CFD Modeling of Mixing Enhancement in a Pitted Micromixer by High Frequency Ultrasound Waves

Faezeh Mohammadi, Ebrahim Ebrahimi, Neda Azimi

***Abstract*—**Use of ultrasound waves is one of the techniques for increasing the mixing and mass transfer in the microdevices. Ultrasound propagation into liquid medium leads to stimulation of the fluid, creates turbulence and so increases the mixing performance. In this study, CFD modeling of two-phase flow in a pitted micromixer equipped with a piezoelectric with frequency of 1.7 MHz has been studied. CFD modeling of micromixer at different velocity of fluid flow in the absence of ultrasound waves and with ultrasound application has been performed. The hydrodynamic of fluid flow and mixing efficiency for using ultrasound has been compared with the layout of no ultrasound application. The result of CFD modeling shows well agreements with the experimental results. The results showed that the flow pattern inside the micromixer in the absence of ultrasound waves is parallel, while when ultrasound has been applied, it is not parallel. In fact, propagation of ultrasound energy into the fluid flow in the studied micromixer changed the hydrodynamic and the forms of the flow pattern and caused to mixing enhancement. In general, from the CFD modeling results, it can be concluded that the applying ultrasound energy into the liquid medium causes an increase in the turbulences and mixing and consequently, improves the mass transfer rate within the micromixer.

Keywords—CFD modeling, ultrasound, mixing, mass transfer.

I. Introduction

RECENTLY, micro-structured devices were proposed to achieve efficient mixing with promised benefits of high surface to volume, reduction of effective diffusion path and an increase in the interfacial area of fluid [1]-[3]. Micromixers depending on the method to disturb the fluids are classified into two categories, namely, passive and active mixers [4]. Passive mixers have simple structures and utilize the energy of fluid flow for mixing phenomena and they are not employing any external energy [5]. Active micromixers use a source to generate the external driving force for fluid perturbation and intensify the mixing process. Varieties of active mixing schemes have been investigated in micro-devices and depicted many benefits for mixing enhancement. Several methods for fluid actuation have been illustrated, including applying magnetic field, mechanical stirrers and valves, ultrasonic vibration, oscillatory flow generated by thermal bubble actuation, periodic pressure perturbation in cross-channels [6]-[9].

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The widespread use of ultrasonic waves as a new technology has attracted many researchers [10]. The transfer of ultrasonic energy into a liquid leads to micro-scale physical phenomena resulting from the production of acoustic streams and the cavitation phenomenon [11]. Acoustic cavitation involves the continuous formation, intense growth, and the collapse of a large number of small bubbles in the liquid, results in the formation of alternating cycles of compression and expansion due to wave propagations [12]. Acoustic cavitation and bubble explosion lead to an increase in the mass and heat transfer rate of the fluid. These phenomena are important for many purposes, such as fluid mixing on a molecular scale. At low frequencies, the cavitation phenomenon is very important and the explosion of bubbles caused by this phenomenon results in better mixing. The high frequency ultrasound waves have the ability to create micro streaming and micro-jets in the fluid as well as circulating flows. High frequency ultrasound waves also have lower power consumption, which is important in terms of energy storage. Unlike, many authors have investigated the application of ultrasound waves to enhance the mixing efficiency in the different micro or large-scale reactors; there are still major problems in this field. One reason is the intricacy of comprehension the ultrasound propagation in the liquids. It can be solved by perform the mathematical modeling to understand the distribution of ultrasound waves through the involved system [13]-[15]. The purpose of this study is to analyze the process of mixing intensification and improve the transfer of liquid-liquid liquid in a pitted micromixer by employing ultrasonic waves using CFD modeling. CFD data will be compared with the experimental data. Modeling have been done in two steps involves the presence of ultrasonic waves and the absence of ultrasonic waves.

II. Experimental Work

A. Martial and Methods

In order to quantify mixing of two liquid phases, the organic phase (n-butanol, 99.8% from Mojallali chemical laboratories, Iran) and an aqueous phase (deionized water) were purchased. Table I shows the properties of two phases that used in modeling.

B. Experimental Setup and Procedure

The experiments were carried out in a pitted micromixer that was made of Plexiglass plates. In this research, CFD modeling of mixing of two immiscible phases have been performed in a pitted micromixer, in which the junction of two inlet flows is Y-shaped. Inlet and outlet channels in the micromixer have square cross section with 0.4 mm in depth and 0.8 mm in width. The bottom wall of the pit of micromixer is a ceramic piezoelectric transducer with a frequency of 1.7 MHz, which acts as an ultrasonic emitter. Fig. 1 shows the geometric shape of the pitted micromixer. The length of inlet and outlet channels was 30 mm and diameter of cylindrical pit was 50 mm and length of 0.4 mm.

