Simulation of Wing-shaped Passive Micromixers using COMSOL

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Abstract—We have designed the interior of a wing-shaped micromixer in such a way that it forces the liquids flowing through it to undergo a combination of the converging and diverging micromixing. In this paper, we have evaluated and compared the response of design parameters on the performance of wing size planar passive micromixers. For this purpose, we have simulated the flow of liquids whose Reynolds number lie in the range between 0.01 and 100, through two micromixers with different design parameters. COMSOL software has been used to execute the finite element analysis based simulation and the resulting mixing efficiency was improved by applying different types of mesh on the geometry of the micromixer. An ultimate mixing efficiency value of 87% with a pressure drop 71. 782 kPa at the outlet of the micromixer has been found for a liquid with a Reynolds number 60. We found that the induced constriction in the flow controls the degree of mixing. The micromixer with a wing size of 100 µm gives better mixing efficiency than the micromixer with 75 µm wings.

Keywords-passive micromixer; micromixing; microfluidics; COMSOL

I. INTRODUCTION

Microfluidics deals with the fluids at sub-milli or micro scale and manipulates accurate control of it (1). Microfluidic technology offers an opportunity of replacing large or miniaturized conventional laboratory equipment, decrease consumption, reduce cost, operating on a massive parallel scale and making analysis faster (2, 3). The potential of microfluidic systems have gained diverse and widespread attention for their chemical and biological applications over the past few decades (4).

Mixing in microscale is one of the significant technologies for miniaturized analysis systems (5). The term micromixing is used to describe the degree of mixing at a molecular scale (6). Mixing of a liquid in microfluidic devices is a challenge when theflow is laminar. Mixing of the fluids is dominated by molecular diffusion instead of turbulence at micro-scale. Hence, it is essential to find a method to achieve, fast and compact mixing at micro-scale.

Micromixer is an important component. Depending on the type of mixing mechanism, micromixers are classified as active and passive. Active micromixers use moving parts or some external agitation or energy for the mixing. They require complex fabrication procedures and are difficult to operate, clean, incorporate with micro systems and expensive too. There are various types of active micromixer such as Magnetic energy (7), electrical energy, temperature-induced, electrohydrodynamic, dielectrophoretic, electroosmotic (8), electrokinetic (9), magnetohydrodynamic (10), pressure driven disturbance, acoustic (11) and ultrasonic (12, 13) mixing can be used to stir fluids. Recently, time dependent pulsatile flows have been used for the fast and efficient mixing (14, 15). One important advantage of active micromixer is that they can be activated on-demand. However, these require external power sources and hence are more complex in packaging and control. Therefore active micromixer is not much convenient.

Passive micromixers do not have moving parts or actuators and don’t use any external energy except the mechanism of pressure head or pump to drive the fluid flow at a constant rate. They have low production cost, more convenient to fabricate and easily integrated into micro-devices.

There are many ways to enhance mixing of the fluids in passive micromixer such as to induce flow separation-recombining and secondary flows by introducing the sharp bends, twist, obstructions, junctions and discontinuities in the path. When fluid stream passes through a sharp bend, secondary flow perpendicular to the flow path takes place. Any separation of the boundary layers leads to the formation of vortices. The curling and breaking of the stream layers create the vortices. This makes the diffusion distance to decrease and gives better mixing performance.

