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EFFECT OF BAFFLE GEOMETRY ON MIXING PERFORMANCE IN THE PASSIVE MICROMIXERS[*]

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Abstract– Micro and nano-fluidic mixing nowadays is a very important area in research due to its crucial role in new technologies and applications such as biomedical and biochemical synthesis. Due to the low velocities associated with microscale flow, it is often very difficult to mix fluids in a rapid and homogeneous manner. One of the methods of enhancing fluid mixing is to obstruct the fluid flow using vanes or panels known as *baffles*. In this paper, a Computational Fluid Dynamics (CFD) approach is used to study the effect of baffles on the mixing performance in a passive micromixer. The numerical method is verified by comparing its obtained results with experiments and numerical results published earlier. Rectangular, semi-circular and triangular baffles have been considered for investigating the effects of baffle geometry on mixing performance. Furthermore, the effects of channel inlet angle and baffle~~s~~ offset in mixing performance are studied. As the results show, there is a two-fold increase in mixing performance in the baffled cases as opposed to the simple case.

Keywords– Computational fluid dynamics, passive micromixer, baffle, mixing index, FEM

1. INTRODUCTION

Microfluidics is a synergy of science and engineering applied to fluid mechanics, involving characteristic dimensions in the micron scale. Examples of application areas include chemical analysis, biological interfacing, medical diagnostics, energy conversion and toxin detection. Characteristic dimensions such as channel widths or orifice diameters are typically on the order of 10 to 100μm. In lab on chip or Micro Total Analysis Systems (μTAS), it is often necessary to mix reactants. For example in biology, in order to identify proteins in an unknown sample, proteins are fragmented by mixing them with enzymes. Proteins can then be characterized using mass spectrometry analysis of the resulting fragments.

Rapid and effective mixing is the basic requirement for a successful biochemical analysis. To reduce the analysis time, rapid mixing and improved procedure control can be carried out in μTAS [1].

Microfluidic micromixers can be categorized into two major groups: Active and Passive micromixers. In active micromixers external energy is given to system in order to accelerate the mixing performance. This external energy can be acoustic [2, 3], magnetic [4, 5], electrokinetic [6, 7], mechanical [8] or thermal [9]. Generally, active micromixers have better efficiency but energy consumption and moving parts in such mixers cause a challenge. Despite active micromixers, passive mixers consume no energy and need no moving parts but have less mixing performance. To optimize the mixing performance in passive micromixer several works have been performed in recent decades. Francesco Penella et al. report a new low-cost passive Microfluidic mixer design, based on a replication of identical mixing units composed of microchannels with variable curvature (clothoid) geometry [10]. Yu Cheng Lin et al.

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proposed a new design of a passive micromixer employing several J-shaped baffles in T-channels to enhance mixing [11]. Jyh Jian Chen et al. present a parallel laminar micromixer with staggered curved channels for homogeneously mixing two fluids by Dean Vortices [12]. Shou-Shing Hsieh et al. present a micro mixer structure fabricated by an interesting technique using embedded twisted threads in polydimethylsiloxane (PDMS), which is polymerized and cured [13]. Nassim Ait Muheb et al. showed that the cross-shaped micromixer could improve the mixing process in comparison with the micromixers having T-geometry [14]. Yongbo Deng et al. discussed a flexible layout design method of passive micromixers based on the topology optimization of fluidic flows [15].

Subtractive processes (or equivalently, material removal processes) are perhaps the most intuitive among fabrication strategies, microscale or otherwise. For making baffled configurations of microchannels, substractive processes such as wet etching, dry etching, directed beam processes and so on can be used.

In this paper, four possible geometries for passive micromixers are considered. A wide range of Reynolds number and diffusion coefficient is considered and their effects on mixing performance are also evaluated. The effects of inlet channel angle and offset are also considered.

2. NUMERICAL MODEL

In this study, four geometries for the mixer are considered. These geometries are shown in Fig. 1. The channel width, height and length equals 200, 150 and 2250 micrometers in all cases and the volume of the baffles is the same in all cases.

