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Mixing Behavior and Pressure Drop Analysis of Micromixer with Different Geometric Conditions

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Abstract: A 3-D design of and analysis of fluid flow in the micromixer with different configurations is carried out in this dissertation. The main purpose of this research is to obtain minimum mixing length as rapid mixing is essential in many of the micro-fluidic systems used in biochemistry analysis, drug delivery, sequencing, or synthesis of nucleic acids. Also effect on various parameters such as mixing behavior, volume flow, mixing length, maximum velocity, maximum pressure, pressure drop, and velocity distribution were analyzed by changing the mixing angle between inlets. Micromixers with square cross-section rectangular mixing chamber with various types of obstacle placed in fluid flow paths such as rectangular obstacles, elliptical obstacle, and circular obstacle in split and recombination manner were designed for the analysis. The micromixer has 3 inlets and 1 outlet. Water and ethanol were used as working fluids. For computational fluid dynamics analysis, COMSOL Multiphysics 5.0 is used. From various results, we have found that size, the geometry of mixing chambers and obstacles, and mixing angle affect mixing length, pressure, and velocity. With a decrease in mixing angle mixing length, pressure drop, and maximum velocity decrease i.e. it gives better mixing performance. Also with an increase in the number of obstacles mixing length and maximum velocity decrease and pressure drop increases. Micromixer with mixing angle 60 degree and circular obstacles gives minimum mixing length than any other models consisting rectangular or elliptical obstacle and mixing angle greater than 60 degrees.

Keywords: Micro-mixing length, pressure drop, obstacles, mixing chamber, velocity distribution, pressure distribution, mixing behavior, mixing angle

I. INTRODUCTION

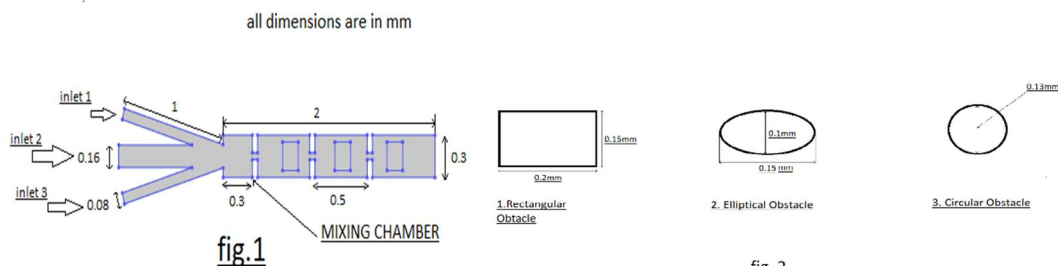
Micro-fluidics is a branch of science that includes the study of fluid flow in channels whose dimensions are in micrometers. It has a wide range of research as microfluidic tools it provides applications in pharmaceuticals, biomedical, lab-on-chip(LOC), drug delivery and DNA sequencing, etc. This technique has the advantage over the standard bench-top method as it requires a low volume of reagents and cost. Micro-mixer is one of the very essential tools in microfluidics. It is a device that mixes two or more fluids at the micro-scale. The main purpose of microfluidic mixing is to achieve fast, complete, and through-out mixing of multiple fluids. In many devices mixing is achieved by enhancing the diffusion effect. There are two types of micromixers as active and passive type. In the passive type, micromixer diffusion is achieved by external force or disturbance. In the passive type, diffusion is achieved by improving area contact, structure configuration, or adding obstacles and baffles in the flow path. In simple T and Y shape mixing takes place by slow molecular diffusion. This mixing does not require any external source for mixing. Various research data showed that Low Reynolds number ($Re < 20$) causes that mixing is only by diffusion so mixing efficiency is low. Also by increasing Reynolds number mixing index is also increased for proposed designs. The final result showed that the YRCSAR mixing efficiency is 99% at $Re=100$ (Imran Shah et.al, 2018). Therefore to improve mixing performance this research is concentrated on micromixers with different obstacles. The high values of wall shear rate, in the crossing zone, confirm the near-wall disturbance created by the impingement of flow and the appearance of vortices which allowed to improve the fluid mixing. The results of the study showed that the \dagger shaped system can improve the mixing process in comparison with the micromixers having Υ geometry (Nassim Ait Mouheb et. al, 2009). Also, the mixing can be improved by suitably choosing geometric parameters of the groove, such as the depth, the width, and the oblique angle (Yeng-Yung Tsui et. al, 2008). The early initiation of vortices in the inlet streams of a T-shaped micromixer by either symmetric or antisymmetric VIOs in the inlet channels can lead to improvements in mixing efficiency (Chih-Yang Wu et. al, 2020).