Many researchers have experimented on various chaotic designs of converge-diverge passive micromixer to enhance the mixing process of the fluid. Sigma micromixer (16) has been designed to study the effect of the laminar velocity profile and its variation. The self-circulating flow micromixer (17) having circular mixing chamber induces mixing even at low Reynolds number. It was found that as the constriction channel becomes narrower, the mixing performance increases with the pressure drop. The sharp turn helps in better mixing as demonstrated by comparative study of zig-zag, square and curved structures of micromixer (18). The square mixer showed improved mixing performance because of the sharp turns. Another example (19) is the curved microchannel with the rectangular grooves on the side wall. The mixing index was found to be sensitive to the width of the grooves for Re range, but not to the depth of the grooves. The 3D chaotic serpentine microchannel showed better mixing results (20). Similar type of simulation was performed (21) and it showed better results with 3D serpentine microchannel due to the presence of the obstacles. Non-periodic fractal pattern were introduced in slanted ridges at the channel bottom (22) and the mixing index based on entropy was measured. The effects on the mixing of the positions at interfaces fluid stream in a rectangular microchannel was studied by Ansari (23). It was observed that bended structure in the microchannel enhance the mixing performance at a shorter length (24). The rectangular chambers with hexagonal and round corner shape with different obstacle were investigated to obtain optimum micromixer with short mixing length (25). Asymmetrical micromixer was demonstrated by inserting the two constriction element alternately at the junction of two rhombi (26).

In the present work, we have investigated the Wings protrusion on the side walls of the microchannel to increase the mixing of the fluids. The inward wing shaped protrusion helps in mixing at short distance. The mixing index and pressure drop has been investigated with different type of mesh through numerical simulation and compared their performance. In section II, we present specification of dimensions of proposed micromixers. In section III, we discuss the equations used to simulate fluid flow. The section IV shows the characteristics of micromixers and meshing, whereas in the last section, the results of intensive simulations are discussed.

II. GEOMETRY OF MICROMIXER

The proposed micromixer models have been created by using the CAD tool of the COMSOL multiphysics 5.0 (27, 28) for analysis. The geometry specifications of the straight channel are as follows: both the inlets have length, width, and depth of 1300 µm, 300 µm, and 150 µm respectively. The leading channel illustrated in Fig. 1(a) has length, width, and depth is11000 µm, 300 µm, and 150 µm, respectively.

The geometries of the inward wing shaped channel with different wing size are shown in Fig. 1(b & c): the inlets, outlet, thickness and total length of the channel are of same size as that of straight channel. All the geometries of the microchannel are supplemented with an apposed T-junction. The length of the entrance of the leading channel is 400 µm; two sizes of the inward wings on the side walls of the channel are considered viz.75 µm and 100 µm at the inner side of the channel; the length of the exit of channel after the last wing is 500 µm. The sharp corners in the geometry, leads to singularities causing a higher pressure drop (25). To avoid this, the sharp corners of the wing or the tip of the wings are flattened by 30 µm; fillet is used to round the outer corners of the micromixer with a radius of 40 µm to optimize the design, illustrated in Fig. 2(a & b). There are a total of 15 wings on both the sidewalls, a pair of the wings makes a mixing unit, and likewise it creates a total of 15 units in the channel.

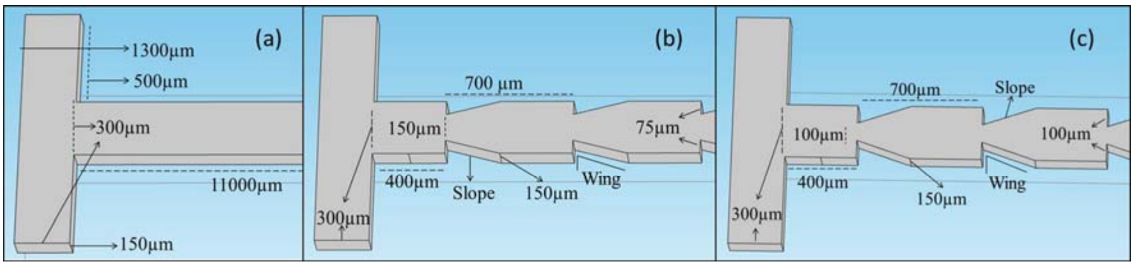

Figure 1.Geometry of (a) Straight, (b) Wing-75, and (c) Wing-100 micromixers.

