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CFD modeling of mixing intensification assisted with ultrasound wave in a T-type microreactor

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ABSTRACT

This paper aims to demonstrate the effect of ultrasound wave on mixing in a T-type microreactor. In order to create vibration in this microreactor, a low frequency (42 kHz) piezoelectric transducer was used. A well-known parallel-competitive reaction (Villermaux–Dushman reaction) was employed to study the mixing in the microreactor and the segregation index values were found for layouts with and without sonication. Results show that the ultrasound waves have a significant favorable influence on product distribution and the segregation index at various total flow rates. In all cases, the segregation index decreased with increase in total flow rate. The results reveal that the segregation index improved up to 10–20% by consuming a low energy (2.45 W Kg^{-1}) by the piezoelectric transducer. Finally, the computational fluid dynamics (CFD) modeling was carried out to explain the observed experimental results.

1. Introduction

Microchannels are new mixing devices which have caused a revolution in the processes involved with mixing [1]. A microreactor or microchannel reactor with dimensions below 1 mm is a device that can cause an efficient mixing [2]. Using reactors in micro size hasmany advantages such as safety and process intensification beside process cost reduction. Microreactor have different applications in various fields like chemical, biological and pharmaceutical industries [1,3,4].

In recent years, the advantages of microchannel and microreactor in various applications have been investigated. As an example, the impact of multi-scale networks on catalyst reaction in wall coated parallel microreactors was studied by Saber et al. [5]. Their results showed that using parallel channels promote the overall reaction selectivity performance by controlling flow uniformity. In another study, Naher et al. [6] investigated the effect of microchannel geometry on fluid flow characteristics and mixing efficiency without reaction and revealed that the mixing efficiency strongly depends on channel geometry. Kockmann et al. [7] presented an investigation on convective mixing for various mixer structures integrated on a silicon chip using Villermaux/Dushmann reaction. They proposed new dimensionless numbers to characterize a mixing device effective.

On the other hand, in many studies the effect of ultrasonic waves on mixing efficiency were investigated [8–14]. The influence of low-frequency (20 kHz) ultrasonic power of on micromixing in a continuous reactor in aqueous and viscous solutions was studied by Monnier et al. [15]. Their results demonstrated that the characteristic micromixing time can be significantly reduced, using ultrasonic waves compared with conventional mixing. Moreover, Liu et al. [16] used ultrasonic waves in a biological activated carbon membrane reactor to remove organic pollutants. They showed that the ultrasonic wave power could enhance the mixing efficiency, which can raise the biological activity for this purpose. Further, sonication process was used in other different fields such as waste activated sludge treatments [17] and aza-Michael reaction in water [18].

In some studies, in order to increase process efficiency, mixers equipped with various vibrators were utilized. Ito and komori [19] used a mechanical vibrator as an active technique in a microchannel to promote liquid mixing and chemical reaction. In their study, the feed streams were oscillated before entering the microchannel, using a small vibrating motor. They showed that fluid mixing efficiency is remarkably improved by vibration. In addition, they found that complete mixing and reaction could be achieved at frequencies more than 90 kHz.

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Nomenclature

A	light absorption
A(t)	The wave amplitude, μm
A_0	vibration amplitude, μm
C_μ	empirical dimensionless coefficient
C_j	concentration of species j, mol/l
Cj,s	surrounding concentration of species j, mol/l
D_h	hydraulic diameter, m
f	friction factor
g(t)	growth function of incorporation law
I	ionic strength, mol/m^3
K_{eq}	equilibrium constant
k_I	kinetic constant
l	cell length, m
L	length, m
M	concentration, mol/l
n	the coordinate normal
P	pressure drop difference, Pa
Q	volume flow rate, m^3/s
e	Reynolds number
rj	total producing rate of the types j in the reaction, mol/m^3 s
T	temperature, K
t	time, s
t_m	characteristic micromixing time, s
u	velocity, m/s
u_s	velocity at a solid surface, m/s
V	volume of fluid in the channel
V_{acid}	volume of acid at t, m^3
$V_{acid,0}$	initial of volume of acid, m3
X_S	segregation index
y(x,t)	movement, m
Y	selectivity of iodide
Y_S	selectivity of iodide at total segregation

