Increasing the efficiency of microfluidic micromixer with gaps and baffles using design of experiments based on Taguchi method

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ABSTRACT

In this study, the geometrical parameters of a micromixer with gaps and baffles are optimized by using design of experiments based on the Taguchi method. Design of micromixers with gaps and baffles to increase the mixing efficiency is crucial in various biological applications such as DNA analysis. The arrangement of gaps and baffles significantly affects the fluid flow structure and mixing. In some cases, arrangement of obstacles outweigh design of framework. The effects of four design parameters are investigated on two important characteristics of a mixer namely mixing efficiency and pressure drop. A weighted profit function is defined to combine these two characteristics. The computational fluid dynamics (CFD) is used to simulate the fluid flow and mixing in three-dimensional models. For this numerical study, the commercial CFD package, COMSOL, is used. The analyses of the numerical results are then shown in signal to noise (S/N) ratio plots indicating which combination of parameters leads to a maximum profit. It is found that a micromixer with the optimized geometry compared to its initial design increases the mixing index by 15% on average in the Reynolds numbers ranging from 1 to 10.
Keywords: Micromixer, Taguchi, Mixing Index, Pressure Drop, Optimization,

1. INTRODUCTION

Mixing is a crucial part of many microfluidic systems like lab on a disk or lab on a chip. Micro total analysis systems (µTAS) are another excellent example that requires integrated mixing units with ability of mixing small sample volumes in a short time [1]. Due to the small characteristic dimension of the channel and low fluid velocities, the flow regime is laminar and the Reynolds number (Re) is usually less than 100. So the inertia effect plays less important role compared to the viscous in small hydraulic diameter channels. Additionally, the scaling effects including surface roughness, entrance effect and slippage phenomena have remarkable effect on the transport of the mass, momentum and heat in the micro scale [2].

Micromixers can be divided into the two different types including active and passive. The active types basically depend on external provocation or energy to reinforce the mixing of fluid samples. Pressure disturbance, magnetic energy, temperature, and electrical energy are all kind of these provocations. Despite the high mixing efficiency and utilization in complex structures, these micromixers cannot easily be integrated with total micro-analysis systems. However, passive micromixers by using and exploiting geometry, produce complex flow leading to effective mixing. They can be fabricated in both planar and three-dimensional configuration [3]. A quick glance on review papers shows that passive micromixers are basically rely on following mechanism: flow separation, chaotic advection, split-recombine flow, and hydrodynamic focusing [1].

Various kinds of micromixers have been reported to increase mixing efficiency and reduce the mixing time, the microchannel length and pressure drop. The mixing efficiency could be increased by adding obstacles in the microchannels; nonetheless the pressure drop and consequently power consumption rises. Therefore, pressure drop should be considered in designing micromixers with mixing efficiency [4]. S Bhagat et al [5] investigated micromixers with gaps and baffles and studied about different chambers and obstacles to obtain an optimum design. Although all these works are effectual and useful for designing desirable micromixers, local optimization and

optimum length, width, and also height of gaps and baffles didn't be considered. It means considering just arrangement of the baffles, isn't enough to get desirable design. As a result, considering local optimization, as final stage, to design favorable micromixer with high mixing efficiency and low pressure drop is unavoidable.

In this study, local optimization based on Taguchi method on the design of the micromixer to enhance optimum efficiency, have carried out. Because of indirect relationship of mixing efficiency and pressure drop, weighted profit function is introduced to solve the problem. After that, analysis of Taguchi method on S/N ratio diagram is taken to get optimum geometrical parameters.

2. MICROMIXER DESIGN

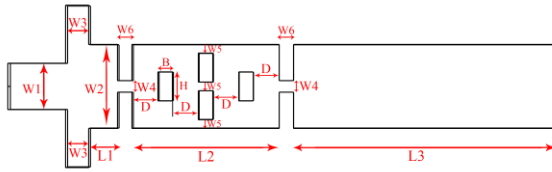Figure 1 shows the micromixer design containing four obstacles as well as two gaps.

Figure 1 Geometric parameters of the micromixer

As can be seen, the first fluid, flows into the micromixer by the main, left inlet and the second fluid, enters into the micromixer by two upper and bottom inlets. Then, they immediately contact each other. At that moment in time, there is a small molecular diffusion between them. After that the two fluids are squeezes into the first gap. Due to the baffle's location, the streams are separated and recombined and at last, the fluids flow into the straight enough channel. These separation and combination help mixing for better efficiency and baffles location is due to this point.

