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Mesoscale modeling of emulsification in rotor-stator devices Part I: A population balance model based on EMMS concept

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HIGHLIGHTS

- Only Alopaeus breakage or adding Prince coalescence model fails for dilute systems.
- Stability condition offers new mesoscale constraint to population balance equations.
- Correctors on droplet breakage rate are derived from EMMS approach for CFD-PBM.
- Without fitting parameters, the new model greatly improves prediction of droplet size.
- Breaking higher dispersed phase content needs more outer rings of rotor-stator gaps.

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ABSTRACT

Droplet size distribution represents one of the key parameters of emulsification products and emulsification efficiency. While there is a large number of computational fluid dynamics and population balance model (CFD-PBM) simulation for droplet size distribution in various emulsification devices, fitting parameters or empirical correlations were always involved to generate the reasonable simulation. In this study, we applied the Energy-Minimization Multi-scale (EMMS) approach for the liquid-liquid flow in rotor-stator (RS) mixing devices. The so-called mesoscale energy dissipation for droplet breakage was derived to close the population balance equations through a breakage rate corrector. The correction factor was then integrated into the fully-coupled CFD-PBM simulation for a surfactant-free MCT-oil/water system. Compared to the original Alopaeus breakage model or the combination of Alopaeus model and Prince coalescence model, this new model could greatly improve the prediction of droplet size distribution, Sauter mean diameter, median diameter and span of size distribution for both the dilute and the dense systems of dispersed oil phase.

1. Introduction

Rotor–stator high-shear mixing devices are well-known for the ability to generate very high shear stress with highly-focused delivery of energy and to control the droplet size and product quality. The devices are thereby widely used in chemical, pharmaceutical, biochemical, agricultural, cosmetic, health care and food processing industries for homogenization, dispersion, emulsification, grinding, dissolving, performing chemical reactions with high selectivity, cell disruption and shear coagulation. For example, droplets less than 20 μm are usually generated in rotor-stator (RS) devices during emulsification, and droplet size distribution represents one of the key parameters of emulsification products and emulsification efficiency.

In addition to the experimental studies on flow regime, droplet size distribution (DSD) and performance of different devices, there have been many computational fluid dynamic (CFD) studies, focusing on flow pattern, power characteristics, pumping capacity and distribution of turbulence kinetic energy dissipation rate in rotor–stator mixing devices of single-phase flow (Calabrese, 2002; Utomo et al., 2008; Özcan-Taşkın et al., 2011; Cooke et al., 2012; Wu et al., 2014; Xu et al., 2014; Li et al., 2015; Jasińska et al., 2015; Makino et al., 2015; Håkansson et al., 2016; Zhao

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Nomenclature

N_T	total energy dissipation, m^2/s^3
N_{surf}	dispersed phase surface energy, m^2/s^3
N_{break}	breakage energy, m^2/s^3
N_{turb}	energy dissipated in turbulence, m^2/s^3
EMMS	Energy Minimization Multi-Scale
C_{break}	breakage corrector
k	turbulence kinetic energy, m^2/s^2
$\tilde{G}_k$	generation of turbulence kinetic energy k
G_ω	generation of specific dissipation rate ω
Y_k	dissipation of k due to turbulence
Y_ω	dissipation of ω due to turbulence
D_ω	cross-diffusion term
S_k, S_ω	user-defined terms
S_{ph}	the source terms of phase transition
S_b	the source terms of breakage
S_c	the source terms of coalescence
d_i	droplet diameter, m
C_1, C_2 and C_3	fitting parameters
d_S, d_L	diameters of small bubble phase and large bubble phase, m
f_S, f_L	volume fractions of small bubble phase and large bubble phase
$U_{g,S}$, $U_{g,L}$	superficial velocities of small bubble phase and large bubble phase, m/s
$N_{surf,S}$, $N_{surf,L}$	energy dissipated in turbulence of small bubble phase and large bubble phase, m^2/s^3
$N_{break,S}$, $N_{break,L}$	breakage energy of small bubble phase and large bubble phase, m^2/s^3
F_r	centripetal force, N
F_D	drag force, N
m	droplet mass, kg
a	the angular acceleration, N/kg
d	diameter of the droplet, m
r	radial length along the radial direction, m
C_D	drag coefficient
U_C, U_d	superficial velocities of continuous phase and dispersed phase, m/s
T	torque of rotor walls, N·m
N	rotation speed, rps
$u_{d,\ inlet}$, $u_{C,\ inlet}$	real (interstitial) velocities of dispersed phase and continuous phase at the inlet, m/s
$f_{d,\ inlet}$	volume fraction of dispersed phase at the inlet
l_k	Komolgorov size, m
d_{32}	Sauter mean diameter, m
DPA	dispersed phase amounts
min	minimum
RANS	Reynolds-Averaged Navier–Stokes