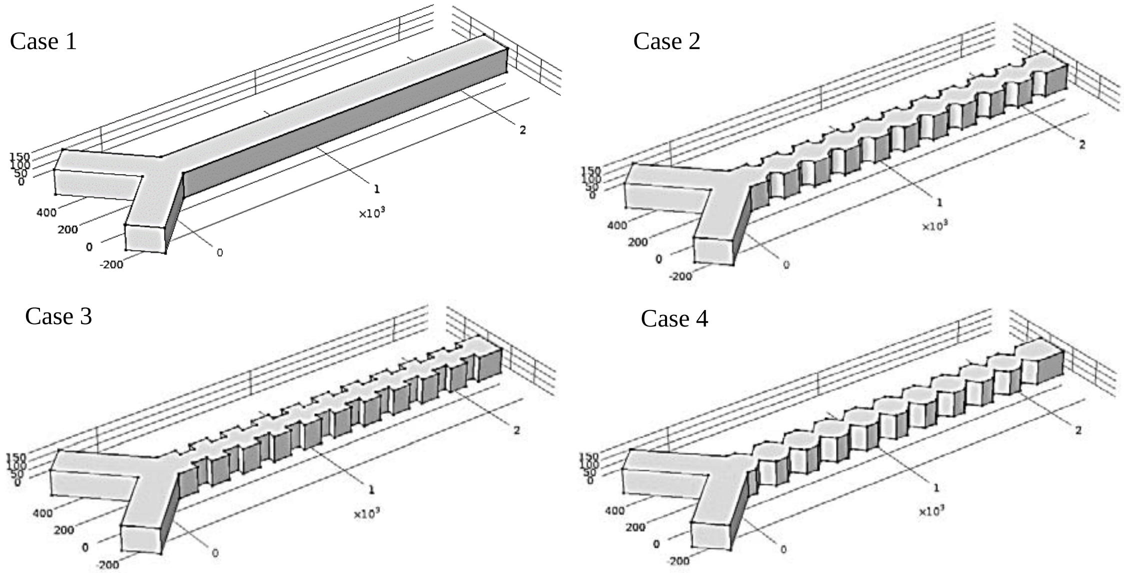

Fig. 1. Geometries of simple and baffled micromixers. All dimensions are in μm

A solution with concentration of 50 mol/m^3 is introduced through one of the inlets, while a pure liquid is infused through the second inlet. To study the mixing, Computational Fluid Dynamics (CFD) is used. Simulations are performed, considering laminar, steady-state conditions and the following equations:

Continuity equation:

$$\nabla \cdot \mathbf{u} = 0 \tag{1}$$

Momentum equation:

$$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla P + \eta \nabla^2 \mathbf{u} \tag{2}$$

Where ρ (kg/m^3) denotes the density of the fluid, **u** (m/s) the velocity vector, P (Pa) the pressure and η (Pa.s) the dynamic viscosity of the fluid.

Diffusion-convection equation:

$$\nabla.\left(-D\nabla c_s\right) = \mathbf{u}.\nabla c_s \tag{3}$$

where, D is the diffusion coefficient (m^2/s) and c_s (mol/m^3) is the species concentration.

The Finite Element Method (FEM) is used to reduce the governing partial differential equations (PDEs) to a set of algebraic equations. This method has been applied as a powerfull tool for simulating the engineering problems [16, 17]. In this method, the dependent variables are represented by polynomial shape functions over a small area or volume (element). These representations are substituted into the governing PDEs and then the weighted integral of these equations over the element is taken where the weight function is chosen to be the same as the shape function. The result is a set of algebraic equations for the dependent variable at discrete points or nodes on every element. To solve the equation~~s~~ set, the generalized minimal residual method (GMRES) which is an iterative method for the numerical solution of non-symmetric systems of linear equations is used. The geometric multigrid (GMG) solver was used for velocity and pressure correction and also species and V-cycle was chosen for multigrid cycle. The stopping criterion of iterative computation is that the relative residual for each variable reaches a value less than 1e-6. For grid sensitivity test, the grid density could be gradually increased until a stable solution is reached. The total number of meshes for a stable solution of 3D model is approximately 570,000 for case 1 and approximately 850,000 for other cases.

All the physical properties of the fluids at the two inlets are considered the same except for their concentrations. The density and dynamic viscosity of both species are considered to be 998.2 kg/m^3 and 0.001003 Pa.s, respectively.

