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CFD-PBM simulation of dense emulsion flows in a high-shear rotor–stator mixer

Vipin Michael[a,*], *Robert Prosser*[a], *Adam Kowalski*[b]

[a] *School of Mechanical, Aerospace & Civil Engineering, The University of Manchester, Manchester M13 9PL, UK*
[b] *Unilever R&D, Port Sunlight Laboratory, Quarry Road East, Bebington, Wirral CH63 3JW, UK*

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ABSTRACT

Computational fluid dynamics (CFD) is coupled to population balance modelling (PBM) for the simulation of turbulent drop dispersion and evolving rheology in concentrated oil–water emulsions flowing through a Silverson 150/250MS mixer. Unsteady Reynolds averaged Navier–Stokes (URANS) simulations on a sliding mesh were performed for the fluid dynamics, linking the $k-\omega$ SST turbulence model to the population balance equations. The quadrature method of moments (QMOM) approach is used to solve the population balance equations. Breakage kernels based on the multi-fractal theory of intermittent turbulence have been modified to include the effect of turbulent shear and close packing of drops at high phase volume. A previously developed rheological model is used to calculate the emulsion viscosity. Emulsion drop size is shown to be influenced by rotor speed and phase volume fraction. Flow curves characterising the rheology of the emulsion show shear thinning behaviour and viscosity build after a single pass through the mixer.

1. Introduction

High-shear in-line rotor–stator mixers are widely used in industry for the manufacture of emulsion based formulated products. The properties of these emulsions are process sensitive, with drop size and distribution affecting the physical stability and viscosity of the product. However, industrial practice is still largely based on experimental results and empirical rules (Calabrese et al., 2000), as understanding of the underlying process mechanics undergone in these devices is limited (Atiemo-Obeng and Calabrese, 2004).

Simulations and experiments of drop dispersion in a Silverson 150/250MS rotor–stator mixer have focussed on low phase volume emulsions (Hall et al., 2011; Jasińska et al., 2014). Hall et al. (2011) have experimentally investigated emulsion systems with dispersed phase volume fractions up to 50%. It was found that rotor speed and dispersed phase viscosity have a significant effect on the droplet size, while flow rate, inlet droplet size, viscosity ratio and dispersed phase volume have a lesser effect. Computational simulations of the fluid flow and drop dispersion by Jasińska et al. (2014) gave results that agree qualitatively with experimental data demonstrating that CFD-PBM approaches are useful for the design of high-shear rotor–stator mixers.

In concentrated emulsions, the dispersed phase volume fraction plays an important role in the emulsification process. As pointed out by Pal (2003), rheology of emulsions is intimately linked to the deformation and orientation of drops suspended in the continuous phase. Fine emulsions have much higher viscosities and stronger shear thinning behaviour than coarse emulsions for the same dispersed phase volume fraction. There is a limited amount of literature on the viscosity of high internal phase emulsions, and semi-empirical models such as Hershel–Bulkley and Cross correlations have often been used to characterise the viscosity in such systems (Princen and Kiss, 1989; Dubbelboer et al., 2016; Jansen et al., 2001). The theoretical modelling of the viscosity behaviour has to take into account deformation and orientation of drops suspended in the continuous phase. The

* *Corresponding author.*
E-mail address: vipin.michael@manchester.ac.uk (V. Michael).
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Nomenclature

α	multi-fractal scaling exponent
β	probability distribution of daughter sizes
$\dot{\gamma}$	strain rate (1/s)
ϵ	turbulence energy dissipation rate (m^2/s^3)
$\eta_K = (\nu_e^3/\epsilon)^{1/4}$	Kolmogorov length scale (m)
η_r	relative viscosity of the emulsion
Γ	total diffusivity (m^2/s)
μ_c	continuous phase dynamic viscosity (Pa s)
μ_d	dispersed phase dynamic viscosity (Pa s)
μ_e	emulsion dynamic viscosity (Pa s)
ν_e	emulsion kinematic viscosity (m^2/s)
ω	specific turbulence dissipation rate (1/s)
ϕ	dispersed phase volume fraction
$\phi_m = 0.8$	maximum packing fraction
ρ_c	continuous phase density (kg/m^3)
ρ_d	dispersed phase density (kg/m^3)
σ	interfacial surface tension ($N\,m^{-1}$)
τ	turbulent stress (Pa)
d	drop diameter (m)
d_i	abscissa of Gaussian quadrature
D_R	diameter of rotor swept volume (m)
$d_{32} = m_3/m_2$	Sauter mean diameter (m)
g	breakage frequency (1/s)
k	turbulent kinetic energy (m^2/s^2)
$K = \mu_d/\mu_c$	viscosity ratio
$L = k^{3/2}/\epsilon$	integral length scale (m)
m	moment of drop size distribution
n	number density of drops
N_Q	number of nodes of Gaussian quadrature
N_{Ca}	capillary number
Q_M	inlet mass flow rate (kg/h)
R	drop radius (m)
R_z	equivalent radius of emulsion (m)
t	time (s)
u_i	velocity vector (m/s)
v	velocity scale of turbulent flow (m/s)
w_i	weights of Gaussian quadrature
x_i	physical coordinate vector (m)
N	rotational speed (rpm)