The micromixer based on the SAR process is more effective at low Reynolds numbers than devices based only on molecular diffusion (Mohammad Nimafar et. al, 2012) therefore the research design includes models based on the SAR technique. Micromixers with ellipse-like micropillars have a well-mixing status when their mixing efficiency is higher than 80% as ≤ 1 . This micromixer has shown the improved performance of the previous micromixer (T-mixer) at a low Reynolds number (Tran-Minh et. al, 2014). The flow regime of symmetrical 1:1 mixing in T-shaped micromixers ranged from straight laminar flow for Re numbers lower than 10 over vortex creation to symmetry break up of engulfment flow. Also for Re numbers larger than 240, the flow showed temporal fluctuations at the entrance of the mixing channel, starting with periodic pulsations. With increasing Re number, the regularity of the pulsations is disturbed by higher frequencies leading to chaotic flow behavior at $Re = 1000$ (Norbert Kockmann et. al, 2007). A bend in the microchannel induced stirring and it also enhanced mixing performance. In case of square wave microchannel number of bend is higher than the zig-zag microchannel therefore it has higher mixing efficiency (Sharhawat Hassain et. al, 2009). The CFD based results showed that the mixer efficiently stirs the fluids, generates secondary vortex flows in the microchannels which results in higher mixing index. The results also revealed that baffles can break the fluid streams, produce fluid convection and increase the contact area of the fluid by folding and deflecting fluid streams which in turn helps to improve the mixing index (Ranjitsinha R. Gidde et. al, 2019). Also because of the reversed area, the mixing performance of TPZ has an highlighted advantage over the zigzag micromixer's and mixing index are all beyond 93% for a wide range of Re ($Re \geq 5$ or $Re \leq 0.5$). The reversed area enhanced the intensity of molecular diffusion. Also the pressure drop in TPZ is bigger than the zigzag micromixer at each Re inevitably (Xueye Chen et. al, 2016). The mixing analysis of different configurations of channel under various operating conditions were carried out using CFD software (Shinde et al). With the respect of pressure drop, teardrop obstacle-based micromixer showed less pressure drop. Both mixing index and pressure drop increase with increase in aspect ratio of the obstacle (Ranjitsinha R. Gidde, 2019). Various results also showed that, the mixing angle, or equivalently the tilt angle, in arrow mixers also has a strong impact on the mixing performance at relatively high values of Re in unsteady periodic regimes, and it appeared that a small downward tilt angle leads to an improvement in the mixing performance compared with classical T mixers that is robust toward variations in the operating conditions up to the transition to chaotic dynamics (Simone Camarri et. al, 2020). It is necessary to improve mixing performance and study the effect of various parameters because of its applications in the chemical industry, fuel cells, micro-reactors, and biomedical. Therefore, in the present work, we studied different types of micromixers consisting of rectangular, elliptical, and circular obstacles for comparing the mixing performance of each micromixer using COMSOL Multiphysics 5.0. Also, various parameters such as pressure drop, velocity, and pressure distribution were studied in this paper.

II. CFD MODELLING AND FORMULATION

A. Micro-mixer Model

For simulation and analysis purposes three models of passive micromixer of SAC type with the rectangular, mixing chamber, and different shaped obstacles such as rectangular, elliptical, and circular are designed in COMSOL Multiphysics 5.0 as shown in fig (1). Micromixer has 3 inlets of 1mm length and 1 outlet of 2 mm length. The Width and Height of inlet 1 and 3 are 0.08 mm and 0.15 mm and of inlet 2 are 0.160 mm and 0.150 mm. . Width and Height of the outlet are 0.3 mm and 0.2 mm respectively. The Length, width, and height of the rectangular chamber are 0.5 mm, 0.3mm, and 0.15mm respectively. The Connector between the rectangular chamber has the Length, width, and height of the rectangular chamber are 0.05 mm, 0.05mm, and 0.15mm respectively. For inlet 1 and 3 water is working fluid and ethanol for inlet 2. The Width, height, and length of a rectangular obstacle are 0.2 mm, 0.15 mm, and 0.15 mm respectively. The major and minor axis of an elliptical obstacle is 0.15 mm and 0.1 mm respectively. The Radius of a circular obstacle is 0.13 mm as shown in figure(2).