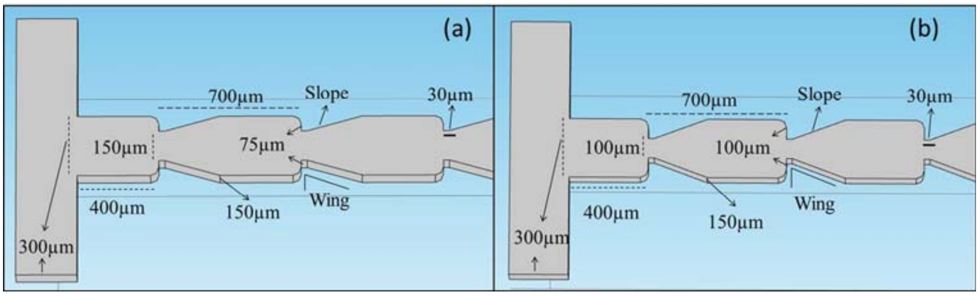

Figure 2. Geometry of (a) Wing-75 and (b) Wing-100 micromixers with flattened wing tip and rounded outer corner.

III. GOVERNING EQUATIONS

Reynolds number is defined as the ratio of inertial force to viscous force, it is denoted by Re and is dimensionless number. It helps to predict the flow characteristics in different fluid flow situation. When Re is less than 2000, laminar flow occurs where viscous effects are dominant and is characterized by smooth, slow, and constant fluid motion. When Re is greater than 2000, turbulent flow occurs where inertial forces are dominant and tends to produce chaotic eddies, vortices and other flows instabilities.

$$Re = \frac{\rho v l}{\mu} \quad (1)$$

Where ν is velocity, ρ is density, μ is dynamic viscosity of the fluid, and l is the length scale of the channel.

The Computational Fluid Dynamics (CFD) simulation based on the finite element method (FEM) has been used to numerically solve the governing equations for 3D laminar incompressible flows in steady state in a microchannel. It uses the Navier Stokes equation, continuity equation and convection diffusion equation, in order to obtain the concentration of the two liquids and their degree of mixing.

Navier Stokes Equation is a fundamental equation to analysis the fluid flow in channel is given below:

$$\rho \left[\frac{\partial u}{\partial t}(u.\nabla)u\right] = -\nabla p + \mu \nabla^2 u \quad (2)$$

Continuous Equation or Conservation of mass (divergent of velocity) is

$$\nabla u = 0 \quad (3)$$

Convection Diffusion Equation is

$$\frac{\partial c}{\partial t} = D\nabla^2 c - u.\nabla c \quad (4)$$

Where ρ is the density, μ is fluid viscosity, p is fluid pressure and u is velocity, c is the species concentration and D is the diffusion coefficient of the species.

The variance of the mass fraction of the mixture of fluids on a cross-sectional plane to the flow direction is given as:

$$\sigma = \sqrt{\frac{1}{\mathrm{N}}\sum_{\mathrm{i}=1}^{\mathrm{N}}\left(\frac{c_i - \bar{c}}{\bar{c}}\right)^2} \quad (5)$$

where σ is the variance, N is the total points at the cross-sectional plane, ci is the molar fraction values at the sample point i and $\bar{c}$ is the mean molar fraction value in the case of complete mixing.

Mixing Index defined to analyze the mixing performance of the micromixer, denoted by M is given as:

$$M = 1 - \sigma \quad (6)$$

Where, σ is the standard deviation. The mixing index (0) means completely unmixed and mixing index (1) means completely mixed. As the mixing index increases, it gives better mixing performance.