To study the effects of the Reynolds number and the diffusion coefficient, a wide range of Reynolds number (0.2 to 20) and diffusion coefficients (10^{-10} to 10^{-8}) are considered. The boundary condition at the outlet is set to atmospheric pressure as well as no-slip velocity at the walls and also uniform inlet velocity.

To evaluate the mixing quality, Danckwerts' intensity of segregation is used which is defined by:

$$I = \frac{\sigma^2}{\sigma^2_{\max}} \tag{4}$$

$$\sigma^2_{\max} = \bar{c}\left(c_{\max} - \bar{c}\right) \tag{5}$$

$$\sigma^2 = \frac{1}{A}\int (c_i - \bar{c})^2 dA \tag{6}$$

$$M = 1 - \sqrt{I} \tag{7}$$

Where $\bar{c}$ and $c_{\max}$ denote the mean and maximum values of concentration. σ^2 and $\sigma^2_{\max}$ denote variance (square of standard deviation) and maximum variance and M is the mixing index. The quantity M reaches a value of 0 for a completely segregated system and a value of 1 for the homogeneously mixed case.

3. RESULTS AND DISCUSSION

In this study, a wide range of Reynolds number along with mixing indices computed at different Reynolds numbers are considered. Streamlines and concentration changes along the channel length are shown in Figs. 2 and 3.