B. Governing Equations

The CFD software COMSOL Multiphysics 5.0 is used to capture the characteristics of the flow features and mixing in the three-dimensional model. The flow of water and ethanol liquid in micromixers and mixing can be described by the Navier–Stokes equation, continuity equation, and species convection-diffusion equation are represented as Eqs. (1), (2), and (3), respectively (Gidde et al. 2018c).

$$\nabla U = 0 \tag{1}$$

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

$$\frac{\partial c}{\partial t} = D \nabla^2 c - u \cdot \nabla c \tag{3}$$

Where u is the fluid velocity, p is fluid pressure, ρ is the fluid density, μ is fluid viscosity, D is diffusivity, and c is molar concentration.

C. Boundary Conditions and Material Properties

The inlet velocity of water and ethanol is 0.5 m/s and set to be uniform and constant across the inlet cross-section of the micromixer. At the outlet, the pressure value is set to atmospheric pressure, and no-slip boundary conditions are used at fixed walls of the micromixer. The molar concentration of water is set to 0 and ethanol to 20 to define the mixing length of the micromixer. When the mixing takes place, the molar intensity of ethanol decreases from 20, while on the other side molar intensity of water will increase from 0 and will become 10 after complete mixing and at that point will give the mixing length of the micromixer. Viscosity of water is 0.001 Pa.s, diffusion coefficient is $1 \times 10^{-10} \text{ m}^2/\text{s}$ and molar concentration is 1000 kg/m^3 . Viscosity of ethanol is 0.00126 Pa.s, diffusion coefficient is $1 \times 10^{-10} \text{ m}^2/\text{s}$ and molar concentration is 500 kg/m^3 . A uniform mass flow inlet and a constant inlet temperature were assigned at the channel inlet of the micromixer.

D. Meshing of Geometry

The structured meshing method is used for meshing the geometry in Comsol Multiphysics. The 3D geometry of the micromixing channel with extremely coarse mesh. Material properties are defined in the material database in Comsol Multiphysics

III. PERFORMANCE PARAMETER

A. Pressure Drop

One of the most important design considerations for a micro-fluidic channel design is to minimize the pressure drop. The equation used to determine the pressure drop is as given below,

$$\Delta P = \left[\frac{f \times RE}{2} \right] \times \left[\frac{\mu \times V \times L}{D_h^2} \right]$$

Where p is the pressure difference within the channel, L is channel length in mm, μ is the dynamic viscosity of a fluid in Pa.s, V is the average velocity, $(f \times Re)$ is Poiseuille number. Also, pressure drop can be evaluated in simulation analysis as shown below,

$$\Delta P = P_i - P_o$$

Where P_i is inlet pressure and P_o is outlet pressure. The difference between inlet and outlet pressure will give the pressure drop.

B. Velocity of Flow

When a fluid is moving through a microfluidic channel, we can see that there is a velocity gradient across the cross-section of the channel. Since a fluid is defined as a substance that will deform continuously under the application of shear stress and know that the flow structure of fluid in a microfluidic channel is laminar. Newton's law of viscosity can be used to show the relationship between shear stress and deformation rate as below,

$$\tau = \mu \frac{du}{dy}$$

Where τ is the shear stress, μ is the viscosity of the fluid, u is the velocity of the fluid in the x-direction and du/dy is the velocity gradient in the y-direction in the above expression. This results in the highest velocity being in the portion of the fluid that is furthest from the wall. Also, there is a no-slip condition for the portion of the fluid that is adjacent to the wall of the channel where the shear force is the greatest.