IV. NUMERICAL STUDY OF PROPOSED MODELS

The simulation has been carried out by using the software COMSOL Multiphysics 5.0 version and microfluidic module based on finite element method (FEM). For this study, the values of density, dynamic viscosity, and diffusion coefficient of water were taken as - 1000 kg m-3, 10-3 kg/m s and 1.2 × 10-9 m2/s, respectively at 25º C (298.15 K). The above parameters were kept constant throughout the simulation and the flow was presumed to laminar. It is believed that the dilute species is transported by Newtonian fluid in an incompressible flow and the simulation has been performed as time non-variant. The concentration at the first inlet was assumed to be 0 mol/m3 while at the second inlet it was kept at 1mol/m3. Boundary conditions were set for the geometry. The fluid flow has been assumed as steady, with no-slip at the wall. The inlets were assigned to have normal velocity while the outlet is assigned to have zero pressure. So, if the concentration at the outlet is found to be 0.5 mol/m3, it should be considered as 100% mixing. The values of the Reynolds number considered for our study were 0.01, 0.1, 1, 5, 10, …, 100.

Various type of mesh has been studied. At first, the geometry of straight microchannel, Wing-75, and Wing-100 with sharp corners microchannel are meshed by using physics controlled normal mesh, it is denoted as M1, as shown in Fig. 3(a, b, & c). The second mesh was implemented on the modified design of earlier microchannel i.e. Wing-75 and wing-100. These have a rounded corner with flattened tip and the mesh was calibrated to fluid dynamic with global size normal mesh. The free triangular was kept high with respect to the boundary condition and free tetrahedral for the remaining geometry. It is denoted as M2, as shown in Fig. 4(a & b). The third mesh refined and applied only on the Wing-100 microchannel which is similar to second mesh with global size set to fine, it is denoted as M3. The straight microchannel is compared with Wing-75 and Wing-100 to show the effects of the chaotic advection on the mixing of the fluids. Later the Wing micromixers are optimized to be compared again and checked their performance. The results are compared to study the behavior of the fluid mixing with respect to the wing size.

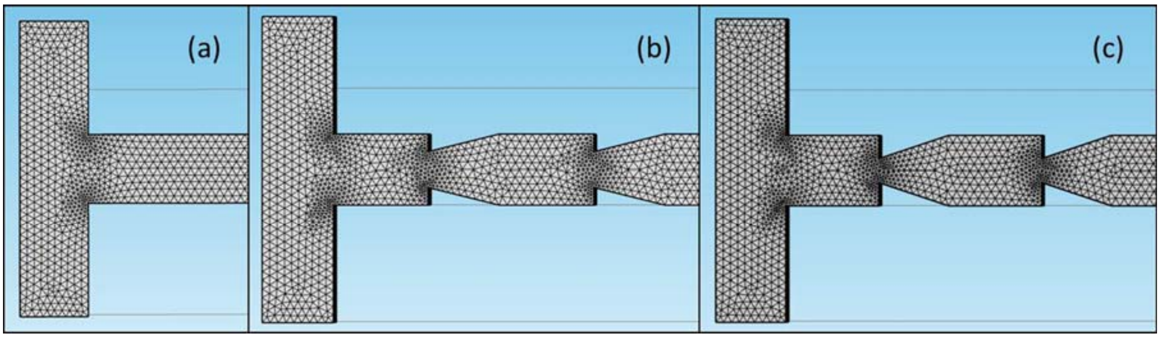

Figure 3. (a) Straight, (b) Wing-75, and (c) Wing-100 micromixer mesh M1.

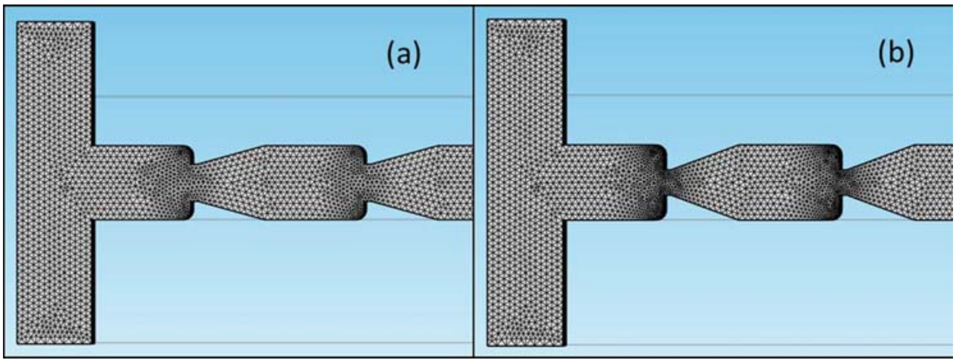

Figure 4.The refined meshing of (a) Wing-75 and (b) Wing-100 micromixer using mesh M2.