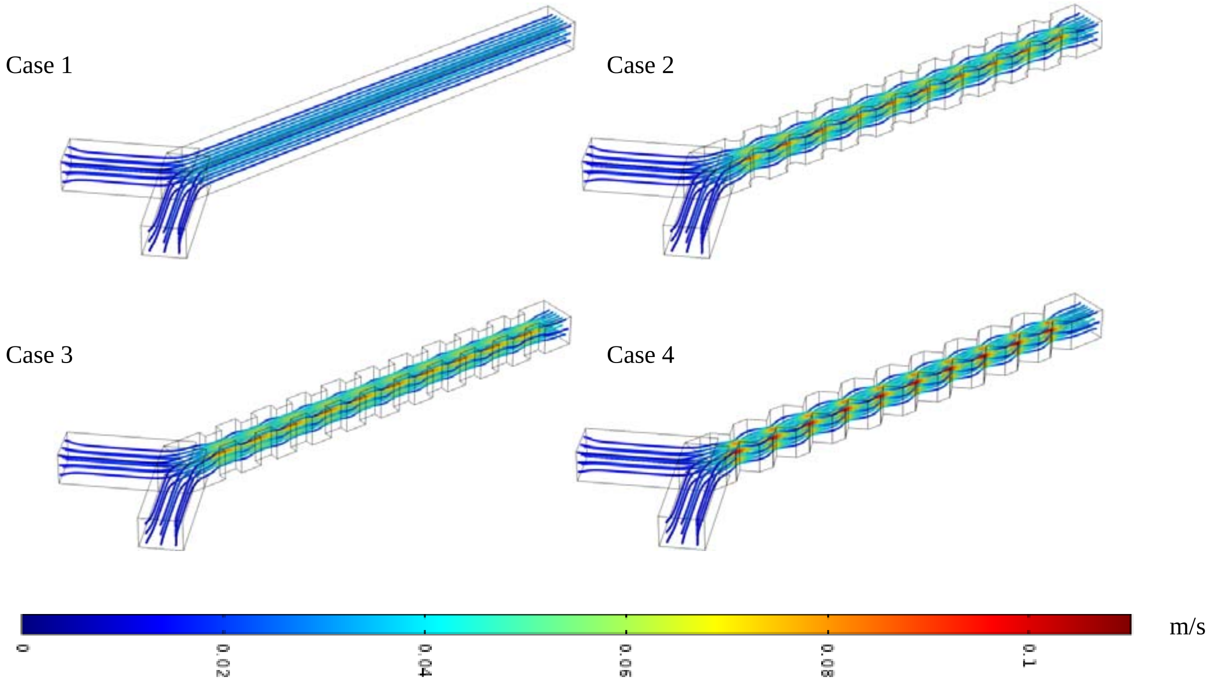

Fig. 2. Velocity Streamline

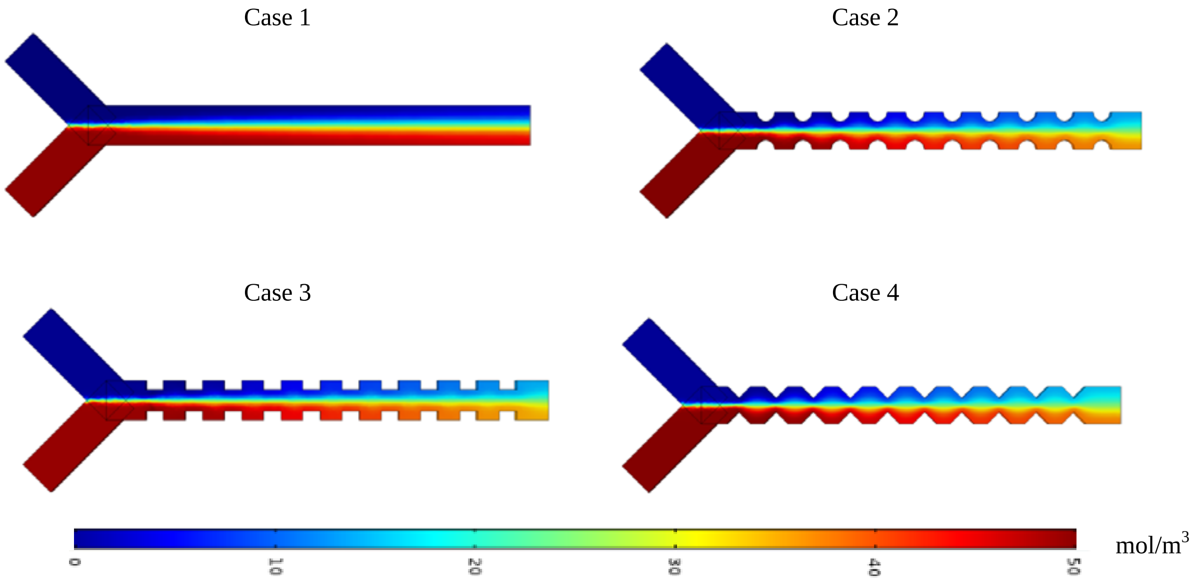

Fig. 3. Concentration contours

The dependency of mixing index to Reynolds number is shown in Fig. 4. The mixing index is more than twice that in the baffled cases in comparison with the simple case. The mixing index in cases 2 and 3 is about the same in all Reynolds ranges but the value of mixing index is the highest in case 4.

Besides the calculation of mixing index, it is necessary to calculate the pressure drop to ensure the applicability of the design. Unfortunately, the value of pressure drop is much higher in cases that have a good mixing index. The value of pressure drop versus Reynolds in all cases is shown in Fig. 5. As it is expected, the value of the pressure drop is proportional to the square of velocity, therefore, the pressure drop is increased as the Reynolds is increased. However, the rate of increase in pressure drop is not the same in all cases.