The main parameters of micromixer for validation are listed below:

Table 1 Geometric values of the micromixer (µm)

Parameters	W1	W2	W3	W4	W5	W6	L1	L2	L3	H	D	B
Values	160	290	80	40	30	50	100	510	910	100	90	50

In this study, Taguchi design of experiment is used to optimize the mixing efficiency. The parameters that will be optimized are shown in Figure 2. Improving the way that fluids split and recombine is a way for increasing the mixing efficiency [6], because of that just four parameters are used in optimization.
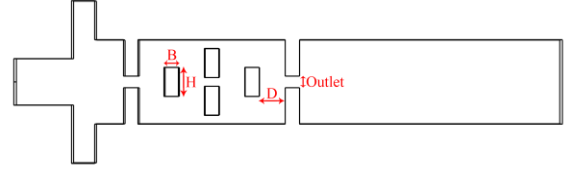

Figure 2 Selected parameters for optimization

The selected geometries are all plotted in XY plane, so for 3D simulation and experimental works, the height of micromixer was regarded as 100 µm in Z direction. The total length of the micromixer is considered as 1900 µm.

3. METHODS AND SIMULATIONS

3.1 Numerical Simulation

Simulations were carried out using COMSOL multiphasics 5.2, a commercial CFD package based on finite element volume approximation. The governing equations include continuity equation, three-dimensional Navier-Stokes equation and species convective-diffusion equation [7].

$$\nabla . V = 0 \qquad (1)$$

$$\rho \frac{\partial V}{\partial t} + \rho V . \nabla V = -\nabla p + \mu \nabla^2 V \qquad (2)$$

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

Where V is the velocity vector, ρ is the density, p is the pressure, μ is the viscosity, C is the species concentration and D is the diffusion of the species. In this study, one stream is pure deionized (DI) water, while the other one is labeled with black ink (diluted to 0.025 g/ml in DI water). Steady-state, Newtonian and incompressible conditions are assumed during solving the governing equations and also gravitational force is neglected. The density and viscosity of the water are 998.2 kg/m^3 and 0.00097 kg/(m.s), respectively and the diffusivity between water and ink is 3.23×10^{-10} m^2/s. the three inlets are set as velocity inlets and the outlet is a pressure outlet where zero static pressure was specified at the outlet. The adiabatic and no slip boundary conditions were applied at the walls. The molar concentration of two fluid species was set as 0 and 1 while uniform mixing

was achieved as molar intensity of two species reached the value of 0.5. Reynolds number (*Re*) is defined as:

$$Re = \frac{\rho U D_h}{\mu} \tag{4}$$

Where U is the average velocity and D_h is the hydraulic diameters of the mixing channel. The Reynolds number of 0.1 to 60 are calculated based on the physical parameters of the main stream (water) and the characteristic length of bottom inlet. The temperature was set to 20°C in the simulation. Grid study was performed to examine the sensitivity of the simulation to the number of the mesh elements. The associated error between two kinds of mesh is:

$$e\% = \left| \frac{G_2 - G_1}{G_1} \right| \times 100 \tag{5}$$

Where G_2 and G_1 are to correspond grids. The cells are meshed with a hexahedral grid and the meshes are assorted from 92210 to 1672911 in the grid independence test that shown in the Table 2.

Table 2 Mixing Index with different grids (Re=10)

Grids	92210	339770	1672911
Mixing Index	0.6213	0.6052	0.6017
e%	2.18	0.58	0

As can be seen, the optimum grid number with beneficial computer cost is 339770 where no significant changes in the results due to grid size are observed.

In order to show the mixing index as a standard evaluation for mixing performance, expression below could be valuable:

$$M = 1 - \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left(\frac{k_i - \bar{k}}{\bar{k}} \right)^2} \tag{6}$$

Where M is mixing efficiency, n is the total number of sampling points, k_i is the mole fraction distribution over the whole outlet cross section and the last term that is $\bar{k}$, is the average mole fraction. M varies from 0 to 1 where $M=0$ corresponds to no mixing (0% mixing) and $M=1$ is a complete mixing (100% mixing).