Greek letters

ε	energy dissipation rate,W/kg
ω	angular velocity, rad/s
β	slip length, m
μ	dynamic viscosity, Pa s
ρ	liquid density, kg/m^3
λ	wavelength, m^{-3}
ε_{353}	molar extinction, mol/m^3
μ_T	turbulent viscosity, Pa s

In another study carried out by Yang et al. [20], a continuous flow ultrasonic micromixer was introduced. They used a diaphragm, which was etched on the silicon side of a plate, and 60 kHz piezoelectric transducer were installed on the diaphragm. They illustrated the positive impact of ultrasonic waves on mixing.

A combination of ultrasound waves at 28 kHz and a simple capillary microreacter were examined by Aljbouret al. [21]. In their study, the hydrolysis of benzyl chloride in a biphasic system was investigated. The effect of ultrasound vibration on the mixing process enhancement was illustrated. In other research, Zhang et al. [22] used combined capillary microreactor and ultrasound irradiation for an intra molecular direct arylation of various aryl bromides. Their experimental data demonstrated that ultrasound waves can solve the clogging problem, which was created in microreactor by solid-forming reactions.

Furthermore, various investigations were carried out on numerical modeling of mixing and diffusion in microchannels. Gobby et al. [23] using computational fluid dynamics (CFD) to study the effects of aspect ratio on mixing in T-micromixers. Their results indicated that at constant width, the required channel length for efficient mixing is independent from the aspect ratio. However, they showed for constant hydraulic diameter, the mixing length decreases with increase in aspect ratio. In another study, Kumar et al. [24] and Qian and Lawal [25] investigated the hydrodynamics of the Taylor flow in a microchannel using volume of fluid (VOF) model.

In the present work, the influence of ultrasound wave propagation on reaction efficiency in a *T*-shaped microchannel was investigated. For this purpose, the Villermaux–Dushman reactions consisting of a neutralization reaction coupled with the iodide–iodate reaction were used. A 42 KHz peizoelectric transducer, placed below the channel, was utilized. The effect of sonication on micromixing performance at various operational conditions including total flow rate and acid concentration were investigated. The CFD modeling employs to compute the velocity and pressure fields to explain experimental results. For this purpose, an advance CFD methodology is developed to examine the liquid mixing in a *T*-type microchannel by considering the wall characteristic.

2. Experimental work

2.1. Reactions descriptions

There are various methods to demonstrate the micromixing performance [26–29]. The segregation index in a parallel–competing reaction [30] is used as an inexpensive and simple test method to show mixing performance in many research [31–33]. In the present work, a method based on a parallel–competing reactions, called Dushman reactions, was used. This reaction includes three parts as follows [34]:

$$H_2BO_3^- + H^+ \rightarrow H_3BO_3 \qquad \text{(Quasi - instantaneously)} \quad (1)$$

$$5I^- + IO_3^- + 6H^+ \rightarrow 3I_2 + 3H_2O \qquad \text{(Very Fast)} \quad (2)$$

$$I_2 + I^- \Leftrightarrow I_3^- \qquad \text{(Equilibrium reaction)} \quad (3)$$

The proton source for first and second equations was sulfuric acid and the reaction rate equations for Dushman reactions with sulfuric acid at 25 °C were considered as follows [35]:

$$r_1 = k_1[H^+][H_2BO_3^-](\mathrm{k_1 = 1011 l.mol^{-1}s^{-1}}) \quad (4)$$

$$r_2 = k_2[H^+]^2[I^-]^2[IO_3^-] \quad (5)$$

$$\text{If} I \le 0.166M \log_{10}k_2 = 9.28105 - 3.664\sqrt{I}$$

$$\text{If} I \ge 0.166M \log_{10}k_2 = 8.383 - 1.5112\sqrt{I} + 0.237I$$