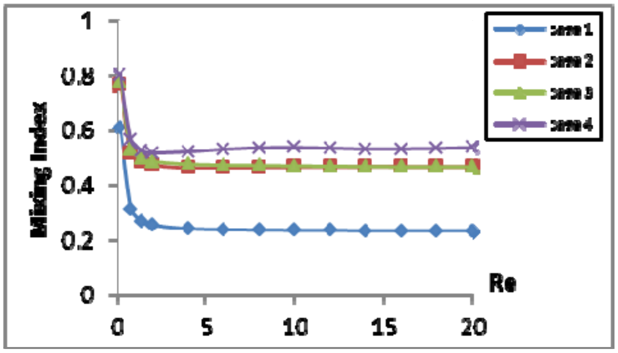

Fig. 4. Relation between Reynolds number and mixing index

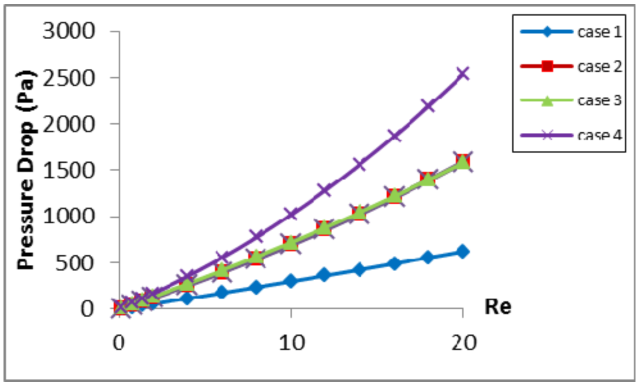

Fig. 5. Effect of Reynolds number on pressure drop

The study is also done in a range of diffusion coefficients to investigate its effect on the mixing behavior. In this situation the Reynolds is kept at 0.2. The effect of diffusion coefficient is shown in Fig. 6. This figure physically means, using baffles will enhance mixing index. In addition, diffusion coefficient has its own effects and greater diffusion coefficient means better mixing.

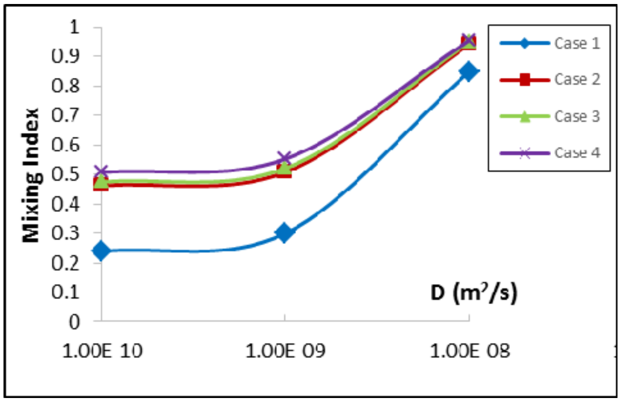

Fig. 6. Effect of diffusion coefficient on mixing index

To study the effect of the channel inlet angle, 5 different angles are considered and the profiles of concentration along the channel width outlet are sketched. It can be seen from the concentration profiles that there is no considerable change in the mixing concentration with the variation of inlet flow angles. Moreover mixing index along channel length is sketched for simple T-mixer in Fig. 8. It can also be concluded that microchannel inlet angle has no considerable effect.