IV. SIMULATION AND RESULTS

A. Mixing length of Micromixers

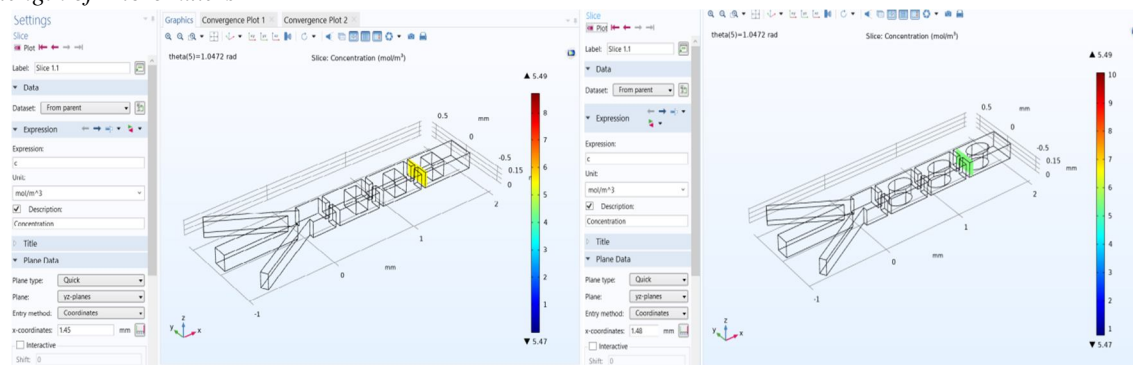


Fig 3: Mixing Length of Micromixer having Rectangular Obstacle

Fig 4: Mixing Length of Micromixer having Elliptical Obstacles.

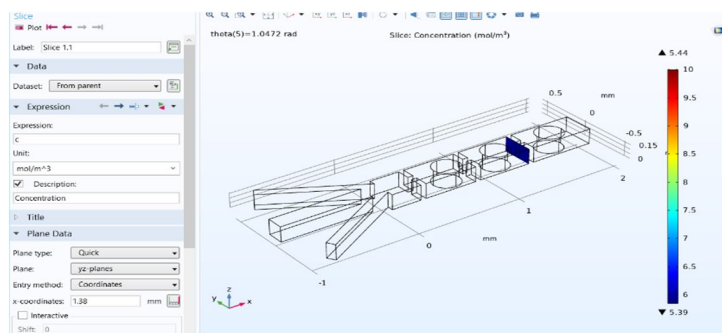


Fig 5: Mixing Length of Micromixer having Circular Obstacles.

The above figures show the mixing lengths of the micromixers having rectangular, elliptical, and circular obstacles. There are two fluids, one is ethanol, and the other is water, ethanol has more molar concentration and water has lesser molar concentration. So the complete mixing takes place whenever the concentration of two fluids becomes equal or near about the same. Mixing lengths for micromixers having rectangular, elliptical, and circular obstacles are 1.45mm, 1.48mm, and 1.49mm respectively as shown in figures 3, 4, and 5. From simulation analysis, it can be seen that for micromixer with a circular obstacle shows a minimum mixing length than a micromixer with a rectangular or elliptical obstacle as it has smooth edges which cause turbulent flow and produce vortices inflow.