TABLE I
THE PHYSICAL PROPERTIES OF ORGANIC AND AQUEOUS PHASES USED IN THIS WORK

Materials	Density (kg/m^3)	Viscosity (Pa.s)	Interfacial tension between two phases (N/m)
Deionized water	981.7	0.00105	0.00225
n-butanol	837	0.00334	

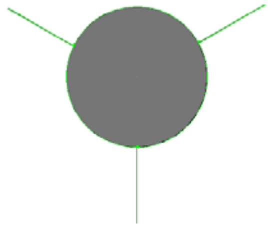


Fig. 1 The schematic photograph of the pitted

The mixture of aqueous and organic phases was remotely excited by subjecting them to ultrasound waves induced by 1.7 MHz piezoelectric transducer.

C. CFD Modeling Strategy

In this work, in order to model surface vibration of piezoelectric transducer, dynamic mesh model was used. In order to introduce the time-dependent velocity equation of PZT vibration, a user defined subroutine (UDF) according to (1) [16]:

$$\xi(t) = \omega A_0 \sin(\omega t)\cos(\frac{2\pi X}{\lambda}) \tag{1}$$

where t is time, ω angular frequency X is the coordinate that is perpendicular to PZT surface and A_0 is the maximum transducer face displacement.

III. NUMERICAL SIMULATION

Understanding the complex structure of mixing of two immiscible phases and hydrodynamic due to ultrasound propagation is quite important to analyze the experimental observation. For this purpose, the three dimensional CFD modeling is implemented in commercial software FLUENT 6.3 [17]. The liquid-liquid mixing adopted in this work is based on mixing of n-butanol as organic phase and water (aqueous phase).

A. Description of VOF Approach

The VOF method and the piecewise linear interface calculation (PLIC) scheme were used to simulate the dynamics of two immiscible liquid flows in a pitted micromixer under laminar flow conditions. The fluids were modeled as incompressible and Newtonian. Water assumed as phase 1 and the n-butanol based-ferrofluid was used as secondary phase.

B. Continuity Equation

The continuity equation of a multiphase immiscible flow in FLUENT is solved only for the secondary phase (here, organic phase), which has the following form [17]:

$$\frac{\partial(\alpha_{or}\rho_{or})}{\partial t} + \nabla.(\alpha_{or}\rho_{or}\overrightarrow{v_{or}}) = 0 \tag{2}$$

The volume fraction (α) equation will not be solved for the primary phase; the primary-phase volume fraction (α_{aq}) will be computed based on the following constraint:

$$\alpha_{or} + \alpha_{aq} = 1 \tag{3}$$

C. Momentum Equation

Momentum equations are given by [17]:

$$\frac{\partial(\rho\vec{v})}{\partial t} + \nabla.(\rho\vec{v}\vec{v}) = -\nabla p + \nabla.(\mu\left(\nabla\vec{v} + \nabla.\vec{v}^{T}\right)) + \rho\overline{g} + \overline{F}_{\sigma} \tag{4}$$

The above equation is dependent on the volume fractions of two phases through the properties ρ and μ. ν is the fluid velocity and P is the static pressure. ρ and μ are the volume-fraction-weighted density and viscosity, respectively, which are defined as:

$$\rho = \alpha_{or}\rho_{or} + (1-\alpha_{or})\rho_{aq} \tag{5}$$

$$\mu = \alpha_{or}\mu_{or} + (1-\alpha_{or})\mu_{aq} \tag{6}$$

The flow patterns of two immiscible fluids are depending on the interfacial tension, viscous forces, and inertial forces. However, the effects of gravity on flow pattern become negligible at the micro scale devices. Therefore, modeling of surface tension and wall adhesion effects are important in this studied case. The surface tension force ($\overline{F}_{\sigma}$) used in (4) was calculated as [17]:

$$\overline{F}_{\sigma} = 2\sigma\left[\frac{\rho k\hat{n}}{\left(\rho_{or} + \rho_{aq}\right)}\right] \tag{7}$$

where σ is the coefficient of surface tension is the surface normal, and κ is the local surface curvature, which is calculated as [17]:

$$k = \nabla.\hat{n} \tag{8}$$

where $\hat{n} = n/|n|$ and $n = \nabla.\alpha_{or}$.

The geometric reconstruction scheme (Geo-Reconstruct) based on piecewise linear interpolation (PLIC) was used for the reconstruction of the interface.

