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Simulation and Fabrication of Microfluidic Chips Using Glass

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Authors

Mirchi, Arman¹
Kazemeini, Mohammad¹
Hosseinpour, Vahid¹

¹ Department of Chemical and Petroleum Engineering, Sharif University of Technology, Tehran, Iran
arman.mirchi98@sharif.edu
kazemini@sharif.edu
hosseinpour.vahid@gmail.com

* Correspondence

Address: Department of Chemical and Petroleum Engineering, Sharif University of Technology, Tehran, Iran.
Phone: -
Fax: -
kazemini@sharif.edu

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ABSTRACT

Microfluidics has a wide range of applications in various fields, especially experimental sciences, chemical industries, microelectronics and pharmaceuticals. Given flow chemistry's advantages over traditional batch approach and wide applications, continuous-flow approaches using microreactors and other microfluidic devices have gained significant attention in recent years from academia and industries. This research studied the design and simulation of the proposed micromixers and microreactors using computational fluid dynamics (CFD) and COMSOL Multiphysics software. During the simulations, transport of dilute species and laminar flow physics were applied, with water used as the operational fluid, entering the microchannels with two different concentrations. Additionally, the mixing index was used as the objective function to quantitatively compare the performance of the microchips, which were calculated at four residence time levels: 20, 30, 40, and 100 minutes for each design. Based on the simulation results, microreactor 1 demonstrated a significantly better mixing index compared to microreactor 2, with its mixing index reaching 92.6% and 99.8% at residence times of 40 and 100 minutes, respectively. Following, microchips that indicated better performance were selected for the fabrication process using glass and CO₂ laser engraving technique. After that, a leakage test was performed to ensure the appropriate fabrication method. Finally, an experimental mixing test was performed on the fabricated micromixer to show the good agreement between experimental and simulation outcomes.

Keywords: Microfluidic-chips, microreactor design, CFD, Flow chemistry.

1 Introduction

Microfluidics is a relatively new field that represents the technology of systems involving channels ranging from a few tens to several hundred micrometers in size. This field has wide applications in chemistry, biology, microelectronics, and pharmaceuticals. Microfluidic devices are useful tools for performing operations such as reactions, separations, or detecting various compounds. Microfluidic chips can be produced using a wide range of materials and different manufacturing methods depending on their application [1, 2]. The revenue from microfluidic devices in 2014 was \$1.8 billion, which increased to approximately \$7.7 billion by 2020 [3]. Micromixers are important components of microfluidic systems that mix two or more fluid species together. The mixing mechanism in micromixers is mainly divided into molecular diffusion and chaotic advection [4]. Micromixers are generally divided into active and passive micromixers. Active micromixers use an external energy source for mixing. These micromixers require only a short time to complete mixing; however, their disadvantages include complex structure and costly fabrication processes.[5-7] Passive micromixers, also known as static micromixers, do not rely on external energy sources and only use the pumping energy of the fluid. They offer several advantages over active micromixers, such as ease of fabrication, relatively low cost, and easy integration with microfluidic systems. The performance of passive micromixers largely depends on the geometry of the microchannels.[8] Microreactors are small devices for performing chemical reactions continuously, where the reactants pass through channels with at least one dimension smaller than 1 millimeter [9]. Microreactors can be classified into three main categories: chip-based microreactors, coil microreactors, and packed-bed microreactors.[10] Here, some of the most important advantages of using microreactors compared to batch reactors are mentioned. First of all, the surface-to-volume ratio in microreactors increases significantly. This increase in the surface-to-volume ratio enhances mass and heat transfer in microreactors. [11] Microreactor systems can dramatically reduce mixing time, enabling nearly complete mixing in a very short period (less than 1 minute), whereas achieving rapid mixing in a traditional batch reactor remains challenging.[12] Also, using microreactors leads to increased automation of laboratory and process systems, facilitating feedback control, optimization, automated screening, and data collection. The

integration of logical and feedback control in microreactors enables the performance of various experiments in a fully automated manner. Therefore, continuous processing has the potential to carry out operations entirely automatically. [13, 14] Additionally, the reduced volume in microreactors leads to shorter residence times, and due to improved temperature control and shorter residence times, many potential hazards can be minimized or eliminated. As a result, the use of microreactors enhances inherent safety.[15] Some of the other advantages of microreactor technology include improved process control, the ease of integrating flow systems with other units, the ability for rapid reaction condition screening, laminar flow, and reduced energy consumption.[13, 16]