3.2 Description of the Taguchi method

Taguchi is the developer of the Taguchi method and suggested that engineering optimization of a process could be accomplished in a three stage approach, i.e. system design, parameter design, and tolerance design. System design is which engineers use scientific and sophisticated knowledge to design and produce a basic model design. All material selections, components, equipment, etc. are involved in this stage. Inasmuch as this stage only deal with system design, optimization of cost and quality is far from it. Therefore, parameter design come to end this problem. The objective of second stage as parameter design is to obtain the optimum value for parameters in the case of quality and cost. Eventually, the last stage (tolerance design) is used to determine and analyze tolerance around the optimal sitting recommended by parameter design [8].

Classical experimental design methods are complex and not easy to be used. Additionally, when the number of parameters are increased, a large number of experiments have to be done. These problems solved by Taguchi method. Taguchi method uses orthogonal arrays to study the entire parameter space with a small number of experiments. The results are transformed into a signal-to-noise (S/N) ratio and analyses are carried out. The number of experiments require thorough analysis in the case of four three-level parameters can be reduced from 81 to 9. The way that 9 is gained is up to Taguchi method. As it's obvious in Figure 2, the base and height of obstacles are major parameters to do optimization. Because our chaotic advection based on the obstacles. The width of outlet could make acceleration effects and vortices so another important parameter is the width of outlet. The way how to two last streams recombine together and the way that they continue their pass through outlet depend on the space between the last obstacle and outlet. So another important parameter to evaluate is D parameter that have shown before. Table 3 shows the values of four parameters in three level.

Table 3 Variety of control parameters used in Taguchi

Level	H (μm)	B (μm)	Outlet (μm)	D (μm)
1	80	30	20	70
2	100	50	40	90
3	110	70	60	110

The square of standard deviation of concentration (σ^2) and signal to noise ratio (η, S/N) were calculated by below equations:

$$\sigma^2 = \frac{1}{n}\sum_{i=1}^{n}(c_i - \bar{c})^2 \qquad (7)$$

$$\eta = \frac{S}{N} = -10\log\sigma^2 \qquad (8)$$

There are three categories of quality in analysis of the S/N ratio, i.e. the lower-the-better, the-higher-the-better, and the-nominal-the-better. Here, we set our analysis to the-higher-the-better, so the higher signal to noise ratio means better mixing efficiency or fluid mixing.

3.3 Weighted Profit Function

Major output and the main function of all micromixers is high mixing index. Another important factor that have main role in the cost and power consumption is pressure drop. In all cases, pressure drop and mixing efficiency have direct relationship; i.e. for larger mixing efficiency the pressure drop is bigger. To solve that problem, some ways are proposed such as Multi Objective Genetic Algorithm (MOGA). In this study, we use Weighted Profit Function (WPF). In this method, all numbers range from 0 to 1. Then a weighted factor multiply to each function and our Weighted Profit Function would be built.

$$\text{WPF} = \alpha \times MI + \beta \times PD \qquad (9)$$

Where WPF is the Weighted Profit Function, MI is the Mixing Index, PD is the Pressure Drop, and α and β are the weighted factors. In this case, due to reverse effect of Pressure Drop, we define PD as:

$$PD=1-(PD)^{'} \qquad (10)$$

Equation above, give same direction to Mixing Index and Pressure Drop where the value corresponds to 1 is benefit for us as higher Mixing Index and lower Pressure Drop. The WPF varies from 0 to 100 (in %) where 0 means the lowest Mixing Index and the Highest Pressure Drop and 100 means the best Mixing Index and the lowest Pressure Drop.

α and β are arbitrary factors. Because PD can be solved by micropump but destructive effects of MI is irrecoverable, in all cases, usually MI outweigh to the PD. So for this study we choose 0.8 for α and 0.2 for β. It's obvious that summation of all weighted factors have to be 1.

4. RESULTS AND DISCUSSIONS

4.1 Validation of the results

This section purpose is to check the validity of the presented study with experimental model of ref [4]. Geometrical properties were exactly same as the experimental study. For this purpose, geometry of Figure 1 with parameters of Table 1 with three inlets and one outlet were considered. According to the initial and boundary conditions, comparison of the simulation and experimental model is shown in Figure 3.

