NUMERICAL INVESTIGATION OF THE EFFECT OF MIXING ON THE PERFORMANCE CHARACTERISTICS OF A MICRO-REACTOR

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Abstract- In this work, we investigate suitable microchannel to carry out reactions and separations. For this, various microchannel geometries are considered such as T, Y and Arrow shaped. Here, the mixing is analyzed at first by sending two fluids having different temperature. The time at which two fluids attain steady state is considered to be the mixing time. This is further verified by sending a liquid mixture with different concentrations. Mixing efficiency is quantified for these microchannels and found Arrow to be the suitable reactor to investigate the progress of reaction. The resulting flow behavior in these system enhances reactions. The mixing was found to be better when the angle formed between inlet and outlet channel is in the range of 90° and -45°.

Index Terms- CFD , Microchannel, Mixing efficiency, Simulation.

INTRODUCTION

Over the past decade, microfluidics has developed at a fast pace. The main driving forces for this research are applications in several emerging technological areas such as chemical synthesis, micro separation processes, nanoparticle synthesis, and polymerization reaction [1]. The main advantage of this system is the increase in surface area to volume ratio with the decrease of the system feature size of micro-devices and some physical phenomena which are insignificant in the macro domain become prominent in the micro domain. Mixing is a transport process for species, temperature, and phases to reduce inhomogeneity. Various studies have been carried out to understand mixing in microchannels [2-7]. The characteristic channel width are of 100 to 500 μm. The channel height is of the order of channel width. In comparison to molecular size scales, the length scale and volume scale of micromixers are very large. This fact leads to two key characteristics of micromixers. Firstly, designing micromixers relies on manipulating the flow using channel geometry or external disturbances. Secondly, while micromixers bring advantages and new features into chemical engineering, molecular level processes such as reaction kinetics remain almost unchanged.

A. Soleymani et.al. [3] carried out numerical and experimental investigations of liquid mixing in T- type micromixers. They considered mainly T-type channels with different geometrical parameters such as aspect ratio, mixing angle and throttle size. Here simulations were performed for different operating conditions. The prediction shows that the development of vortices and it is essential to achieve good mixing performance. Furthermore, it has been shown that the development and occurrence of vortices strongly depends on flow rate. It was found that with increase in flow rate, the flow pattern changes from stratified to vortex and then to engulfment flow. The mixing efficiency is found to be higher during engulfment flow.

John T. A., and Adeniyi L., [8] investigated on T-shaped channels. The performance of such a channel is analyzed by the RTD.

The performance of mixing in different micro-channel geometries has been further analyzed by K. D. P. Nigam et.al [7]. They used both active and passive mixers. The effect of different geometries (rectangular, circular, and triangular) on friction factor, laminar-to-turbulent transition, and the effect of roughness are analyzed in their study. The differences in the uncharacteristic behavior of the transport mechanisms through micro-channels due to compressibility and rarefaction, relative roughness effects were discussed. The micro-mixers were quantified based on Reynolds number (N_{Re}) and Peclet number (N_{Pe}) and mixing characteristics.

Computational fluid dynamics (CFD) is an important tool for the development of micro-fluidic system. CFD has been used extensively to investigate and understand flow regimes in micro-channels [10-11]. Here, the flow in micro-channel is predicted by Computational Fluid Dynamics (CFD) to find suitable micro-channel to carry out reactions and separations. The micro-channels considered have different mixing angles and it is analyzed by commercial software Ansys Fluent 13. The aim of our article is to analyze and quantify mixing in such microchannels for various N_{Re} using 2D model.