B. Pressure Drop across Micromixers

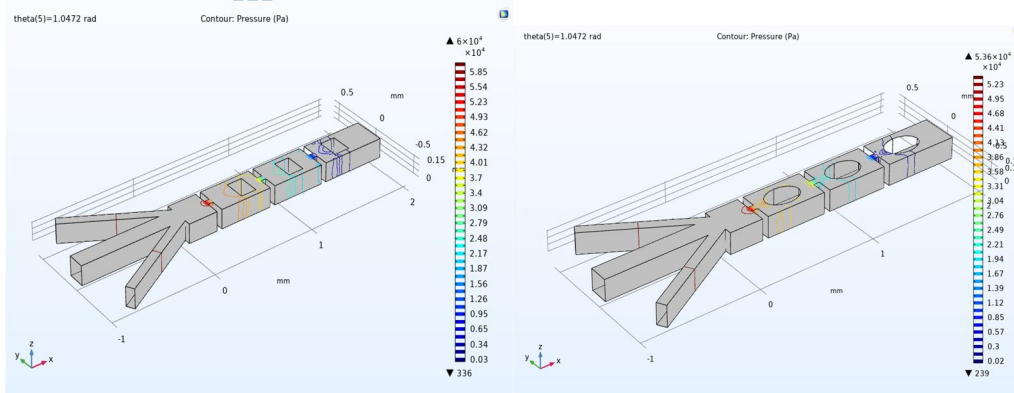


Fig 6: Pressure Drop of Micromixer having Rectangular Obstacle

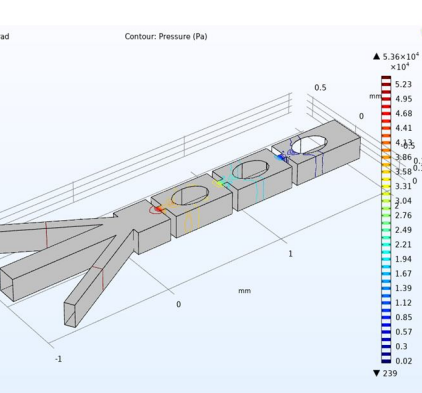


Fig 7: Pressure Drop of Micromixer having Elliptical Obstacles

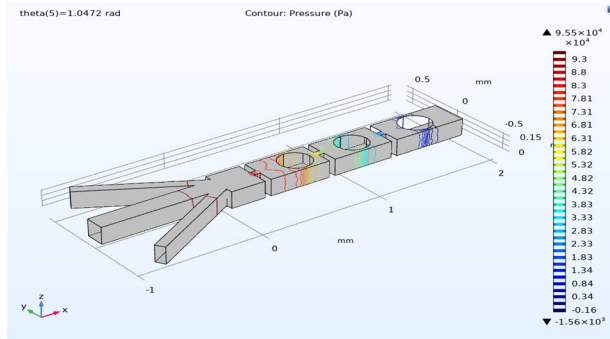


Fig 8: Pressure Drop of Micromixer having Circular Obstacles

The above figures represent pressure distribution along with various points in the model. Maximum pressure is indicated by dark reddish color and the minimum pressure is indicated by dark blue color. For micromixers having rectangular obstacles, inlet pressure is 6×10^4 Pa and outlet pressure is 336 Pa. So the pressure drop for that micro-mixer is 3.9×10^4 Pa. For micromixers having elliptical obstacles, inlet pressure is 5.36×10^4 Pa and outlet pressure is 239 Pa. So the pressure drop for those micromixers is 5.3×10^4 Pa. For micromixers having circular obstacles, inlet pressure is 9.55×10^4 Pa and outlet pressure is -1.56×10^3 Pa. So pressure drop for micromixers is 9.7×10^4 Pa.

C. Velocity Distribution across Micromixers:

Figures show velocity variation at different sections and points with the help of different colors. The red color indicates maximum velocity. The maximum velocity of micromixers with a rectangular obstacle is 2.62 m/s and for micromixers with an elliptical obstacle is 2.18 m/s. For micromixers with a circular obstacle is 2.19 m/s. At the walls of the channel, there is minimum velocity and it is denoted by blue color. Maximum velocity is maintained at the center of geometry as there is no resistance which will be provided by walls of geometry.