Greek letters

ω	specific dissipation rate, s^{-1}
ε	turbulent kinetic energy dissipation rate, m^2/s^3
ρ_C, ρ_d	densities of continuous phase and dispersed phase, kg/m^3
σ	droplet surface tension, N/m
μ_d	viscosity of dispersed phase, Pa·s
ω	angular velocity, rad/s
μ	viscosity of fluid particles, Pa·s

et al., 2016; Håkansson et al., 2017a, 2017b, 2017c; Håkansson and Innings, 2017). In the earlier studies, Calabrese (2002) reported a two-dimensional numerical simulation of the single-phase flow in rotor–stator mixers. Utomo et al. (2008) simulated the three-dimensional flow in a lab-scale batch-operated Silverson mixer, and investigated the effects of rotor speed and stator geometry on flow field and distribution of turbulence energy dissipation rate. The simulations were reported to be in good agreement with experiments, though the modeling of flow and power properties at transitional regime remains an unresolved issue. Moreover, the turbulence modeling for RS systems is also challenging. Mortensen et al. (2018) reported that the turbulence dissipation rate could only be qualitatively captured by the two-equation RANS turbulence models.

From a macro-scale point of view, DSD is determined by the operational parameters of rotor-stator devices and physical properties of materials in liquid-liquid emulsification. At the mesoscale, DSD is the result of the frequencies of droplets breakage and coalescence, both of which are relevant to the complex interactions between turbulence eddies and droplets and to the interfacial adsorption of emulsifiers in rotor-stator high-shear devices. In general, population balance model (PBM) equations, together with the CFD models, are required to model the droplet size distribution. In PBM, the so-called kernel function models, which correlate turbulence energy dissipation rate and droplets breakage or coalescence rates (Luo and Svendsen, 1996; Lehr and Mewes, 1999; Kostoglou and Karabelas, 2005), remain a challenging issue. Droplets are modeled to break up when the energy content of the colliding eddies is greater than the corresponding increase of surface energy during breakage and the dynamic pressure of eddies is greater than the capillary pressure of smaller daughter droplets. Droplets are modeled to coalesce when the film drainage time is smaller than the contact time of droplets. A number of parameters, e.g., turbulent velocity of eddies, collision frequency of eddies and droplets, breakage probability, daughter particle size distribution and coalescence efficiency, require to be modeled, as reviewed by Liao and Lucas (2009, 2010). One of recent development is the extension of the fluid-particle breakage and coalescence closures to the entire spectrum of isotropic turbulence and a wider range of Reynolds number based on the statistical isotropic turbulence theory (Han et al., 2014, 2015; Solsvik and Jakobsen, 2016a, 2016b; Solsvik et al., 2016). Another method for simulating droplet dynamics is the direct numerical simulation. For instance, Li et al. (2016) investigated the splashing phenomenon in slag–metal molten bath under real oxygen steel making conditions through the multi-fluid VOF model combined with the blowing number theory.

A large number of CFD-PBM simulation have been carried out for emulsification processes. However, fitting parameters or correlations were always involved in most simulations to give the better simulation of droplet size, and the extrapolation to systems of different geometries, phase and physical properties are still doubtful. Jasińska et al. (2014) reported that the breakage model proposed by Baldyga and Podgórska (1998) could well predict the DSD at some operating conditions. Alopaeus et al. (2002) developed a multi-block simulation and proposed a droplet breakage model for a dense liquid-liquid dispersion in a stirred tank. Dubbelboer et al. (2016) presented a population balance model for high internal phase emulsions for the manufacturing of mayonnaise in a colloid mill. They considered the variable number of fragments in daughter droplet size distribution and the interaction of viscosity and droplet size. Carrillo De Hert and Rodgers (2017) investigated the effects of dispersed phase viscosity, stirring speed and mean residence time on the droplet size distribution for dilute systems