ}{\Delta P / \rho U^2} \tag{9}$$

where, MQ and ΔP are the mixing quality and pressure drop through the mixing unit, respectively. The ΔP is a measure of head loss or pumping power. Also, ρ and U indicate density and inlet velocities of the fluid flows.

3.5 Grid independence study

The governing equations with the associated boundary conditions have been numerically solved using the finite element-based commercial codes COMSOL Multiphysics (version 5.2a). As shown in Fig. 2, unstructured triangular elements are used to discretize the computational domain in this study. The grid size is finer around the walls and sharp parts of the channel due to the intense gradients in these regions. The grid independence study is essential to obtain the independent results of grid size. The grid independence study is performed for five different elements number containing 17,858, 22,154, 26,480, 29,440 and 34,225. The results are presented in Table 1 for average concentration at the channel outlet. Also, concentration distribution on channel outlet is depicted in Fig. 3. Results in Table 1 and Fig. 3 indicate that the difference between the concentrations in grid numbers of 29,440 and 34,225 is

Table 1 The average concentration at the channel outlet versus the mesh grids number

Grid	Number of elements	C_{ave} (mol/m ³)
G1	17858	0.49425
G2	22154	0.49743
G3	26480	0.49865
G4	29440	0.49962
G5	34225	0.50023

Table 2 The constant parameters used in the numerical simulation

Parameters	Values
D, Diffusion coefficient (m ² s ⁻¹)	10 ⁻¹⁰
ν , Kinematic viscosity (m ² s ⁻¹)	10 ⁻⁶
Inlet velocity, (m s ⁻¹)	0.04
μ , Viscosity (kg m ⁻³)	1 × 10 ⁻³

Table 3 The mixing quality comparison for one-period micromixer when the same conditions in Fang et al. (2012) are used

	Present work	Fang et al. (2012)
Mixing quality (%)	21.79	21.90

negligible. Therefore, the cells number of 29,440 (G4) is used for the rest of this research to reduce the computation running time and memory requirements.

3.6 Validation

The validation will consist of reproducing the results by Fang et al. (2012) with the same governing parameters, mixing unit and mesh they used. The physical properties used in our simulation are listed in Table 2. Table 3 represents the mixing quality for the case of one mixing unit compared with the numerical results obtained by Fang et al. (2012). Obviously, results in Table 3 match very well with the mentioned results. Also, Fig. 4a illustrates the concentration profile at the channel outlet compared with the reference data (Fang et al. 2012). As it is clear, there is good conformity between them. From Fig. 4 it is obvious that concentration value varies between 0 and 1 (mol/m³) as expected. Furthermore, concentration contour for the one-period micromixer with oblique flat obstacles is shown in Fig. 4b. It declares that two fluids with different concentrations flow inside the main channel from two different inlets and after passing through the mixing unit exit the channel. It is observed that one-period mixing unit causes less mixing.

4 Results and discussion

At first for the geometrical study, different types have been presented; then, their mixing quality is investigated to find out the best configuration of the obstacle’s curvature for Newtonian fluid; finally, the same simulation has been done on the efficient type with non-Newtonian operating fluid.

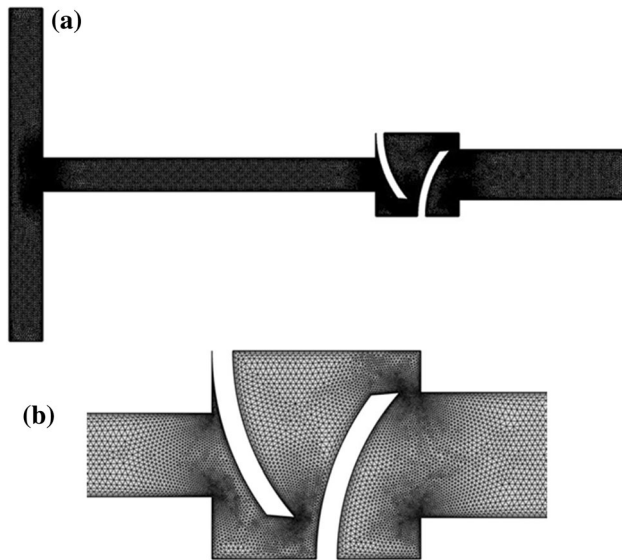


Fig. 2 **a** Geometrical discretization of type I channel with one-period mixing unit. **b** Magnified figure of mixing unit