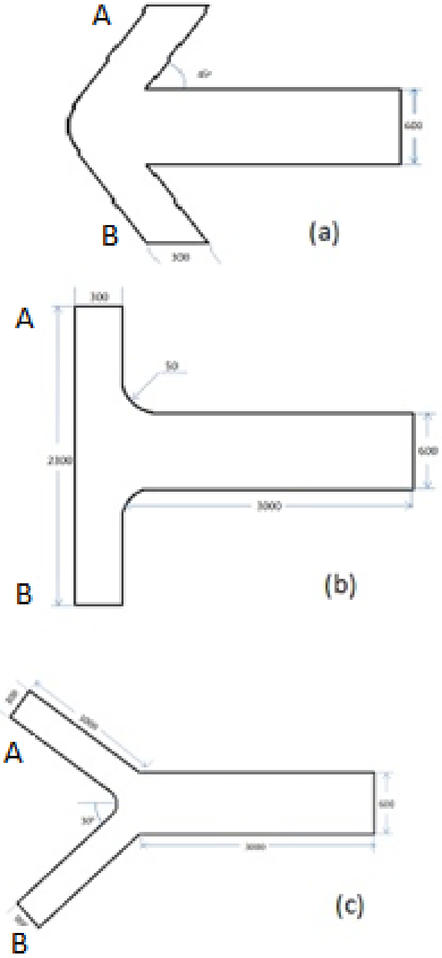

Fig. 1. Schematic representation of (a) Arrow, (b) T and (c) Y-Shaped microchannels. A and B are the inlets. (all dimensions are in mm)

I. CFD MODELLING

Newtonian liquid in microchannels can generally be described by Navier-Stroke equation and continuity equation [9].

$$\frac{\partial V}{\partial t} + V.\nabla V = -\frac{1}{\rho}\nabla p + \vartheta \nabla^2 V$$

(1)$\nabla . V = 0$

(2)Where V is the velocity vector, ρ is the density of the fluid, p is pressure and ν is kinematic viscosity of the fluid. The species transport on the other hand can be described by diffusion- convection equation.

$$\frac{\partial C}{\partial t} + (V.\nabla)C = D\nabla^2 C$$
(3)

where C and D are concentration and diffusion coefficient of the species, respectively. The energy balance for the system can be described by the energy equation [12].

$$\rho C_p\left(\frac{\partial T}{\partial t} + (V.\nabla)T\right) = k\nabla^2 T$$
(4)

where C_p is the specific heat, k is thermal conductivity coefficient and T is temperature of the fluid.

II. SIMULATION METHODOLOGY

To simulate such micro-channels, no slip boundary condition was imposed on the walls of the microchannel and a gauge pressure of zero was considered at the outlet of the channels. A uniform velocity profile was specified by setting the desired mass flow rate at the inlet zones.

The CFD results may depend strongly on the employed mesh. In order to check grid independency three different meshes employing roughly (i) 312, (ii) 25177 and (iii) 100850 grid cells, revealing that the intermediate one is sufficient to describe hydrodynamics with a good accuracy. It has therefore been retained (10^{-5} m) for all the further simulations.

Second order upwind discretization is adopted in the CFD together with the SIMPLE algorithm for pressure-velocity coupling. A typical CFD simulation requires roughly 2 days of computing time on a standalone desktop PC (2 GB RAM, 32 bit, Pentium IV processor). Here transient simulations were performed with a time step of 10^{-4} s for integration. The simulation are carried out for the flow time of 1 sec, the system usually attained steady state at 0.16 sec.

III. RESULTS AND DISCUSSIONS

A. *Heat transport in liquid phase*

To investigate the flow field in such microchannels, calculated fields of the major flow variable are first discussed. Figure 2 shows contours of velocity magnitude predicted by CFD for N_{Re} of 180. Here velocity magnitude is maximum at the center of the microchannel as expected. dead zones are present in Arrow and T shaped microchannel when comapred to Y shaped microchannel.

To analyze the performance of micro-channel, hot water (360 K) is passed through one inlet (A) and cold water (300 K) through another inlet (B). The physical properties of water considered are shown in Table 1.

Property	**Value (SI units)**
Density (ρ_w)	998.2 kg/ m^3
Viscosity (μ_w)	1.003e -3 kg/m s
Thermal Conductivity (k_w)	0.6 w/m K
Specific Heat Capacity (C_{pw})	4182 J/kg K

Table 1. Physical properties of water considered.

To understand mixing in such microchannel, variation of temperature in the microchannel is analyzed. Here the time at which two liquids attain steady state is considered to be the mixing time. To analyze quantitatively, the spatial variation of temperature at two cross sections along x=1000E^{-6} m and 2000E^{-6} m are studied. For N_{Re} of 180 as shown in Figure 3, it is observed that there is no significant change in temperature across the channel as temperature between the two inlet of the microchannel is very small.