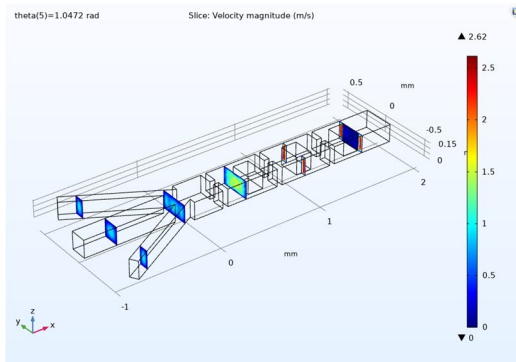


Fig 9: Velocity Distribution micromixer having Rectangular obstacles

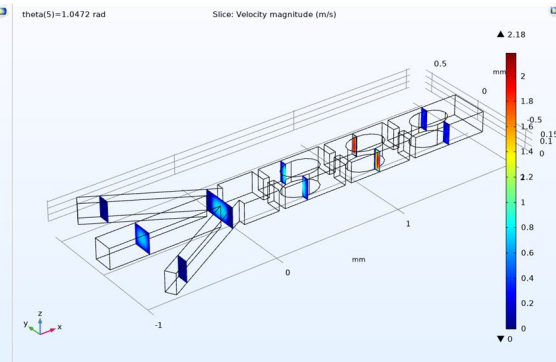


Fig 10: Velocity Distribution of Micromixer having Elliptical Obstacles

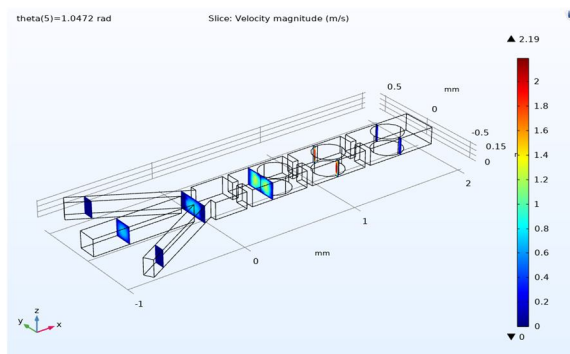


Fig 11: Velocity Distribution Micromixer having Circular Obstacles

Figures show velocity variation at different sections and points with the help of different colors. The red color indicates maximum velocity. The maximum velocity of micromixers with a rectangular obstacle is 2.62 m/s and for micromixers with an elliptical obstacle is 2.18 m/s. For micromixers with a circular obstacle is 2.19 m/s. At the walls of the channel, there is minimum velocity and it is denoted by blue color. Maximum velocity is maintained at the center of geometry as there is no resistance which will be provided by walls of geometry.

D. Mixing Behavior across Length of Micromixer:

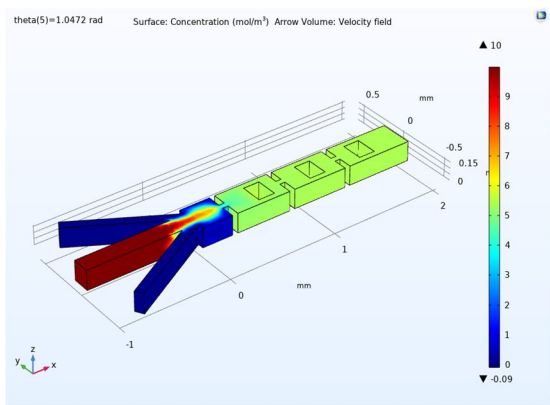


Fig 12:Mixing behavior for rectangular obstacles

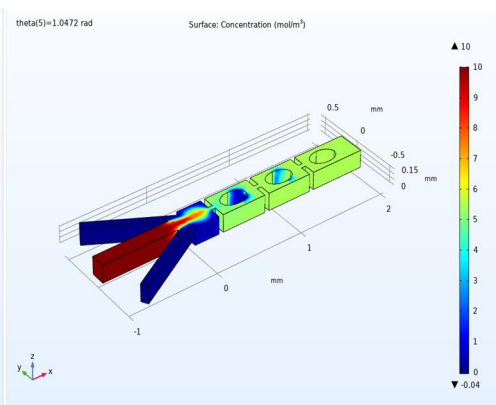


Fig 13:Mixing behavior for elliptical obstacles

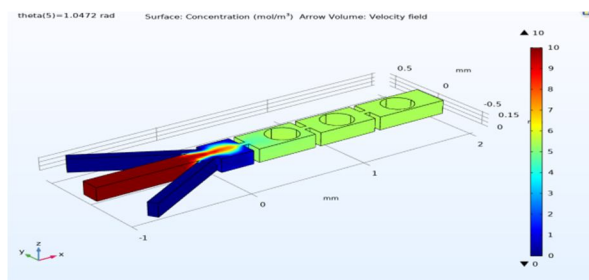


Fig 13:Mixing behavior for circular obstacles

The above figures show mixing behavior across micromixers with rectangular, elliptical, and circular obstacles. Various colors shows vary in concentration as mixing takes place. Water is represented by blue color and ethanol is shown by reddish color. As mixing takes place, the concentration of water tends to increase and ethanol to decrease and finally becomes equal after proper mixing. The uniform mixture has a uniform concentration and shows a uniform color as shown in figures 12, 13, and 14. The presence of obstacles improves the mixing performance as it increases diffusion.

E. Comparison of Mixing Lengths of Obstacle with Varying Mixing Angle:

1) For Micromixer with Rectangular Obstacle

Sr.No	Angle between Inlet 1 and 3(degree)	Maximum Pressure (pa)	Maximum Velocity (m/s)	Mixing Length (mm)	Pressure drop (Pa)
1.	180	7.88×10^4	2.39	1.5	4.4×10^4
2.	150	8.22×10^4	3.76	1.49	4.41×10^4
3.	120	4.81×10^4	2.38	1.47	4.29×10^4
4.	90	4.81×10^4	2.28	1.46	4.29×10^4
5	60	4.81×10^4	2.04	1.45	4.28×10^4

Table I: Results of Mixing Length for Varying Angle of Micromixer With rectangular obstacle.