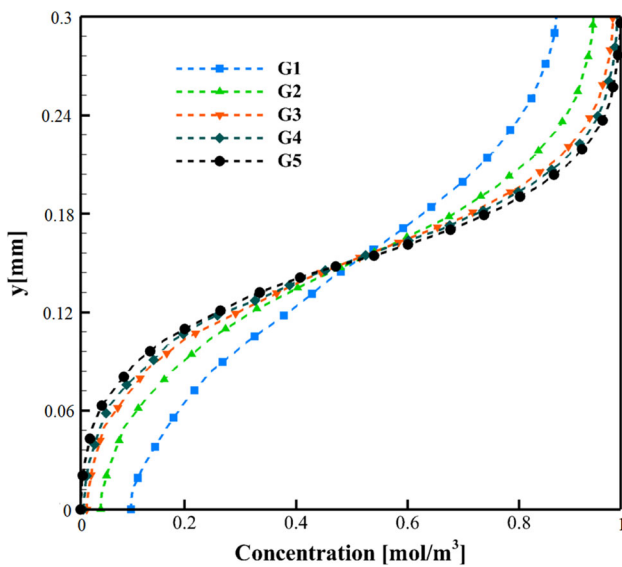


Fig. 3 Concentration distribution at channel outlet for different grid sizes

4.1 Newtonian fluid

Fang et al. (2012) have used period(s) of mixing unit with the oblique flat obstacles to enhance the mixing quality inside a passive micromixer. In current research, it has been shown that the curvature of these obstacles mainly influences the mixing quality. Mixing quality is a factor in the mixing process that evaluates the performance of a micromixer. This factor indicates that how a designed channel could be beneficial. Mixing quality values generally vary between 0 to 100%. The closer values to 100%

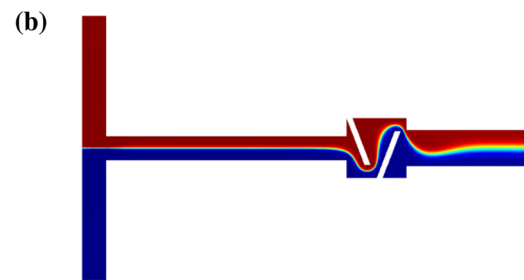
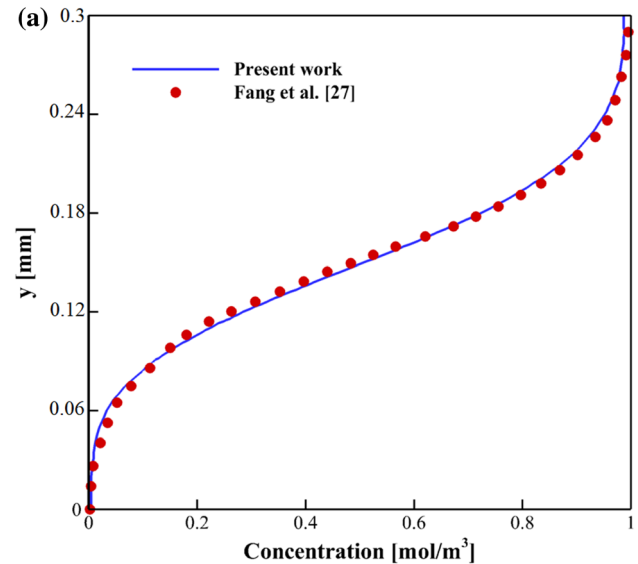


Fig. 4 The concentration comparison at the channel outlet

shows that the proposed model is efficient. At the first step, four channels with different curved obstacles have been presented (Fig. 1) to investigate the mixing quality and hydraulic performance index. Hydraulic performance index of a micromixer is the mixing quality change of the mixer under consideration or pressure loss. This parameter reflects the efficiency of the presented method in increasing the mixing quality per energy cost. Since changing the geometrical characteristics of the microchannels for enhancing the mixing quality may affect the pressure loss, it is essential to study the PI factor. This allows researchers to determine whether the proposed method is cost-effective or not. To find the efficient type, the number of periods for each type is set from 1 to 10 (1, 2, 5, 7 and 10). Next, the performance of the efficient type has been examined in the larger range of periods.

