Computers and Chemical Engineering 60 (2014) 403–412

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

Computational Fluid Dynamics modeling of micromixing performance in presence of microparticles in a tubular sonoreactor

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A R T I C L E I N F O

Article history:
Received 29 May 2013
Received in revised form 10 August 2013
Accepted 14 September 2013
Available online 21 September 2013

Keywords:
Sonoreactor
CFD modeling
Micromixing
Microparticle
Segregation index
Ultrasound

A B S T R A C T

This paper reports the results of CFD modeling for evaluating micromixing efficiency in presence of polymeric microparticles in a continuous tubular sonoreactor. The studied tubular sonoreactor was equipped with four 1.7 MHz ultrasound transducers and micromixing efficiency was analyzed using Villermaux/Dushman reaction. The main objective of this study is to illustrate the simultaneous effects of 1.7 MHz ultrasound waves and polymeric microparticles on micromixing performance from the fluid dynamics point of view. In order to model the presence of these microparticles, the Eulerian multiphase model was applied based on kinetic theory of granular flow. The dynamic mesh method was used to model the vibration of 1.7 MHz piezoelectric transducers. CFD modeling results indicate the positive effects of the presence of microparticles on micromixing efficiency and more efficient velocity distribution inside the sonoreactor. This was interpreted as the ability of high frequency ultrasound waves (1.7 MHz) to move and disperse the microparticles.

1. Introduction

In recent years, the ultrasonic energy applications for intensification of many chemical and mechanical processes is among one of the new techniques that have been attracted more attention (Laborde, Bouyer, Caltagirone, & Gerard, 1998; Matouq & Anber, 2007). Ultrasound can be defined as an acoustic energy at a frequency higher than the upper human hearing limit (20 kHz) (Legay, Gondrexon, Person, Boldo, & Bontemps, 2011).When a liquid subjected to an ultrasound field, one of the main phenomena that will occur is acoustic cavitation (Monnier, Wilhelm, & Delmas, 1999; Parvizian, Rahimi, Hosseini, Madaeni, & Alsairafi, 2012a). Acoustic cavitation refers to the growth of nuclei in a liquid and subsequent collapse of the gas bubbles that formed during alternate compression and expansion cycles in the liquid. It is strongly dependent on the pressure amplitude in the ultrasound field and the gas content in the liquid (Aljbour, Tagawa, & Yamada, 2009; Gondrexon et al., 2010; Parvizian, Rahimi, & Faryadi, 2011). The main effect of bubbles imploding is the release of large magnitudes of energy over a very small location in involved system (Katekhaye & Gogate, 2011; Narducci, Jones, & Kougoulos, 2011; Rooze, Rebrov, Schouten, & Keurentjes, 2012). Transmitting ultrasound energy through a liquid causes the turbulence and the bulk movement of medium (Rahimi, Dehbani, & Abolhasani, 2012). If the high frequency ultrasound (in the range of MHz) passes through the liquid, acoustic streaming is induced (Moholkar, 2009). Acoustic streaming is a steady fluid flow that ensues from the dissipation of acoustic energy (Legay et al., 2011; Lighthill, 1978). In some studies, it was reported that the acoustic streaming increases the rate of heat and mass transport and promoted the chemical processes (Kumar, Kumaresan, Pandit, & Joshi, 2006). These above mentioned effects have been used in many applications such as fields of heat transfer (Kiani, Sun, & Zhang, 2012; Legay et al., 2011), chemical reactions, wastewater, crystallization, extraction, cleaning and most importantly for micromixing improvement (Parvizian et al., 2011). Unlike, using ultrasound waves to improve the mixing efficiency has been considered by many researchers, there are still major problems in use of ultrasound waves in industrial reactors. One reason could be complexity of understanding the ultrasound propagation in liquids. It is clear that mathematical modeling can help to understand the distribution of these waves through the sonoreactor consisting complex reactions. Several studies have been carried out in order to model and theoretical investigation of ultrasound propagation in fluids (Dahlem, Reisse, & Halloin, 1999; Dahnke, Swamy, & Keil, 1999a; Kumar et al., 2006; Vanhille & Pozuelo, 2004; Yasui et al., 2007).

Dahnke and Keil (1999b) presented a model to predict the sound wave distribution in sonoreactor equipped with three transducers by solving the three-dimensional time-dependent wave equation using the finite differences approach. Their model is appropriate to

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http://dx.doi.org/10.1016/j.compchemeng.2013.09.006

Nomenclature

A	light absorption
A_0	maximum displacement of transducer (m)
$C\mu$	k–ε model parameters
$C_{1\varepsilon}$	k–ε model parameters
$C_{2\varepsilon}$	k–ε model parameters
C_D	drag coefficient
d	diameter (m)
$D_{i,m}$	diffusion constant (m^2/s)
D_t	turbulent diffusion coefficient (m^2/s)
e	coefficient of restitution
f	frequency (Hz)
F	molar flux (mol/s)
g	gravitational acceleration (m/s^2)
J	diffusion flux ($mol/m^2\,s$)
k	k–ε model kinetic energy
K	interphase exchange coefficient
l	cell length (m)
P	pressure (Pa)
Q	volumetric flow rate (m^3/s)
R_i	reaction rate i ($mol/m^3\,s$)
Re	Reynolds number
Sc_t	turbulent Schmidt number
S_ϕ	source term
S_q	source mass for phase q
t	time (s)
T	temperature (K)
x	x coordinate (m)
X_i	species mass fraction
X_S	segregation index
Y	selectivity of iodide
Y_{TS}	selectivity of iodide in the case of total segregation
y	y coordinate (m)
Z	z coordinate (m)