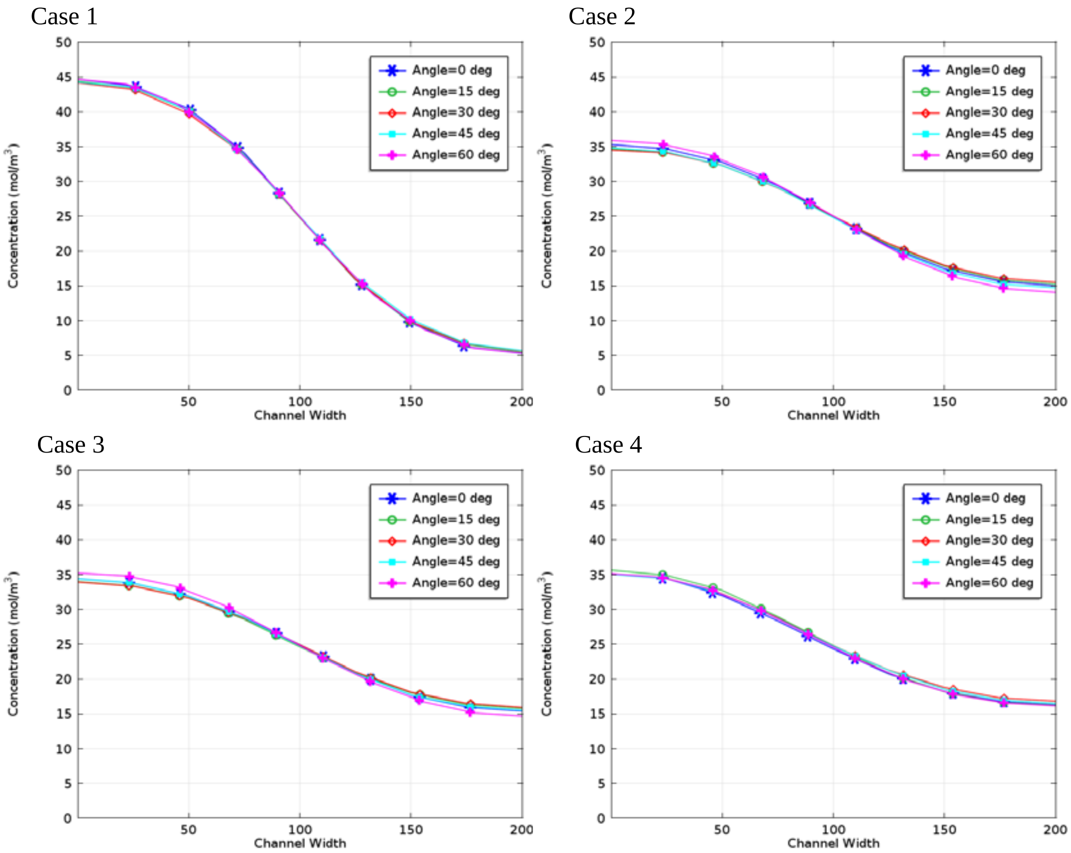

Fig. 7. Concentration profiles across channel width for various channel inlet angles

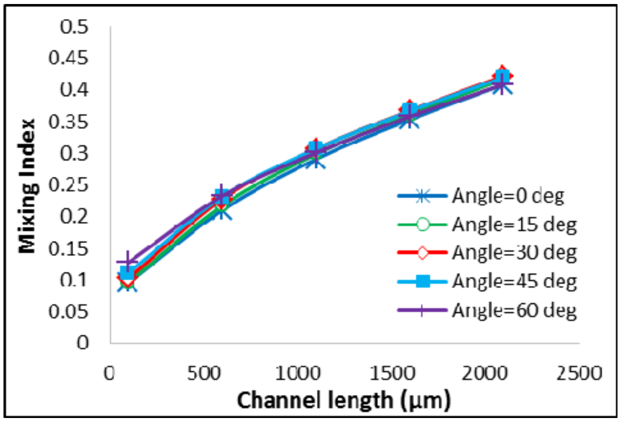

Fig. 8. Mixing index along simple T-mixer for various inlet angles

In the next step, the effect of baffles offset is studied. The offsets with 20, 40, 60, 80 and 100 microns are considered and its effect on the mixing index is shown in Fig. 9. In case 2, offsets between 20 to 40 microns gives the best performance of the mixer. In case 3 offsetting has an adverse effect in the mixing performance, therefore, it is not recommended to use case 3 with offset. In case 4, mixing performance initially increases with the offset but beyond a critical offset distance, it starts to decrease, thus the best offset for case 4 is 20 to 40 microns.

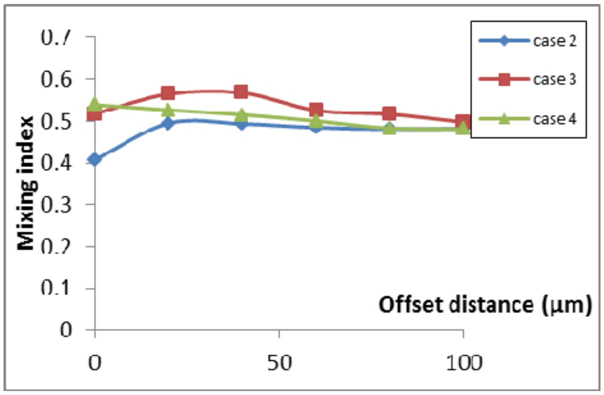

Fig. 9. Effect of baffle offset on mixing index

The pressure drop in the offset cases is shown in Fig. 10. As the results show, offsets decrease the pressure drop.

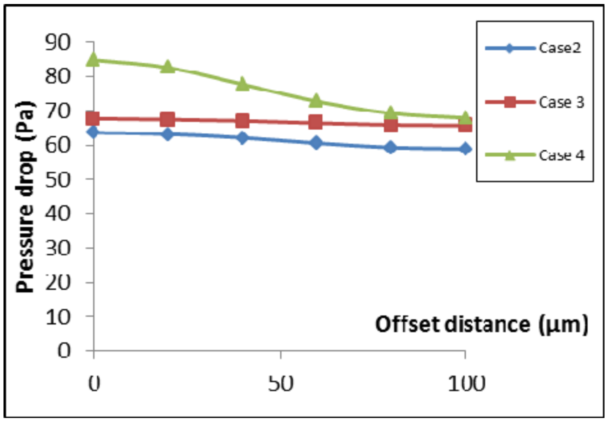

Fig. 10. Effect of baffle offset on pressure drop

4. VALIDATION

This numerical study is validated by comparing the simulation results with experiments done by P. K. Sahu et al. [18]. Experiment and simulation were performed with Rhodamine B with a diffusion coefficient equal to 2.8×10^{-6} cm^2/s. The geometry consists of a Y mixer with two inlets. The dimension of two inlet channels 50×50 microns and the mixing channel is 100×50 microns. The boundary conditions are similar to those of [18].