equilibrium shape and orientation of the drop with respect to the flow direction is governed by a balance between hydrodynamic stress ($\mu_c\dot{\gamma}$) and interfacial stress (σ/R) expressed through the capillary number which is defined as

$$N_{Ca} = \frac{\mu_c \dot{\gamma} R}{\sigma} \tag{1}$$

As the capillary number increases with shear rate, the drop elongates and orientates itself along flow streamlines, organising into planes and thus offering less resistance to flow. Consequently, shear-thinning behaviour is exhibited in these systems. At very high shear rate, drops cannot align any further and the emulsion behaves as a Newtonian fluid with a constant viscosity.

Baldyga et al. (2016) presents a theoretical model for emulsion viscosity as function of the capillary number. This model based on earlier works of Pal (2003) and Palierne (1990), includes the effects of dispersed phase volume fraction, droplet size distribution, interfacial surface tension and shear rate on the relative emulsion viscosity. The model can be combined with PBM and CFD to produce fully coupled simulations (Baldyga et al., 2016).

The statistics of the drop size distribution are controlled to a large extent by break-up, which occurs when the external disruptive forces acting on the droplet are larger than internal cohesive forces resisting deformation. In the context of industrial flows, break-up is strongly influenced by the dynamics of turbulence. Turbulent emulsification is modelled using the Hinze–Kolmogorov theory; denoting the smallest length scales (the Kolmogorov length scale) in the flow as η_K, then the breakage mechanism is predicated on the ratio of η_K to the drop size (d). If the drop size $d > \eta_K$ then the drop tends to be broken by pressure fluctuations from multiple turbulent eddies colliding with it. This case is referred to as turbulent inertial (TI) breakage. If the drop size $d \le \eta_K$, viscous stresses generated by velocity gradients around the drop generate disruptive forces. This case is referred to as turbulent viscous (TV) breakage. The nature of internal forces depends on the viscosity of the dispersed phase. For a low viscosity dispersed phase, the cohesive force comes from interfacial tension, while for high viscosity dispersed phase, there are additional contributions from viscous shear stresses within the drop.

For low dispersed phase viscosity systems, the maximum stable equilibrium drop size when inertial forces are responsible for breakage can be expressed as (Leng and Calabrese, 2004)

$$d \approx \left(\frac{\sigma}{\rho_c}\right)^{0.6} \epsilon^{-0.4}, \tag{2a}$$

whereas if viscous stresses become important for breakage, then (Leng and Calabrese, 2004)

$$d \approx \left(\frac{\nu_c^3}{\epsilon}\right)^{0.25}. \tag{2b}$$

To compare these mechanistic drop size correlations to results obtained from simulations or experiments, the turbulence energy dissipation rate is related to process parameters. In case of rotor–stator mixers, dimensional analysis leads to

$$\epsilon \sim N^3 D_R^2. \tag{2c}$$

Combining Eq. (2c) with Eq. (2a) yields $d \sim N^{-1.2}$ when the drop breakage is dominated by inertial effects or with Eq. (2b) yields $d \sim N^{-0.75}$ when it is dominated by viscous effects.

The aim of the present work is to perform CFD-PBM simulations of an inline high-shear rotor–stator mixer (Silverson 150/250 MS), modelling turbulent drop dispersion coupled to Non-Newtonian viscosity, following the assumptions and methodology of Baldyga et al. (2016). The emulsion system considered is assumed to be non-colloidal, pseudo-homogeneous with constant dispersed phase fraction and stabilised with excess surfactant so that drop coalescence may be neglected. The Peclet number is assumed to be large, i.e., drops are much larger than the distance travelled due to Brownian motions. Turbulent stresses generated within the mixer is expected to exceed the yield stress of the emulsion. The contribution of added surfactant to continuous phase properties are also neglected. The drop breakage model used by Baldyga et al. (2016) is extended to include the effects of turbulent viscous shear and close-packing density of drops occurring at high phase volume fractions. Baldyga et al. (2016)