The performance of a micromixer can be understood certainly by observing the concentration contours and profiles, and other parameters like trend of mixing quality and hydraulic performance index. The concentration contours within the micromixer were observed for mentioned channels with one-period mixing unit in Fig. 5. The streamlines for each type are also demonstrated in Fig. 6. $C = 1$ (mol/m^3) has been illustrated by red color, while the

Fig. 5 Concentration contour for one-period micromixer, **a** type I, **b** type II, **c** type III, **d** type IV

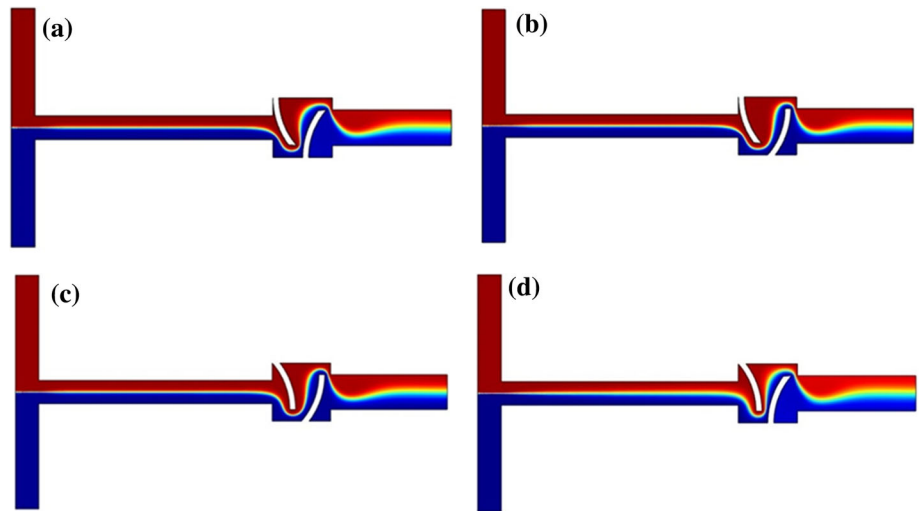


Fig. 6 Streamlines for one-period micromixer, **a** type I, **b** type II, **c** type III, **d** type IV

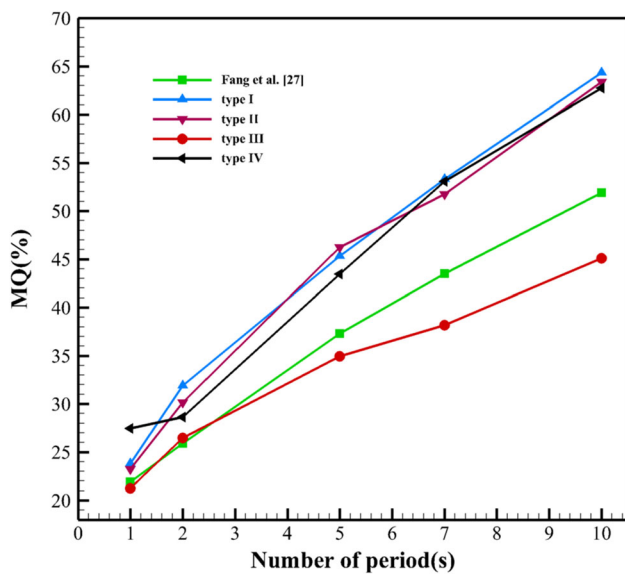
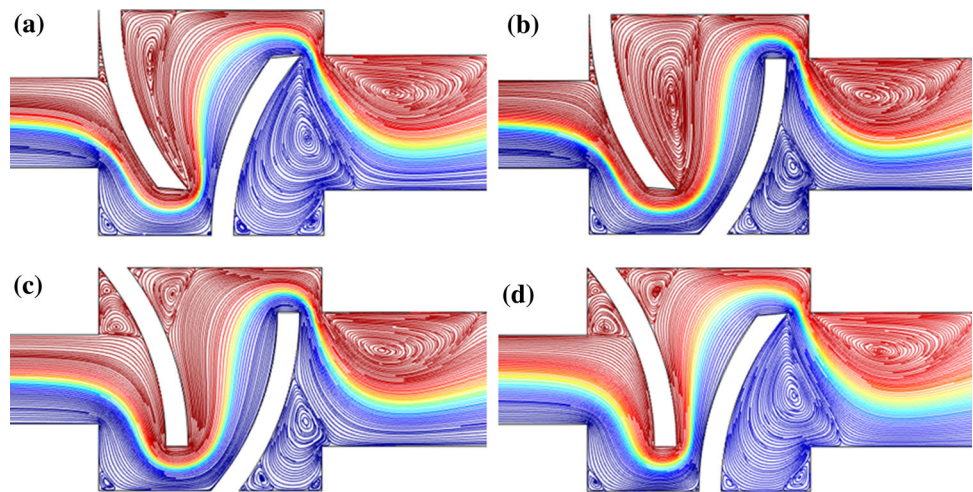