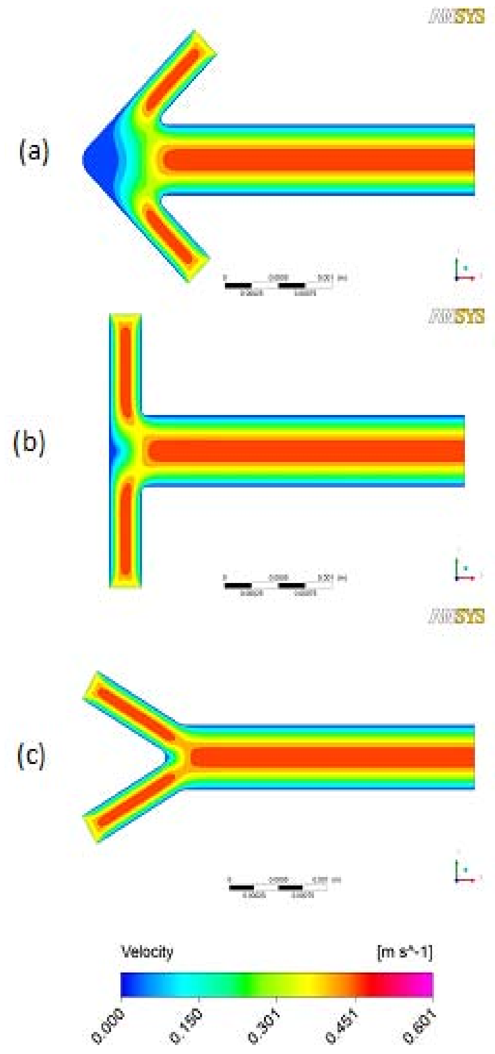

Fig. 2. Comparison of velocity contours for various geometries of micro-channels (a) Arrow (b) T and (c) Y-Shape.

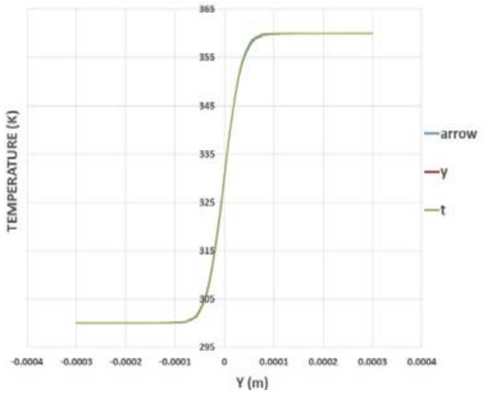

Fig. 3. Spatial variation of Temperature along X = 1000eE^{-6} m in the microchannels.

B. Species transport in gas phase

To find suitable microchannel, further nitrogen and oxygen gases are admitted as into the microchannel. Through inlet A, 0.2 and 0.8 mole fraction of oxygen and nitrogen, respectively are passed and through inlet B inversed mole fractions as that through inlet A is passed. The physical properties of the mixture are as shown in Table 2.

Transport properties	**Value (SI units)**
Density (ρ_g)	1.225 kg/ m^3
Viscosity (μ_g)	1.72E $^{-5}$ kg/m s
Diffusion Coefficient (D)	2.88E^{-5} m^2/s

Table 2. Physical property of gaseous mixture considered.

The spatial variation of concentration of the oxygen at 1000E-6 m and 2000E^{-6} m is analyzed for the microchannels as shown in Figure 4. It is observed that no significant variation was present even when the concentration gradients at inlets were kept large. Observations made can be explained by strong molecular diffusion over the convective transport at this Reynolds number.