V. RESULT AND DISCUSSION

The fluids of two different concentrations enter the channel through the inlets and start flowing in the main channel. The two streams of different concentrations undergo a laminar flow at first. Then get constricted between the first pair of wings, which, converges two streams and forces them to mix together. The slope towards the outer side, increase the width of the channel and help to diverge. Then for some distance the streams flow straight again and reach the next wings where they converge again. Periodic convergence and divergence (or constriction and expansion) of the flow in the microchannel imposed by the wings assists in the mixing of fluids. Simulations have revealed that there are dead zones presents at the corner of the micromixer.

The mesh M1 is implemented on the Straight microchannel, wing-shaped micromixer of wing size 75 μm and 100 μm micromixers. The mixing index was evaluated at the cross section perpendicular to the axial direction as a function of Reynolds number. Fig. 5(a) shows that 100 percent mixing of the fluids occurs at very low Re no. such as 0.01, because the fluids get sufficient residence time for their inter-diffusion. As the Reynold's number increases, the mixing efficiency gradually decreases due to the decrease in the residence time for diffusion. The straight microchannel shows a continuous but very slow decrease in the mixing index with increase of Reynold's number. At a higher valve of Re no. say 100, the mixing index is 87% in straight microchannel. However in the micromixer of wing-75, the mixing decreases from 100% for Reynold's number 0.01 to 92% for Re number 70. Then it increases marginally to 93% for Re no. 80 and remains invariant with further increase of Re number. Micromixer wing-100 shows similar behavior as that of wing-75. At low Re number, mixing efficiency shows 100% for Re number 0.01 and 0.1. It decreases from Re number 1 to 60 and remains invariant. The maximum mixing of fluids flowing through it became 97% for Re no. 70. The straight microchannel always shows low mixing efficiency because of the absence of the chaotic advection. The pressure drop for the straight channel at Re 100 is 89.48 kPa as shown in Fig. 5(b). The pressure drop for micromixer of wing-75 is 107.19 kPa at Re 80. It gives maximum mixing index with minimum pressure drop. The micromixer wing-100 shows 97% mixing with 138.40 kPa at Re no. 70. Due to the sharp wings, it is observed that the pressure drop increases with the increase of the wing size.

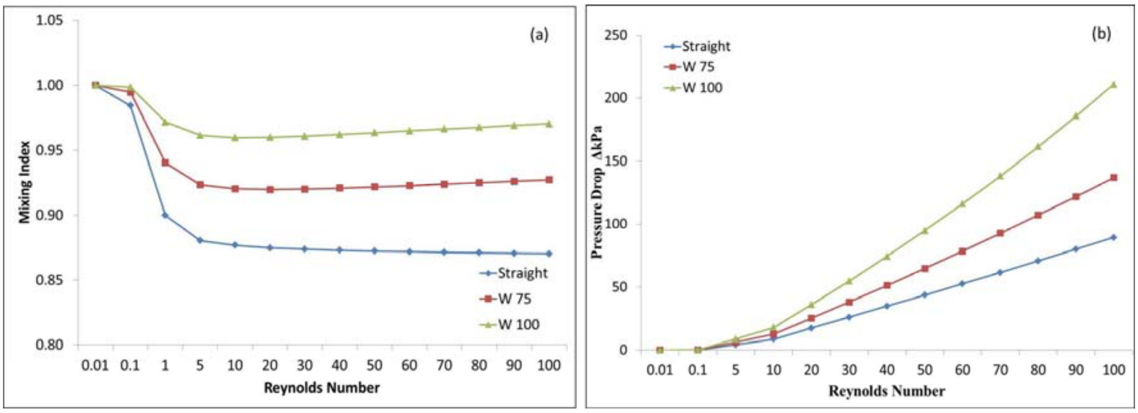

Figure 5.(a) Comparison of Mixing Index of Straight, Wing-75 and wing-100 micromixer; (b) Comparison of Pressure drop of the same; both using mesh M1.