Fig. 7 Mixing quality for each type with particular mixing unit period

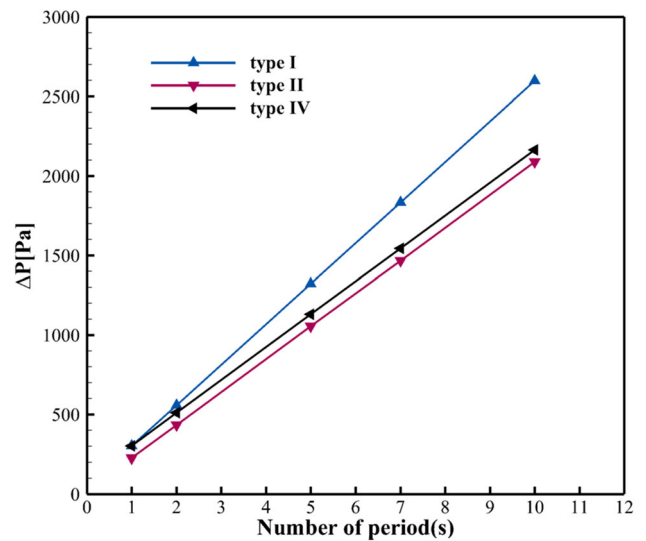


Fig. 8 Pressure drop for each type with particular mixing unit period

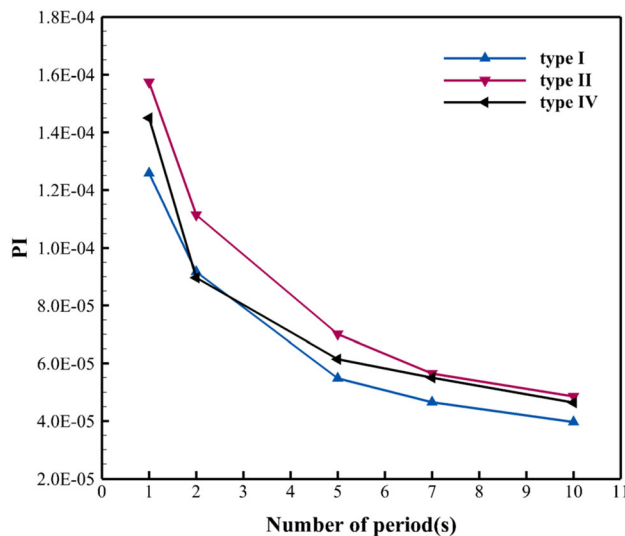


Fig. 9 Performance index for each type with particular mixing unit period

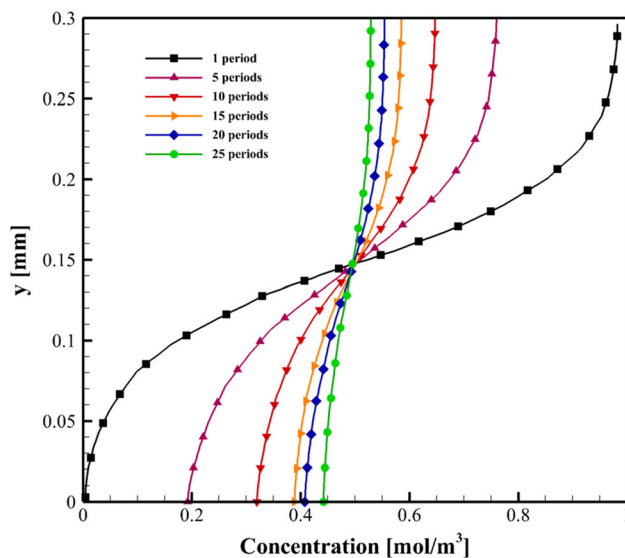


Fig. 10 Concentration profile at the channel outlet for type II channel with different period number

blue color refers to concentration of zero. Using curved obstacles greatly contribute to generate vortices in the corners. Presence of these vortices initially cause the disturbance in the mixing unit (which eventually results in better mixing quality by periodically breaking the fluid flow). At simulation of one-period mixing unit micromixer two fluids existing at the channel outlet are not completely mixed yet. But at higher mixing unit period numbers, the mixed fluid coming from the mixing unit will show an increasing trend in the mixing quality.