Present Study (Re=10)
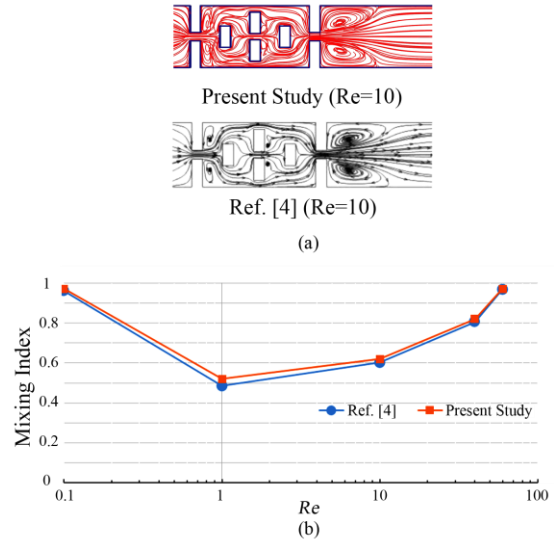
Ref. [4] (Re=10)

(a)

(b)

Figure 3 Comparison of numerical results of the present work with ref. [4]

It can be clearly seen that the numerical simulation remain consistent with experimental results of ref. [4]. As demonstrated in Figure 3-a, stream lines for *Re=10* is shown for presented study and experimental one. The separation vortices that are generated, improve mixing. Also comparison of Mixing Index of presented study and experimental one is demonstrated in Figure 3-b for five Reynolds numbers. Thus, the numerical model is able to precisely predict the experimental setup and the validation have been done.

4.2 Effect of geometrical parameters on the Mixing Index and Pressure Drop

Effect of geometrical parameters on the mixing index and pressure drop is investigated by Taguchi method for optimization in the selected parameter ranges. The results of our simulation with levels that proposed by Taguchi is shown in Table 4.

Table 4 Results of simulation with the levels that proposed by Taguchi method for *Re=10*

Simulations	Height (H)	Width (B)	Outlet	D	Profit Function	Mixing Index
1	1	1	1	1	81.530	0.727
2	1	2	2	2	72.070	0.631
3	1	3	3	3	77.134	0.599
4	2	1	2	3	71.100	0.618
5	2	2	3	1	75.455	0.585
6	2	3	1	2	82.338	0.735
7	3	1	3	2	74.921	0.579
8	3	2	1	3	81.638	0.722
9	3	3	2	1	70.530	0.616
Best	1	3	1	3	83.449	0.745

Figure 4 demonstrated the signal to noise ratio for *Re=10*. In the Taguchi method, the term 'signal' represent the desirable value for output characteristic and the term 'noise' act for the undesirable value. Taguchi uses the S/N ratio to measure the quality characteristic of each geometrical parameter.
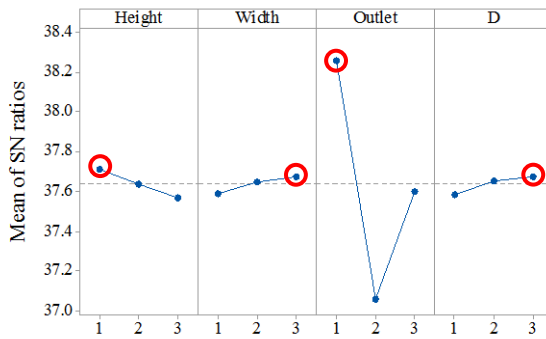
Signal-to-noise: Larger is better

Figure 4 S/N ratio criterion for controllable parameters

As can be seen, sensitivity of four parameters ranks like this:

Outlet > Height > Width ≃ D

The width of outlet is the most sensitive and important factor for weighted profit function for the better mixing index and lower pressure drop. The desired level of outlet as it is illustrated by red circle, is the first one whose values is 20 (Table 1). When the outlet is small enough, it can makes vortices in straight channel and helps to improve mixing with extra power. Area variation through the channel also accelerates the fluids. Therefore, mixing index would be enhanced by extra vortices. Increasing the width of outlet has negative effect on its performance because of pressure drop and it's one the major advantages of the weighted profit function to determine each parameter, even with reverse effect on another parameter. Another important parameter to increase mixing index is the height of each obstacles. Increasing height of each obstacle, because of its edge, make extra chaotic advection that helps to improve mixing index. After all, width of each obstacle and distance of the last obstacle to the outlet are the least sensitive parameters in comparison to others. The best design of micromixer with given ranges is demonstrated in Figure 4, That is the micromixer with four obstacles with height of 80 and width of 70, the width of outlet 20, and distance between the last obstacle and outlet 110. All dimensions are in µm. The results of this is shown in Table 4. As it's clear, the profit function goes to 83.449 and MI is 0.745 in *Re=10*. In comparison to main micromixer with mixing index of 0.60, it's exceedingly favorable. Our optimization have done not only with just mixing index, but also with pressure drop and the results of mixing index just have shown for illustration of our function. It's not a hard work to show the pressure drop just like mixing index.