Reynold's number helps to predict the flow characteristics in different fluids flowing in the micromixer. In this study, the Reynold's number of each inlet is considered for Re values of 0.01, 0.1, 1, 10,…, 100. The effects of the Reynold's number on mixing index are observed at the outlet of the micromixer having a mixing length of 11mm.

The sharp tip leads to poor mesh element quality in the adjacent regions and greater pressure drop. The geometry of winged-shaped micromixer designed by us has sharp tip at the inner side of the sidewall. To diminish this problem, the tip of the wings has been made flat for next 30μm. Further, the outer corner of the rectangle has been made round to avoid the mesh problem as shown in Fig. 2(a & b). Also, the refined meshing is applied on the geometry of both micromixers.

The mixing efficiency of the refined Wing-75 and Wing-100 micromixer with mesh M2 is shown in the Fig. 6(a). For small values of Re<0.1, the mixing efficiency is high in both of the micromixer. As the Reynold's number increases, mixing index of Wing-75 drops sharply first and gradually later fluctuating in between till the Reynold's number reaches 50. Its mixing index stabilizes at about 83% for Re 90 with a pressure drop 60.57 kPa as shown in Fig. 6(b). The mixing index of Wing-100 falls from Re 0.01 to 10 and later rises from Re 20 till it reaches to Re 60 which gives mixing 95% at pressure drop 74.26 kPa. The performance remains same at Re 70 with pressure drop of 88.72 kPa, even though there is slight difference in mixing of 0.0013, but the pressure drop difference is 14.46 kPa. So, the best mixing is considered at Re 60. Mixing efficiency of microchannel is found to improve with increase in the resulting pressure drop across the channel. It is observed that, mixing gets better with increase in the constriction of the flow.

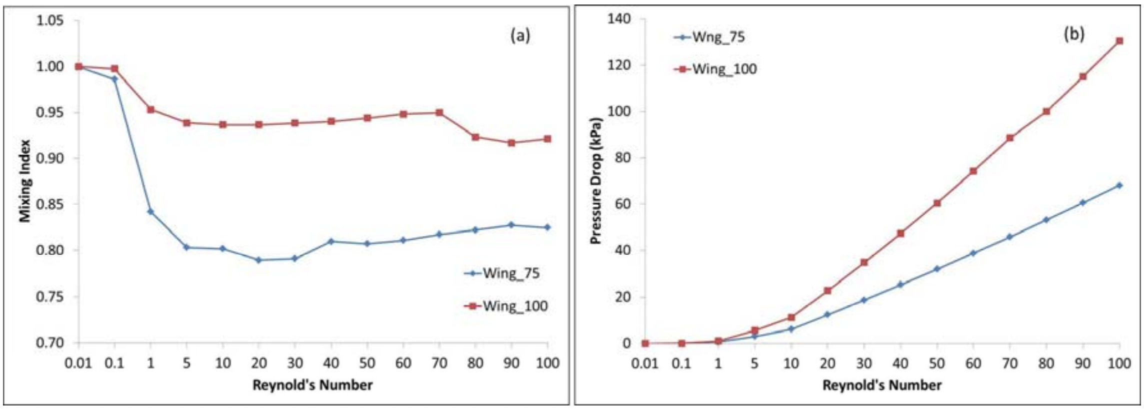

Figure 6. (a) Comparison of Mixing Index of optimized Wing-75 and Wing-100 using mesh M2 and (b) Comparison of Pressure drop for the same.