D.Geometry, Boundary Conditions and Grid Study

The fluid domain was generated in a finite set of control volumes using GAMBIT 2.3.2 software. The volume of the computational domain was meshed using the structured hexahedral cells. For more accurate predictions, the domain that exposed to ultrasound waves was meshed using structured hexahedral cells with the smaller mesh sizes rather than other domains.

1. Initial and Boundary Conditions

The numerical modeling was performed at constant temperature. The initial gauge pressure was set to 0 Pa. The boundary conditions are described as follows:

Aqueous inlet: velocity inlet boundary condition.

Organic inlet: velocity inlet boundary condition.

Outlet: pressure outlet boundary condition (0 Pa).

Solid walls: wall boundary condition (no slip shear condition) for all other boundaries.

IV. Results and Discussion

In this work, CFD modeling was carried for two layouts including the situation with no ultrasound and for mixing in existence of ultrasound. The results obtained from solutions were plotted graphically and discussed below.

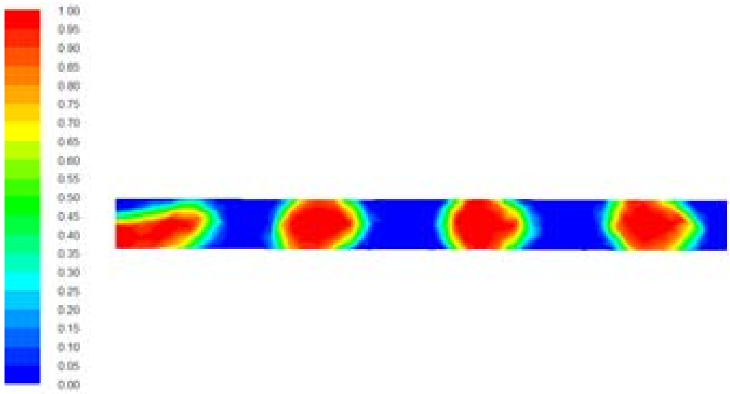
The pattern of two-phases flow inside the micromixer is graphically plotted and further analyzed. In this part of the study, the flow pattern at two flow rates of Q_{or}=Q_{aq}=2 mL/min and Q_{or}=Q_{aq}=6 mL/min have been investigated. Fig. 2 shows the flow behavior of n-butanol and water in the mixing channel of the pitted micromixer in the absence of ultrasonic waves.

The flow rate of organic phase (Q_{or}) was set at 6 mL/min and the flow rate ratio ($R = \frac{Q_{aq}}{Q_{or}}$) was set to 1.

The flow patterns of two-immiscible liquids are depending on the interfacial tension, viscous forces and inertial forces. The effects of gravity on flow pattern become negligible at the micro scale devices. Therefore, in the studied micromixer, interfacial tension and inertial force are dominant stresses, which they can skew the interface of two phases. The importance of interfacial tension and inertial force on the flow pattern in mixing channel can be explained by the Weber (We) number according to:

$$We = \frac{\rho U^2 D}{\sigma} \tag{9}$$

Weber number is the ratio of inertial force to interfacial tension. Fig. 2 (a) shows as the flow rate ratio is high, the slug flow was established.



(a)

(b)

Fig. 2 Effect of Q_{aq} on HD flow regime in mixing channel at vertical slice (y=0), (a) R=1, Q_{or}=2 *m*L/min, (b) R=1, Q_{or}=6 *m*L/min