Greek letters

α	volume fraction
ε	k–ε model dissipation energy
ε_{353}	molar extinction coefficient of three iodate (m^2/mol)
γ	relative segregation index
φ	quantity parameter
μ_{eff}	effective viscosity (Pa s)
μ_t	turbulent viscosity (Pa s)
ρ	density (kg/m^3)
ν	velocity (m/s)
$\bar{\bar{I}}$	stress tensor
λ	bulk viscosity (Pa s)
μ	shear viscosity (Pa s)
$\bar{\bar{\tau}}$	shear stress tensor (Pa)

Subscripts

l	liquid phase
max	maximum value
q	either liquid or solid phase
s	solid phase
t	turbulent

calculate the pressure field in a sonochemical reactor with a sufficient accuracy. In numerical study done by Servant, Caltagirone, Gerard, Laborde, and Hita (2000) a numerical modeling was undertaken to consider the effects of high frequency ultrasound waves (477 kHz) on cavitation bubble dynamics in a cylindrical sonoreactor. They considered the emergence of cavitation bubbles and the effect of pressure amplitude on the generation and the volume fraction of bubbles due to acoustic driving.

The Laborde, Hita, Caltagirone, and Gerard (2000) study included a Computational Fluid Dynamics (CFD) modeling of the acoustic field at low and high frequencies (from 20 to 800 kHz) in a cylindrical sonoreactor. They declared that CFD modeling is an efficient method to simulate the liquid flow in ultrasonic fields. In addition, the CFD modeling was used by Trujillo and Knoerzer (2009) to show acoustic streaming induced by ultrasound horn reactor at powers higher or equal than 30 W. Their results showed that at all power densities, velocity pattern predicted by CFD modeling has a good agreement with the experimental data. The numerical model based on 2D finite-volume modeling was presented by Osterman, Dular, and Sirok (2009) to simulate the collapse of a single bubble in a 33 kHz ultrasound pressure field. The shape of bubbles, which computed by this model, showed a good agreement with experimental data from the literature. In addition, Jamshidi, Pohl, Peuker, and Brenner (2012) used COMSOL software for numerical analyzing of the ultrasonic waves propagation in a sonochemical reactor. Their results showed that ultrasound has a significant effect on the efficiency of the reactor because of acoustic streaming generation. In addition, the acoustic pressure distribution and the sound absorption coefficient in a sonochemical reactor at high frequency (490 kHz) were numerically simulated by Xu, Yasuda, and Koda (2012). They investigated the liquid velocity distribution in a sonochemical reactor for low (10 W), middle (30 W) and high (50 W) acoustic power from the acoustic pressure distribution.

Mixing quality and turbulent transport have significant effects on product distributions in many industrial reactions. Conversion and selectivity of fast chemical reactions are related to micromixing efficiency of reactants (Hjertager, Hjertager, & Solberg, 2002). Thus, in order to improve reactors performance, it is important to characterize micromixing, which it is the mixing at the molecular scale (Su, Chen, & Yuan, 2011) or motion of the components in the abstract composition space (Lakatos & Varga, 1988). In our previous work (Parvizian, Rahimi, Faryadi, & Alsairafi, 2012b), mechanical mixing in a batch sonoreactor equipped with four 1.7 MHz transducers was modeled using computational fluid dynamics. The results from that study had a good agreement with experimental data. In addition, in our two previous experimental works (Parvizian et al., 2011; Parvizian, Rahimi, & Azimi, 2012c), effects of high frequency ultrasound (1.7 MHz) on the mixing performance were considered. The results of these studies showed more efficient micromixing performance. In addition, other researchers declared that ultrasound has a significant effect on mixing processes (Monnier et al., 1999; Monnier, Wilhelm, & Delmas, 2000). Therefore, coupling ultrasound irradiation into a reaction system can significantly reduce the reaction or mixing time and increase the reaction yield (Gogate & Pandit, 2004). In addition, using solid microparticles in the reactors causes stretch and high shear of the fluid elements, increase the interfacial contact area of fluids and reduce the diffusion length between fluids (Su et al., 2011). In another experimental work by the authors (Rahimi, Azimi, & Parvizian, 2013), simultaneous effects of 1.7 MHz ultrasound waves and polymeric microparticles on micromixing efficiency in a continuous tubular sonoreactor were investigated. That study showed that coupling high frequency ultrasound field and microparticles in a reaction system causes additional enhancement in micromixing efficiency.

For this complex structure, it is important to gain better insight into particle motions and mixing rate that are affected by the ultrasound field. In this work CFD modeling was applied to characterize the hydrodynamic and flow pattern of acoustic streams created by high frequency (1.7 MHz) piezoelectric transducers with a