Fig. 7 shows the comparison of mixing efficiency of the Wing-75 and Wing100 micromixer at different mixing units at Re 60. It shows the comparison between the two micromixers at the cross section of every even numbered mixing unit, where both the fluids stream emerge from the constriction region and are about to spread or expand. In Wing-75, more than 50% mixing has been achieved at the sixth unit whereas in Wing-100 an equivalent degree of mixing gets achieved at the third unit only. 70% of mixing is achieved after eleventh unit in Wing-75 while in Wing-100 it happens at sixth unit. 80% of mixing index, which is considered as well mixed, appears in Wing-75 after the fourteenth unit and in Wing-100 after the eighth unit. While Wing-75 micromixer fails to provide a mixing index greater than 85%, Wing-100 micromixer provides 90% of mixing at the twelfth unit itself and it keeps on increasing to 95% at the outlet. We thus conclude that Wing-100 micromixer provides better mixing efficiency.

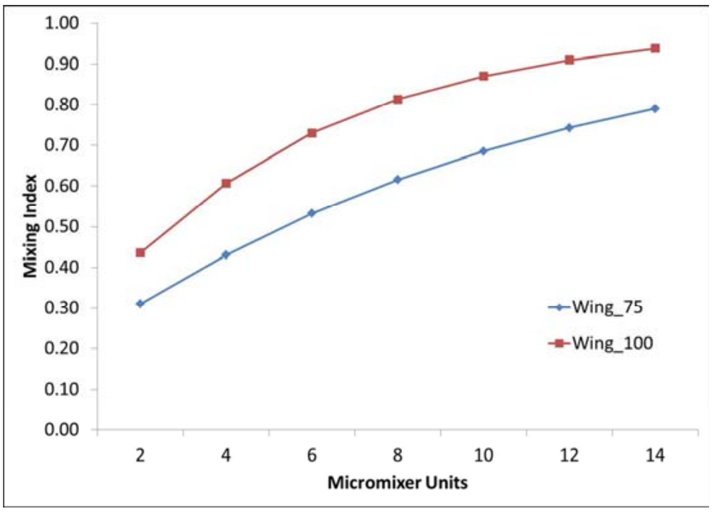

Figure 7.Mixing Index at different units of the Wing-75 and Wing-100 micromixer at Re 60.

Fig. 8 displays the concentration gradient of mixing fluids with Reynolds number 60 flowing through Wing-75 and Wing-100 micromixers at different cross sections located at axial length of 6.2mm, 7.6mm, 9mm, 10.4mm, 11mm. The upper left corner of this picture depicts the cross section (red thin vertical line) occurring immediately after the mixing unit. The mixing index has been evaluated at this location and the axial length corresponding to it has been furnished in the Fig.7. The convergence in flow takes place up to this region and further downstream the fluids are headed to diverge. This region offers a clear view of the concentration gradient. It can be easily visualized that in Wing-100, the mixing is occurring early as compared to that in Wing-75. After the fifteenth unit (axial length 11mm) in Wing-75, two different color bands are visible, indicating that the mixing of fluids is not sufficient. On the other hand, at the same axial length of 11mm in Wing-100 micromixer, the two color bands have merged, which indicates a much better mixing.