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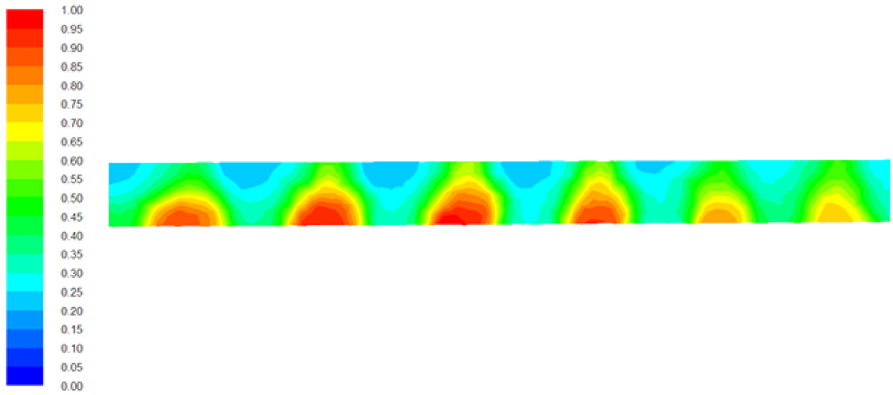
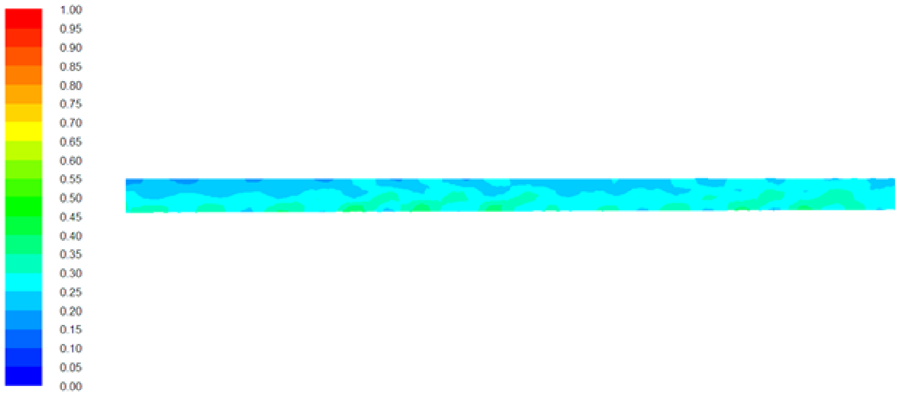
It represents We <1, which demonstrated surface tension is dominating force and being stronger than the viscous and inertial forces. Unlike slug flow, parallel flow (Fig. 2 (b)) offer a limited degree of interface surface area control by changing the values of R. As CFD results show, in the case of low flow rate ratio, parallel flow with wavy interface was established.

Fig. 3 depicted flow pattern in the mixing channel while organic based-ferrofluid was stimulated by ultrasound.



(a)

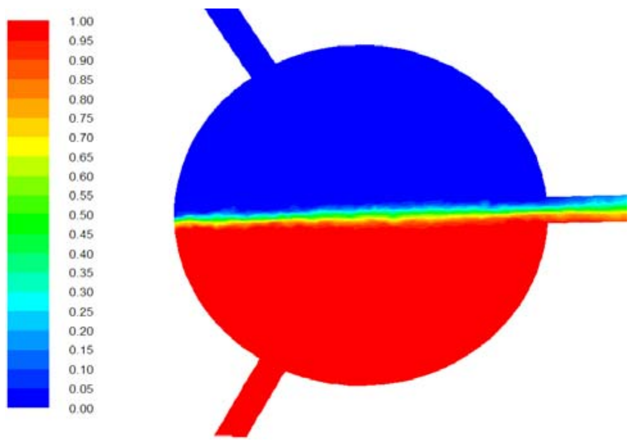


(b)

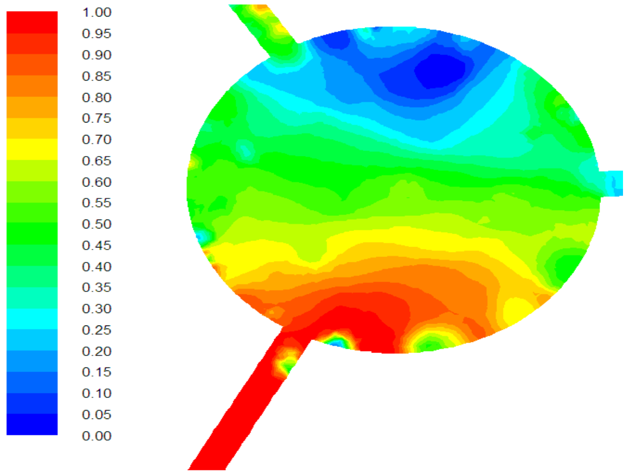
Fig. 3 Effect of Q_{aq} on ultrasound on the flow regime in mixing channel under magnetic field at vertical slice (y=0) (a) R=1, Q_{or}=2 *m*L/min, (b) R=1, Q_{or}=6 *m*L/min

As CFD and experimental results depicted, actuating fluid flow under ultrasound waves in mixing channel results in change in the form of slugs as shows in Fig. 3 (a). It is because fluid flow was affected by both hydrodynamic and ultrasound forces, which it results in convective motion in the direction and perpendicular on flow.