The overall fluid mixing is mainly because of the molecular diffusion and generated vortices at the back of the inserted obstacles inside the mixing units. In this

regard, the number of the mixing unit period is an important factor in examining of the mixing quality. Figure 7 indicates the mixing quality of micromixer in terms of different channels over the range of mixing unit period numbers. For each type, it can be seen that by increasing the number of periods, the mixing quality increase significantly. Difference between mixing quality for all types in current work and reference data (Fang et al. 2012) for one and two-period mixing unit is small. By increasing the number of periods from 2 to 10, type I, II and IV channels show better mixing quality than reference data (Fang et al. 2012) and type III channel. To find the efficient type between type I, II and IV channels, ΔP and also PI factor were presented.

Considering the pressure drop is necessary in micro-mixer designs. Figure 8 shows the CFD simulated pressure drop vs mixing unit period numbers for three types. The pressure drops were calculated using the differences between total pressures on the centerline located at the inlet and exit of the mixing unit. The pressure drop is found to be increasing with increase in mixing unit period numbers for all depicted types in Fig. 8. It is observed from Fig. 8 that pressure drop for type I and IV enhanced up to 24.4% and 4% respectively as compared to type II for the case of 10-period mixing unit. Basically, the pressure drop is higher in type I and IV than in the type II micromixer. The type II channel, which showed nearly same mixing quality throughout the mixing unit period number range considered, is advantageous in terms of pressure drop. Therefore, type II micromixer is preferable in terms of both mixing quality and pressure loss.

Performance index (PI) is the ultimate parameter used for evaluating the use of the curved obstacles, simulation results. The factor is obtained by considering the effect of mixing quality enhancement and the increase of pressure drop for conducted channels. The variation of performance index with mixing unit period numbers of three channels is shown in Fig. 9. Performance index decreases with increasing mixing unit period numbers. As it is obvious, performance index corresponding to the type II is higher than that for type I and IV. This is because of the showing lower pressure drop by type II since mixing quality is nearly same for types I, II and IV. Therefore, type II micromixer has been chosen as the main study object for the rest of this paper due to the showing best PI in comparison to others.

Figure 10 illustrates the concentration profile at the channel outlet for type II channel when the number of periods increase from 1 to 25. The concentration distribution across the channel outlet is gradually close to 0.5 with the increasing of the number of periods. The more the concentration value is near 0.5 (mol/m^3) the more mixing

Fig. 11 Concentration contour of type II channel with different period number; **a** 2, **b** 5, **c** 7, **d** 10, **e** 15, **f** 20, **g** 25-period