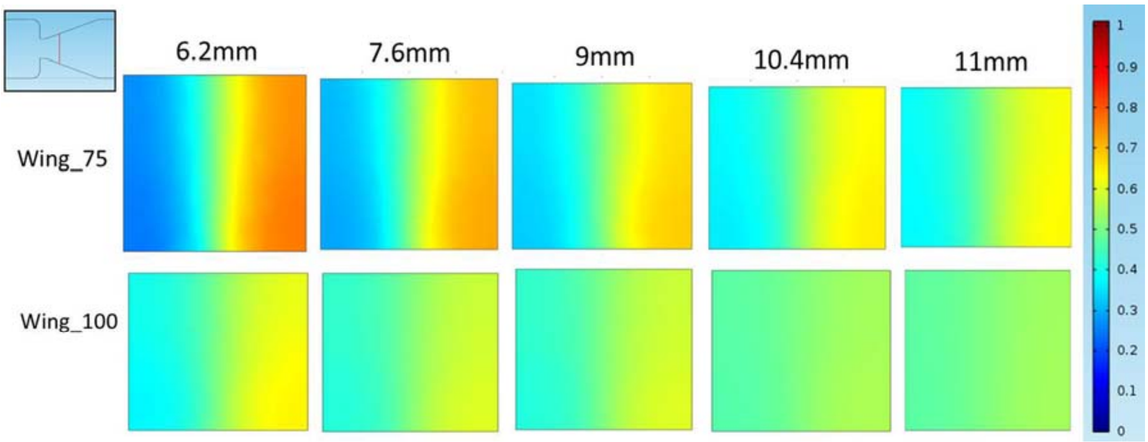

Figure 8.Concentration gradient of mixing fluids (Re 60) at different values of axial length in Wing-75 and Wing-100 micromixers.

The mesh of Wing-100 has been refined to M3. The mixing efficiency of the normal mesh has been compared with that of the fine mesh at Reynolds number 60. This comparison made at the stages of different units of the micromixer is shown in Fig. 9. In the fine meshed microchannel, a mixing index of 80% was achieved at the twelfth unit and it continues to increase until it becomes 87% at the outlet cross section with a pressure drop of 71.782 kPa, at the end of the microchannel. It is observed that the refinement of the mesh has a direct influence on the mixing performance.

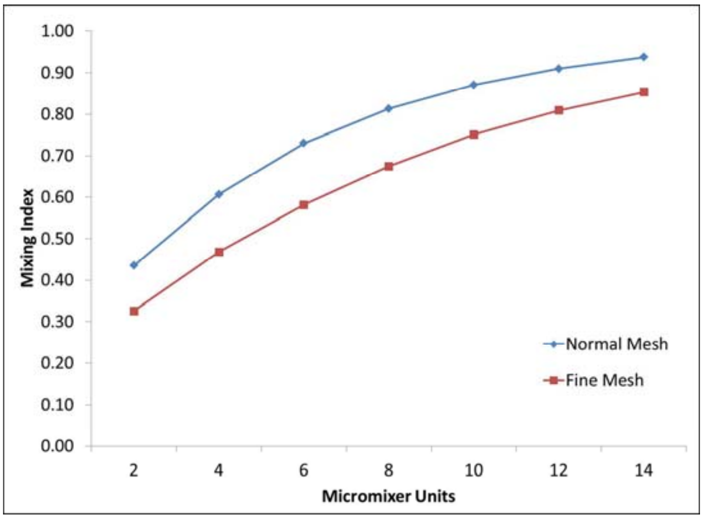

Figure 9.Mixing Index of Wing-100 micromixer with mesh (M2 and M3) at different units at Re 60.

VI. Conclusion

We have investigated the mixing efficiency of the proposed model. In our design, the Wing-100 micromixer designed by us having rounded corner and wing tip flatten with mesh M2 illustrate mixing efficiency of 95% at Reynolds number 60 and a corresponding pressure drop of 74.26 kPa. When Re rises from 60 to 70, it results in only a slight change in the mixing performance but leads to a substantial change in pressure drop between the inlet and outlet. At Reynolds 60 with mesh M3, the mixing efficiency drop to 87% and the pressure drop to 71.782 kPa. We have observed that the mixing efficiency depends on the constriction in the flow. As the size of the wings in the microchannel is increased from Wing-75 to Wing-100, the proximity between their wing tips increases and it enhances the channel constriction. Mixing of fluids flowing around narrower orifice and corners was found to be better although it is accompanied by a bigger drop in the pressure while moving from the inlet to outlet.

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