Micromixers can be made from various materials, including glass, ceramics, silicon, polymers, and stainless steel. The choice of material depends on various criteria, such as operational conditions, physical properties, cost, mass production capability, and ease of fabrication. However, the most commonly used material is glass, which is chemically inert, transparent, and cost-effective[11, 17]. The methods for fabricating microfluidic devices are divided into different types of chemicals, mechanical, laser-based, and other processes. The most common techniques for fabricating microreactors include micromachining, lithography, electroplating, molding (such as lithography, galvanic forming, and embossing), and etching. Depending on the desired complexity, other methods, such as injection molding, soft lithography, photolithography, hot embossing, and electroforming, are also used for fabricating microreactors. 3D printing is also a relatively new and effective approach, providing an easy way to create microchannels.[1, 18]

In the present study, to develop microchips for numerous industrial applications, the design and simulation of novel micromixers and microreactors were initially conducted to compare their performance. Subsequently, their fabrication process was examined using the cost-effective method of CO₂ laser engraving with glass material.

2 Design of proposed chips

Figures 1 and 2 show the geometry of the proposed micromixers and microreactors. For performance comparison under similar conditions, the length and width of the microchannels for the micromixers are 16 millimeters and 800 micrometers, respectively, and for the microreactors, they are 800 millimeters and 800 micrometers, respectively.



Figure 1- Geometries of proposed micromixers

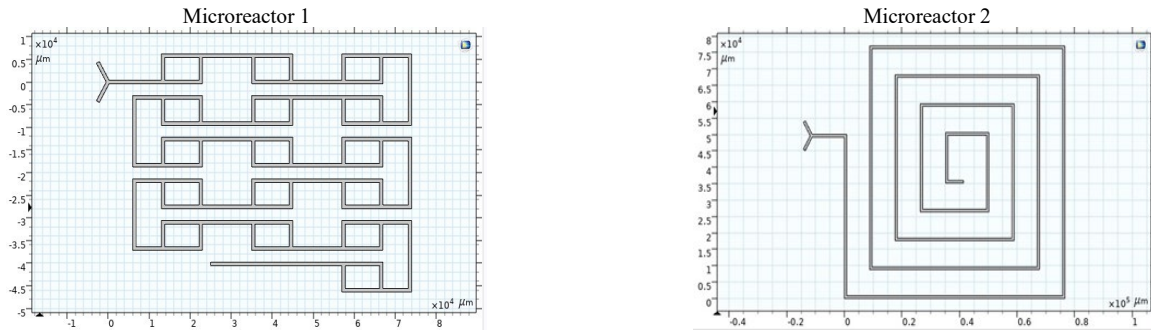


Figure 2- Geometries of proposed microreactors

3 Simulation using COMSOL software

In this study, since momentum transfer and mass transfer phenomena are involved in the simulation, the physics of laminar flow and transport of diluted species are used to simulate the microchips in COMSOL software. In this study, the fluid used has properties similar to water with a diffusion coefficient $D=10^{-10} \text{m}^2 \cdot \text{sec}^{-1}$. The micromixer's upper inlet and lower inlet have a molar concentration of $1 \text{ mol} \cdot \text{m}^{-3}$ and $0 \text{ mol} \cdot \text{m}^{-3}$, respectively. The boundary conditions are uniform velocity at the inlets and zero static pressure at the outlet. A no-slip boundary condition is also assumed for the walls. The flow of both fluids is assumed to be steady, Newtonian, and incompressible. The mixing index (MI) is used to compare the performance of different designs. The mixing index (MI) and residence time (τ) are defined as follows:

$$MI = 1 - \sqrt{\frac{1}{n} \sum_{i=1}^n \left(\frac{C_i - \bar{C}}{\bar{C}} \right)^2} \quad \text{Eq 1}$$

$$\tau = \frac{V}{\vartheta} \quad \text{Eq 2}$$

A mixing index of zero means no mixing, while a mixing index of one indicates complete mixing. Meshing, or grid generation, is also one of the most critical aspects of solving numerical problems. Figure 3 shows the trend for determining the optimal mesh numbers.

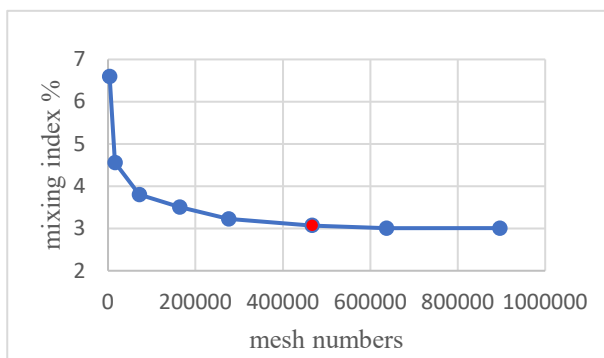


Figure 3- Mesh independency diagram for micromixer 2 at the residence time of 40 minutes.

4 Simulation results

The mixing indexes obtained for micromixers and microreactors at different residence times are shown in Table 1.

Table 1- Mixing indexes (%) of micromixers and microreactors at different residence times.

	Micromixer 1	Micromixer 2	Microreactor 1	Microreactor 2
20 (min)	1.39	4.2	72.99	49.57
30 (min)	1.69	5.16	85.93	64.11
40 (min)	1.94	6.01	92.67	74.38
100 (min)	3.03	9.78	99.85	96.48

According to Table 1, micromixer 2 and microreactor 1 demonstrate better performance in terms of the mixing index. The mixing index for the micromixers at different residence times is low due to the microchannels' length and the short contact time. Additionally, the mixing index is enhanced with increasing residence times in all designs. The concentration profiles of the selected designs at a residence time of 40 minutes are shown in Figures 4 and 5.

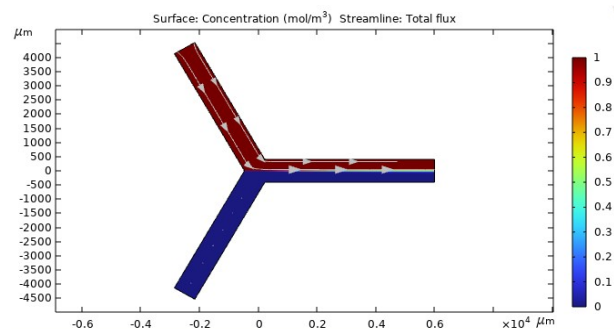


Figure 4- Concentration profile of selected micromixer at a residence time of 40 minutes.

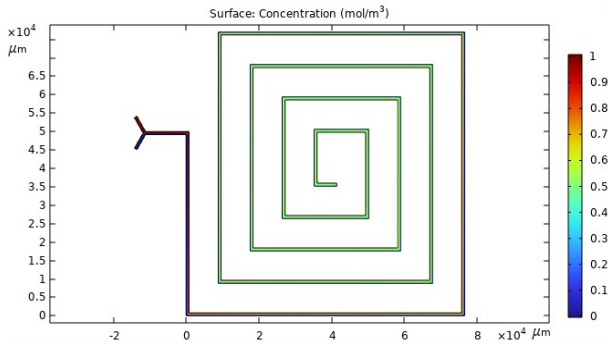


Figure 5- Concentration profile of the selected microreactor at a residence time of 40 minutes.