The table (I) shows various results such as maximum pressure, maximum velocity, mixing length. and pressure drop for micromixer with a rectangular obstacle. When the angle difference is 180 degrees between inlet 1 and 3 then the mixing length is 1.5 mm from the mixing junction. Also for angle difference 150 and 120 degrees mixing length is 1.49 mm and 1.47mm respectively. For 90 and 60 degrees mixing length decreases and becomes 1.46 and 1.45 mm. Results have shown that as the angle between inlet decreases mixing length also decreases. Also, maximum velocity decreases from 2.39 m/s to 2.04 m/s when the mixing angle decreased from 180 degrees to 60 degrees. Pressure drop also showed a decreasing trend as a decrease in mixing angle. It decreased from 4.4×10^4 Pa to 4.28×10^4 Pa. After an increase in the number of obstacles mixing length is decreased to 1.41 mm. That means with an increase in the number of an obstacle, mixing length will decrease.

2) *For Micromixer with Elliptical Obstacle:* Table (II) shows various results of various performance parameters that were studied in this research, for micromixers with elliptical obstacles. When the angle difference is 180 degrees between inlet 1 and 3 then the mixing length is 1.84 mm from the mixing junction. From there the mixing length decreases by a great margin. For angle difference 150 and 120 degrees mixing length is 1.53 mm and 1.51mm respectively. For 90 and 60 degrees mixing length decreases and becomes 1.50 and 1.48 mm. Again the results have shown that as the angle between inlets decreases mixing length also decreases. Also, maximum velocity decreases from 2.34 m/s to 2.18 m/s when the mixing angle decreased from 180 degrees to 60 degrees. Pressure drop has shown a decreasing trend as a decrease in mixing angle. It decreased from 5.87×10^4 Pa to 5.34×10^4 Pa.

Sr.No	Angle between Inlet 1 and 3(degree)	Maximum Pressure (pa)	Maximum Velocity (m/s)	Mixing Length (mm)	Pressure drop (Pa)
1.	180	4.87×10^4	2.34	1.84	5.87×10^4
2.	150	4.81×10^4	3.32	1.53	5.6×10^4
3.	120	4.81×10^4	2.29	1.51	5.65×10^4
4.	90	4.81×10^4	2.25	1.50	5.38×10^4
5	60	4.81×10^4	2.18	1.48	5.34×10^4

Table II: Results of Mixing Length for Varying angle of Micromixer with Elliptical Obstacle.

3) *For Micromixer with a Circular Obstacle*

Sr.No	Angle between Inlet 1 and 3(degree)	Maximum Pressure (pa)	Maximum Velocity (m/s)	Mixing Length (mm)	Pressure drop (Pa)
1.	180	4.87×10^4	2.33	1.66	1.04×10^5
2.	150	4.81×10^4	2.29	1.65	1.03×10^5
3.	120	4.81×10^4	2.27	1.48	1.00×10^5
4.	90	4.81×10^4	2.26	1.38	1.01×10^5
5	60	4.81×10^4	2.19	1.38	0.97×10^5

Table III: Results of Mixing Length for Varying Angle of Micromixer With Circular Obstacle.

The above table (III) contains various results such as maximum pressure, maximum velocity, mixing length, and pressure drop for micromixer with a circular obstacle which was studied in this thesis. When the angle difference is 180 degrees between inlet 1 and 3 then the mixing length is 1.66 mm from the mixing junction. Also, for angle difference 150 and 120 degrees the mixing length is 1.65 mm and 1.48 mm respectively. For 90 and 60 degrees the mixing length equal i.e 1.38mm for both. For a decrease in angle, there is a decrease in mixing length. Which is a positive outcome of results. Also, maximum velocity decreases from 2.33 m/s to 2.19 m/s when the mixing angle decreased from 180 degrees to 60 degrees. Pressure drop also showed a decreasing trend as a decrease in mixing angle. It decreased from 104×10^4 Pa to 9.7×10^4 Pa.