Fig. 4 (a) shows the fluid flow inside the micromixer at a high flow rate for two phases ($Q_{or} = Q_{aq} = 6\frac{mL}{\min}$) in the absence of ultrasonic waves. In this case, the flow pattern of the two phases is parallel, whereas when the ultrasonic waves are applied, Fig. 4 (b), the fluid flow is no parallel and, in fact, the application of ultrasonic waves changes the shape of the flow pattern and better mixing has done. In fact, in this case, the interface of two phases of aqueous and organic is complete and the contact of the two phases has become more intense. The reason for this is that the flow of fluid under ultrasonic force leads to movement in the direction of propagation of waves and perpendicular to the flow. The dynamics of the organic phase in the mixing channel and in the direction of the emission of ultrasonic waves causes a change in the shape of the organic phase transition and causes mixing of the two-phases.

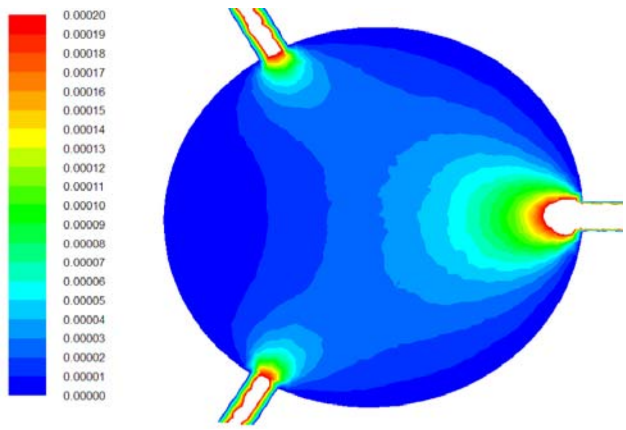


(a)

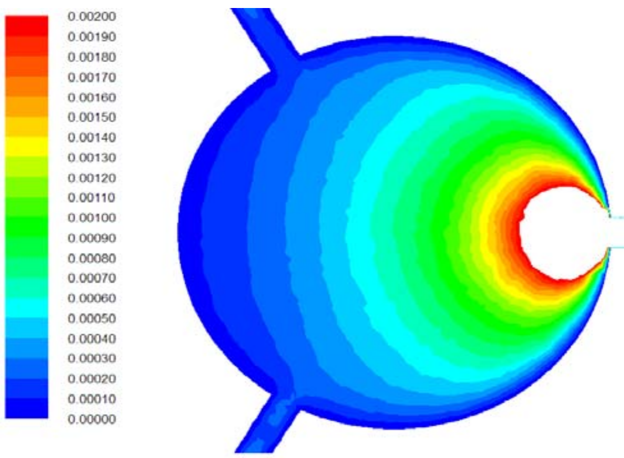


(b)

Fig. 4 CFD results of the flow regime in a horizontal shear (y = 0) in the micromixer in the absence of and presence of ultrasonic waves, R=1, Q_{or}=6 *m*L/min. (a) absence of ultrasound, (b) presence of ultrasound



(a)



(b)

Fig. 5 CFD results of the velocity contour in a horizontal shear (y = 0) in the micromixer in the absence of and presence of ultrasonic waves, R=1, Q_{or}=6 *m*L/min. (a) absence of ultrasound, (b) presence of ultrasound

Fig. 5 (a) shows the flow velocity inside the micromixer in a in the absence and presence of ultrasonic waves. In this case, the flow velocity within the pit is very low, while when ultrasonic waves are applied, the velocity of the fluid increases in this region (Fig. 5 (b)), and in fact, the application of ultrasonic waves causes disturbance in this region and the mixing has improved.

V. Conclusion

In this research, the effect of 1.7 MHz ultrasonic waves on increasing the mixing between two immiscible phases in a pitted micromixer was investigated. In the hydrodynamic model of the micromixer, it can be concluded that in the absence of ultrasonic waves, the mixing is poor. The flow pattern through the micromixer at the low flow rate of two-phases shows that applying ultrasonic waves on the pitted micromixer, the shape of the slugs is changed and mixing enhanced. The reason for this is that the fluid flow is subjected to two hydrodynamic and ultrasonic forces, leading to movement of the movement in the direction and perpendicular to the flow. The dynamic movement of the organic phase in the mixing channel and in the direction of ultrasonic waves causes a change in the shape of the organic phase slug and causes mixing of two-phases. The flow pattern inside the micromixer in a high flow rate for two phases in the absence of ultrasonic waves is parallel, while when the ultrasonic waves are applied, the flows are no parallel and the application of ultrasonic waves change the flow pattern and results better mixing. The applied ultrasonic waves stimulate the flow of fluid and create a secondary flow in a direction perpendicular to the flow. The movement of the fluid toward the propagated ultrasonic waves leads to increase the disturbances, velocity and mixing in the micromixer.

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