5 Fabrication process and experimental section

The optimized micromixer and microreactor were fabricated using glass and CO₂ laser engraving technique, mainly due to ease of manufacturing and cost-effectiveness. For this purpose, two glass pieces with a thickness of 4 mm and identical dimensions were first cut. Then, microchannels were engraved on one of the glass pieces using a laser, while inlet and outlet holes for the fluids were drilled on the other glass piece. Finally, the two pieces were placed on each other and bonded through fusion bonding in a furnace. After the micromixer and microreactor were fabricated, a leakage test was performed to ensure appropriate fabrication and bonding processes (Figure 6). Additionally, for the fabricated micromixer, an experimental mixing test was conducted using the injection of dye substances, blue and red, to evaluate the degree of mixing achieved and compare it with the simulated results (Figure 7).

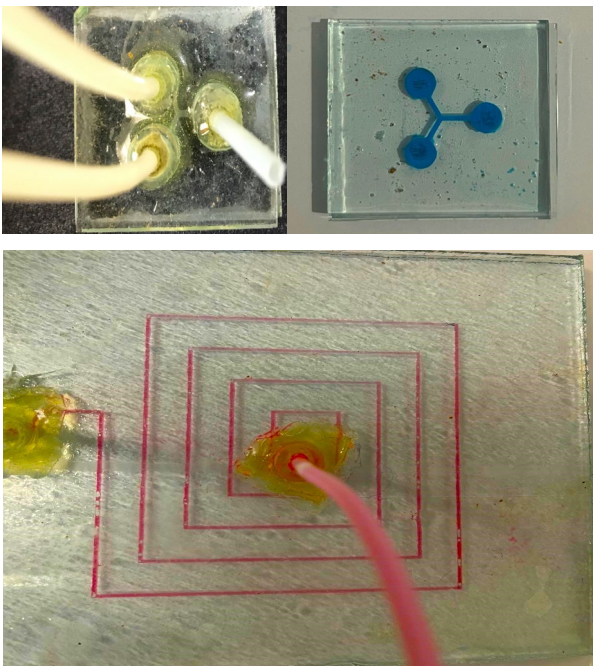


Figure 6- Fabrication of glass microfluidic chips and performing leakage test.

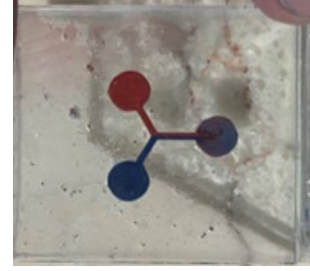


Figure 7- Experimental mixing test of the fabricated micromixer.

6 Conclusion

Given the numerous applications of microfluidics in various fields, this paper focused on the simulation and fabrication of novel microfluidic chips. To achieve this, the proposed micromixers and microreactors were first simulated using COMSOL Multiphysics software. The mixing index was used as the objective function during the simulation to evaluate the microchip's performance, quantitatively. Based on the results, microreactor 1 achieved a significantly higher mixing index at different residence times compared to microreactor 2. Using microreactor 1, the mixing index reached 92.6% and 99.8% at residence times of 40 and 100 minutes, respectively. Following, the optimized micromixer and microreactor were fabricated using glass and laser engraving techniques. A leakage test was conducted to ensure the appropriate fabrication of the chips, and the absence of any leakage after the continuous injection of dye confirmed the effectiveness of the fabrication process. Finally, an experimental mixing test was performed on the fabricated micromixer using the injection of dye substances, and the experimental and numerical simulation results showed good agreement with each other.

Considering the significance of microfluidic systems, future work could focus on simulating and designing a broader range of micromixers and microreactors to achieve better performance. For instance, using active micromixers could effectively enhance the mixing index compared to the passive micromixers studied here. Additionally, the microchip fabrication process could be pursued using other methods, such as 3D printing and photolithography, to compare each approach's performance, advantages, and limitations.

Disclosure of Potential Conflicts of Interest

The Authors declare that there is no conflict of interest

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