F. Comparison Of Results Of Mixing Length Of Micromixer With Rectangular, Elliptical, And Circular Obstacles

Fig 14 shows graph of mixing length to mixing angle between inlets for rectangular, elliptical and circular obstacles. From various results, it can be seen that mixing angle, the shape of geometry, and the shape of obstacle play an important role in minimizing mixing length. Overall results showed that mixing length is minimized as the mixing angle decreases. It showed a great variation in mixing length as the angle decreased from 180 degrees to 60 degrees. The change in the shape of the obstacle also showed a change in mixing length. The graph below shows mixing length vs mixing angle between inlets for micromixers containing rectangular, elliptical, and circular obstacles. Y-axis denotes mixing angle and X-axis denotes mixing length from mixing junction along the length of micromixers. Blue, red and green denotes mixing length for circular, elliptical and rectangular obstacle respectively. For the rectangular obstacles, the minimum length is 1.45 mm obtained at 60 degrees and the maximum length is 1.5 mm at 180 degrees. For the elliptical obstacles, the minimum length is 1.48 at 60 degrees and the maximum length is 1.84 mm at 180 degrees. And for circular obstacles minimum mixing length is 1.38 at 60 and 90 degrees, maximum mixing length is 1.66 mm at 180 degrees. From the results, it can be seen that a micromixer with circular obstacles gave better-mixing performance in terms of mixing length.

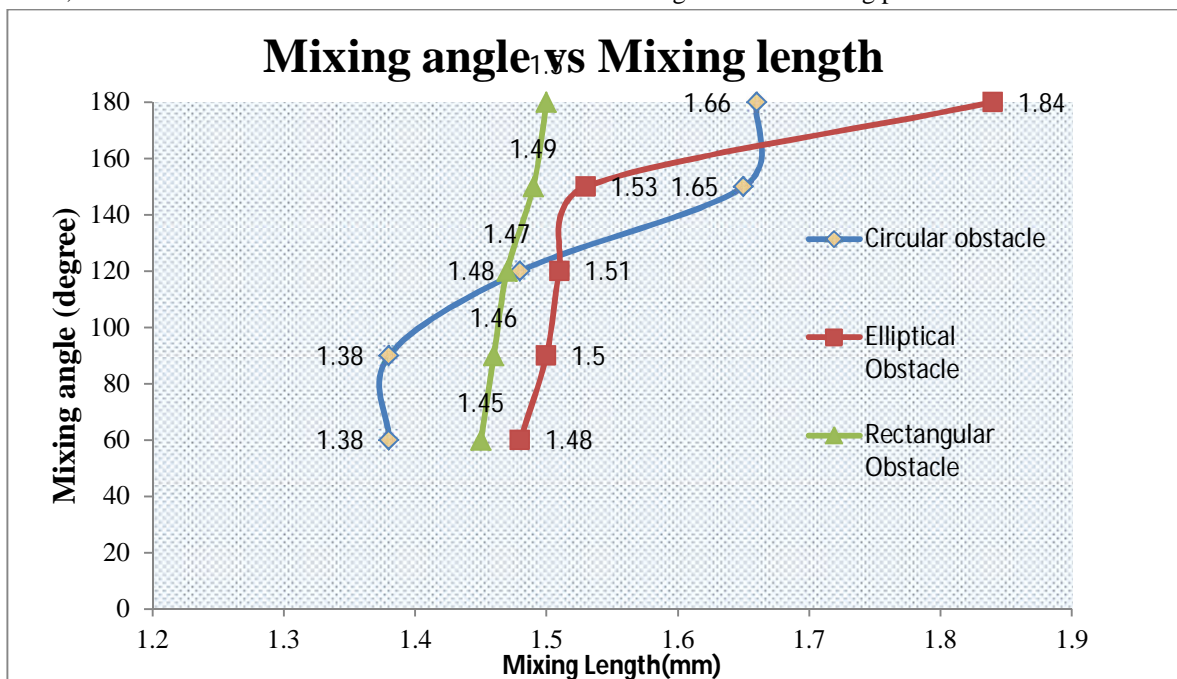


Fig 14: Graph of Mixing Angle vs Mixing Length for Micromixer with Rectangular, Elliptical and Circular Obstacle

V. CONCLUSION

From various results, we have found that size, the geometry of mixing chambers and obstacles, and mixing angle effect mixing length, pressure, and velocity. With a decrease in mixing angle mixing length, pressure drop, and maximum velocity decrease i.e it gives better mixing performance. Also, with an increase in the number of obstacles mixing length and maximum velocity decreases and pressure drop increases. Micromixer with mixing angle 60 degree and circular obstacles gives minimum mixing length than any other models consisting rectangular or elliptical obstacle and mixing angle greater than 60 degrees.

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