Figure 11 shows the variation of dimensionless concentration to dimensionless channel width. As the figure shows, there is a good agreement between numerical and experimental results. This agreement indicates the validity of numerical method.

The work is also validated using results published by Yakhshi-Tafti et al. [19]. The micro-mixer used in the aforementioned article is a simple T-mixer. Dependence of mixing index on mixer length is sketched for experimental results and the numerical results are presented in Fig. 12. In this case the Reynolds number is kept 1.3 and mixing index is evaluated by the method described by Stroock et al. [20]. The obtained results also show the validity of numerical methodology.

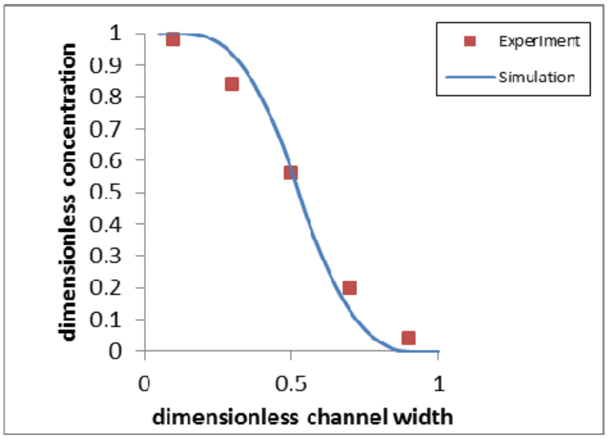

Fig. 11. Comparison with experiments.

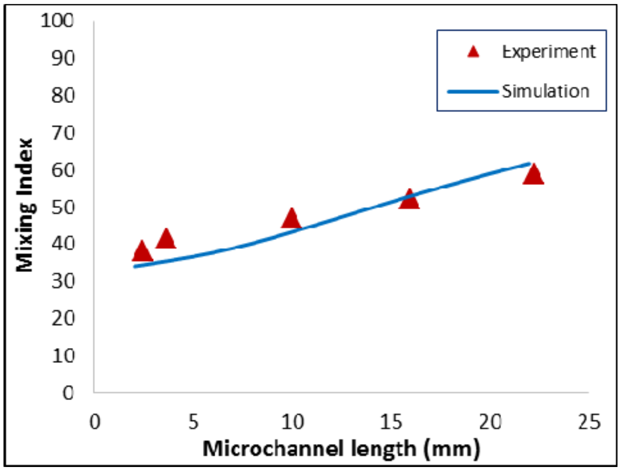

Fig. 12. Comparison of numerical results with Yakhshi-Tafti et al. results

5. CONCLUSION

In this paper, a numerical simulation of fluid flow and mixing in microchannels is presented. The simulations were performed to investigate the mixing process in microchannels by simultaneously solving the mass, momentum and convection-diffusion equations. The simulation results were validated with experiments done by Sahu et al. and Yakhshi-Tafti et al. The results revealed that using baffles in microchannels increases the mixing index by a factor of two, however, it leads to a greater pressure drop. The effects of the diffusion coefficient were also studied. It was shown that the channel inlet angle has no considerable effect on the mixing performance. Furthermore, the effect of baffle offsetting was studied and the optimum baffle offset for each case was calculated. It can be concluded that the current numerical method is a valuable tool for investigating the performance of the micromixers.

NOMENCLATURE

∇	gradient tensor
$\mathbf{u}$	velocity vector
ρ	density
P	pressure

η	dynamic viscosity
∇^2	laplace operator
$\nabla.$	divergence operator
c_s	species concentration
D	diffusion coefficient
σ	standard deviation
$\bar{c}$	mean value of concentration
$c_{\max}$	maximum value of concentration
M	mixing index

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