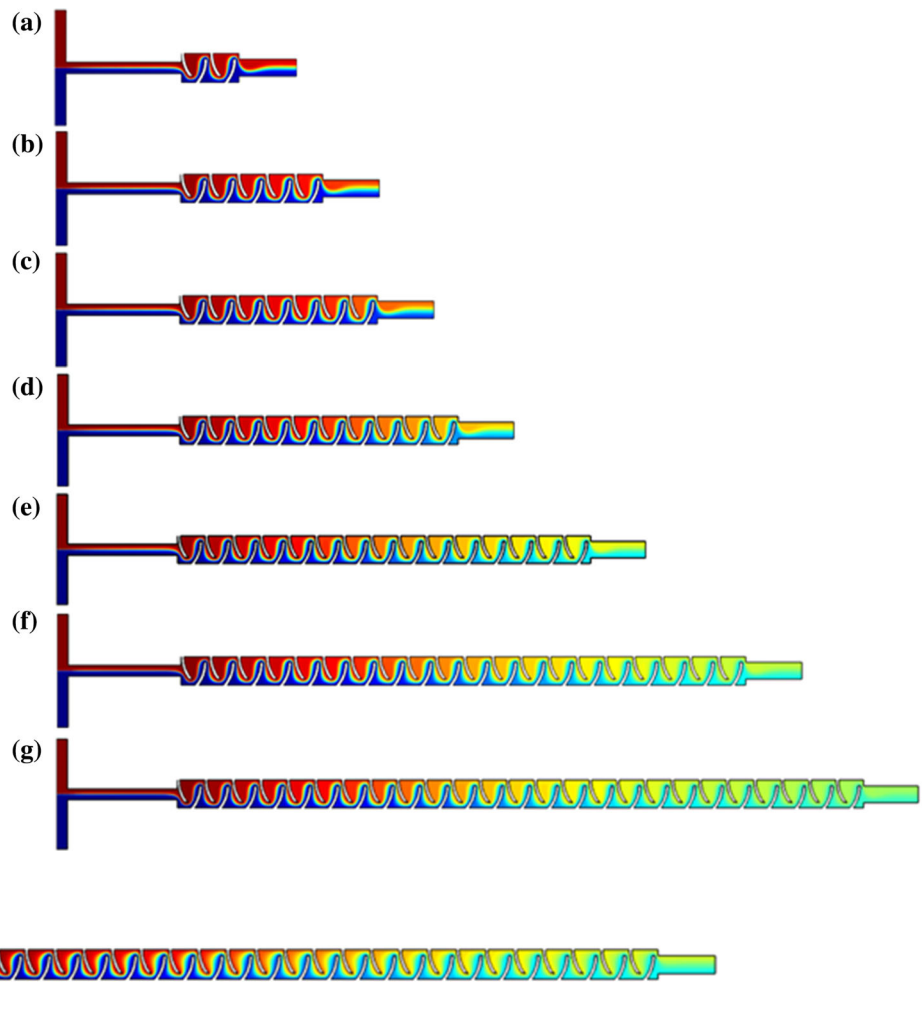


Fig. 12 Concentration contour of type II channel with 25 period and non-Newtonian working fluid

is homogeneous; according to this, 25-period mixing unit gives higher mixing quality than others.

Figure 11 illustrates the concentration contours for type II channel in the large range of periods and it was found that, mixing occurred at the outlet section of the micromixer. The major changes in concentration contours occur after the mixing unit that contribute to the flow variation at the core and promote mixing quality enhancement. Obviously, the mixing increases with increasing the period numbers. In this case, mixing in 25-period micromixer is better than that of others and this is due to the presence of obstacles in the path of fluid. As in the microchannel, mixing depends on molecular diffusion only, presence of any obstacle or confluence in the path of fluid results in uniform mixing at the channel outlet. Finally, it should be mentioned that after 25 periods, fluid reaches to mixing quality of 85.8% which is noticeable in comparison to 79.4% mixing quality in 28-periods micromixer designed by Fang et al. (2012).

4.2 Non-Newtonian fluid

Fluids mixing has many applications in biological and chemical systems; especially, in LOC devices it is necessary to achieve a rapid and uniform mixture of bio-fluids. As the last part of this study, blood has been used as the working fluid instead of water. Blood is an anisotropic, non-homogeneous and polarized fluid which consists a suspension of viscoelastic particles carried in a background liquid known as plasma. The plasma shows different behaviors under shear stresses; hence, the dynamic viscosity of blood is a function of shear rate. The dynamic viscosity of blood could be modeled by Carreau–Yasuda model, Casson model, power-law model and Bingham model (Chakraborty 2005). In current paper, the dynamic viscosity of blood has been modeled by Carreau–Yasuda model (see Eq. (4)), in which zero shear-rate viscosity μ_0 is equal to 0.056 (Pa s), the infinite shear-rate viscosity μ_∞ is 0.0035 (Pa s), λ is 3.313 (s), and $n = 0.3568$ (Johnston

et al. 2004; Cho et al. 1991). Same as what discussed in the previous sections for a Newtonian fluid, blood has been examined as the working fluid in type II channel in this section. Figure 12 shows the concentration contour of type II channel with 25 periods. The mixing quality of 81.2% is achieved at the channel outlet when blood is used.

It should be mentioned that, designed micromixer (type II) is a suitable device in biological application and mixing of non-Newtonian fluids (such as blood) because of showing acceptable mixing quality in using periods of mixing unit up to 25. Also, this device is superior to active micromixers because of their undesirable effects on fluid physical properties.

5 Conclusion

We conducted many intensive numerical simulations to evaluate the mixing quality and PI factor in a passive micromixer with four different type of flow blocking obstacles. The numerical results obtained by the COMSOL Multiphysics (Version 5.2a) software, are presented to analyze the mixing quality enhancement and PI factor. Based on the CFD analysis the main findings can be summarized as following:

1. The results show that the best mixing quality (85.8%) has been obtained when 25-period mixing unit has been used.
2. Noticeable mixing quality (81.2%) has been achieved for blood using the presented model which could make it suitable for all chemical systems.

Additionally, because of simple processing and easy operation, these micromixers have significant applications, especially in the LOC.

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