The main characteristic of the optimized micromixer fluid flow with *Re=10* is shown in Figure 5. In Figure 5-a, controlled stream line is shown with chaotic advection and enough molecular diffusion. The width of inlet is bigger than the outlet so the speed of outlet, is more that inlet and it's accelerate the fluids. Due to acceleration and enough speed, big vorticity regions occur at the straight channel and help mixing. Figure 5-b shows velocity distribution though out the microchannel. In the region of baffle and gaps, total distribution changes rapidly, especially when the stream collide with the baffles or pass near the edges. This also enhance mixing efficiency. As it's clear, optimizing the geometric parameters, distribution and velocity changes across the channel due to the baffles and gaps and at last in the straight channel, fully developed stream occurs. In Figure-c, pressure

contour shows. It was mentioned that zero static pressure was specified at the outlet and shown in the Figure 5. The major problem happens at the end of the outlet and our optimization is based on that to recover pressure drop by correcting the geometrical parameters.
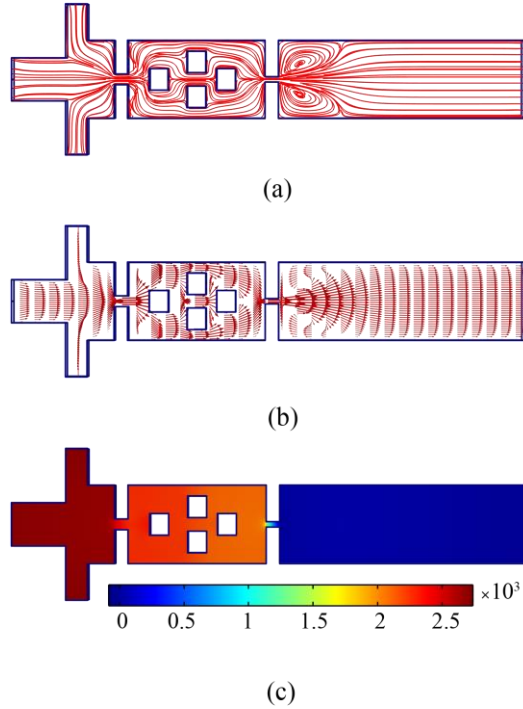

(a)

(b)

(c)

Figure 5 The characteristics of optimized micromixer fluid flow (Re=10): a) stream lines b) velocity distribution c) pressure contour

This optimized configuration is also tested for other Reynolds numbers and the results show in **Error! Reference source not found.**
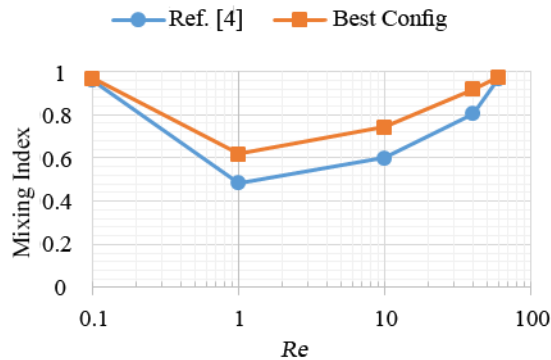

Figure 6 Comparison of mixing index between optimized and initial design

Due to inherent function of microfluidics, their Reynolds number varies from 0.1 to 10 so optimization in that range is crucial. All corresponding analysis like DNA or protein analysis occurs in Reynolds about 1. Thus the optimum geometry would be proposed to them to use it in near future.

5. CONCLUSION

In this paper, the effect of geometrical parameters on the mixing index and pressure drop was studied. A weighted profit function was introduced to combine the effects of these two functions which have reverse effect on each other. Local optimization of geometry with four parameter in three levels have done by Taguchi methods. Analyzing S/N ratio shows that the current micromixer with obstacles with height of 80 μm and width 70 μm, outlet of 20 μm, and distance between the last obstacle and outlet 110 μm are the best configuration. Increasing 15% mixing index is achieved by optimum configuration. The results also show that the lowest pressure drop is happened on this configuration.

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