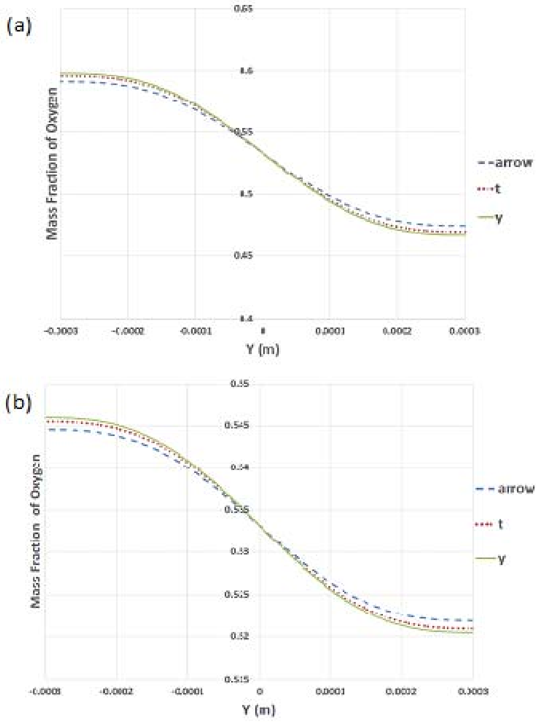

Fig. 4. Spatial **v**ariation of concentration at (a) 1000E^{-6} m and (b) 2000E^{-6} m in the micorchannels.

C. Species transport in liquid phase

The liquid phase species transport system is considered further to investigate the performance of micro-channel. Here, the inputs A and B have the same properties as that of water but are treated as two different liquids with a diffusion coefficient of 2E^{-7} m^2/s. In order to quantify the extent of mixing at a certain distance along the mixing length, mixing efficiency α is defined by

$$\alpha = 1 - \sqrt{\frac{\sigma^2}{\sigma^2_{max}}} \qquad (5)$$

Where σ^2 is variance of concentration and σ^2_{max} is the maximum variance of concentration present in the mixture. Here α=1 for perfect mixing and α=0 for no mixing in the micro channel.

The previous simulations had a strong influence of molecular diffusion and hence the diffusion coefficient of the system was set to 2.0E^{-7} m^2/ s. The simulations are performed for various N_{Re} starting from 24 to 360. The mixing efficiency α is calculated at two cross sections, one at a distance of 1000E^{-6} m and another at 2000E^{-6} m as seen in Figure 1. The calculated values are shown in Table 3 and Table 4.

Reynolds Number, N_{Re}	Microchannels		
	T-Shaped	Y-Shaped	Arrow-Shaped
24	11.21	10.86	13.24
30	9.74	9.45	11.45
60	6.37	6.19	7.46
90	4.97	4.84	5.83
120	4.16	4.08	4.90
180	3.23	3.21	3.84
240	2.70	2.71	3.23
300	2.35	2.38	2.83
360	2.09	2.15	2.55

Table 3. Percentage of Mixing Efficiency for various Reynolds numbers for considered geometries at a cross sectional distance of 1000E^{-6} m.

Reynolds Number, N_{Re}	Microchannels		
	T-Shaped	Y-Shaped	Arrow-Shaped
24	17.40	17.08	19.38
30	14.83	14.57	16.41
60	9.48	9.34	10.37
90	7.39	7.30	8.08
120	6.20	6.14	6.79
180	4.84	4.82	5.32
240	4.06	4.07	4.48
300	3.54	3.56	3.92
360	3.16	3.20	3.52

Table 4. Percentage of Mixing Efficiency for various Reynolds numbers for considered geometries at a cross sectional distance of 2000E^{-6} m.

It is observed that the arrow shaped channel has a better mixing efficiency due to larger dead space as observed in figure 2. In all the cases mixing efficiency (α) has been found to decrease with increase in Reynolds number in all the channels. This is due to the dominance of diffusive effect over convective. These results are concordant with the previous researcher's [3] results.

IV. SUMMARY AND CONCLUSION

Mixing in micro-channels has been investigated quantitatively for various micro-channel using CFD and an approximated 2D model. To carry out this, two fluids with different temperatures are admitted through the inlets of such channels. Here, spatial variation of temperature along the line is considered for investigation. The observations made were inconclusive to decide on the best microchannel due to the strong influence of molecular diffusion.

This is further verified by sending two liquid having different concentration. The system was also influenced greatly by molecular diffusion. For better understanding of the system, two materials with low diffusion coefficient are considered. On simulating this system and quantifying the mixing, it was observed that arrow shaped channel was better than the other considered channels. Here, Reynolds number was varied from 24 to 360. The residence time decreases as velocity is increases and hence mixing efficiency decreases. These observations were observed in 3D models also; hence making the approximation of microchannels to 2D models is valid.

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