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Modeling of turbulent drop coalescence in the presence of electrostatic forces

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ABSTRACT

The influence of ionic surfactant (SDS) on the drop size distribution in stirred liquid–liquid dispersions was considered. The destabilizing effect of a salt (NaBr) on the dispersion was also discussed. A new model for drop coalescence in turbulent flow in the presence of repulsive forces was derived. The film drainage between rigid and deformed droplets was taken into account. The influence of interfacial tension and electrostatic repulsion on the behavior of the dispersion in different zones of a stirred tank was predicted. It was also shown that, additional disruptive stresses, resulting from interfacial tension difference, due to surfactant desorption, increase drop breakage rate. In both breakage and coalescence models local intermittency was taken into account by using the multifractal formalism. Drop size distributions were predicted, by solving the population balance equation, and compared with experimental data.

1. Introduction

Liquid–liquid dispersions find applications in the chemical, pharmaceutical, food and petroleum industries and are involved in numerous operations such as: solvent extraction, multiphase chemical reactions and emulsion polymerization. To generate and maintain a dispersion of one liquid in another mechanical agitation is usually applied under turbulent conditions. The resulting drop size distribution (DSD) and its evolution in time are of great importance, as they are related to mass transfer and chemical reaction rates and, therefore, affect the quality of the final products. The DSD depends on the disperse and continuous phase properties, on the presence of surface active agents, on the type of surfactant, on the presence of electrolytes, as well as on the overall flow field and is the result of two competing processes: drop breakage and coalescence.

The complexity of these processes makes the prediction and control of drop size evolution a great challenge. Both processes are strongly influenced by the turbulence intensity in stirred dispersions. The breakage of drops is considered to be mainly an effect of pressure fluctuations, in the case of droplets of diameter within the inertial subrange of turbulence encountered in stirred tanks, whereas external disruptive viscous stresses can be regarded as negligible (see for example Zhou and Kresta, 1998). Internal viscous stresses (within the drop) can be important, instead, and can damp drop deformation, when the disperse phase viscosity is large enough (Arai et al., 1977; Calabrese et al., 1986; Davies, 1987). However, when the viscosity of the drops is low, the main stabilizing (or shape restoring) stress is due to the interfacial tension. Many breakage rate models, based on the Kolmogorov theory of turbulence, were proposed, including one of the first and most popular one by Coulaloglou and Tavlarides (1977),

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Nomenclature

a	film radius (m)
A_1	defined by Eq. (20)
C, C_1, C_2	constants in the coalescence model
C_g, C_x	constants in the breakage model
D	impeller diameter (m)
d	drop diameter (m)
d_{32}	Sauter diameter (m)
d_{jk}	$= (d_j + d_k)/2$
$E(\upsilon,\upsilon')$	increase in total surface energy (J)
e	unit electron charge (C)
F	force (N)
F_{int}	interaction force in the film (N)
F_{Rp}	repulsion force between flattened droplets (N)
$F_{R\,planar}$	repulsion forces between discs per unit area ($\mathrm{N\,m^{-2}}$)
F_{R_r}	repulsion force between rigid spheres (N)
F_t	turbulent force (N)
$f(\alpha)$	multifractal spectrum
$g(d)$	breakage frequency ($\mathrm{s^{-1}}$)
H	tank height (m)
h	film thickness (m)
h_c	critical film thickness (m)
h_0	initial film thickness (m)
$h(d,d')$	drop collision function ($\mathrm{m^3\,s^{-1}}$)
I	ionic strength ($\mathrm{mol\,dm^{-3}}$)
k	kinetic energy of turbulence ($\mathrm{m^2\,s^{-2}}$)
k_B	Boltzmann constant ($\mathrm{J\,K^{-1}}$)
L	integral scale of turbulence (m)
M	molar concentration ($\mathrm{mol\,dm^{-3}}$)
N	impeller rotational speed ($\mathrm{s^{-1}}$)
N_A	Avogadro number ($\mathrm{mol^{-1}}$)
$n(\upsilon,t)$	number density function of drops ($\mathrm{m^{-6}}$)
n_∞	defined by Eq. (16)
$P(\alpha)$	probability density for α
R	drop radius (m)
R_{eq}	equivalent radius (m)
r	size of eddy, distance (m)
T	tank diameter (m)
T	temperature (°C)
t_{eff}	effective adsorption time (s)
t_{cP}	drainage time for flattened drops (s)
t_{cR}	drainage time for rigid drops (s)
t_{int}	interaction (contact) time (s)
u	velocity, characteristic turbulent velocity ($\mathrm{m\,s^{-1}}$)
z	valency

Greek symbols

α	multifractal exponent
α_{min}	minimum value of the multifractal exponent α
α_x	upper bound of the multifractal exponent α
$\beta(\upsilon,\upsilon')$	daughter drop distribution function ($\mathrm{m^{-3}}$)
ε	energy dissipation rate ($\mathrm{m^2\,s^{-3}}$)
ε_r	dielectric constant
ε_0	electrical permittivity of vacuum ($\mathrm{C\,V^{-1}\,m^{-1}}$)
κ	inverse Debye length ($\mathrm{m^{-1}}$)
$\lambda(d,d')$	coalescence efficiency
μ	dynamic viscosity (Pa s)
$\nu(\upsilon')$	number of daughter drops
ρ	density ($\mathrm{kg\,m^{-3}}$)
σ	static interfacial tension (N/m)
υ	drop volume ($\mathrm{m^3}$)
Φ_R	total potential energy of repulsin (J)
ϕ	dispersed phase volume fraction
Ψ	electrostatic potential (V)
Ψ_0	electrostatic surface potential (V)

Subscripts

C	continuous
D	dispersed
imp	impeller zone
bulk	bulk zone

in which the probability of breakage was derived using a Gaussian distribution for the turbulent velocity, the model of Narsimhan et al. (1979), in which the droplet is interpreted as a one-dimensional simple harmonic oscillator and its extension, proposed by Alopaeus et al. (2002), with included effect of viscous force within the drop. Other developments include the work of Tsouris and Tavlarides (1994) and Luo and Svendsen (1996). Tsouris and Tavlarides (1994) as well as Luo and Svendsen (1996) assumed that droplets can be broken only by eddies smaller than or of comparable size with the droplet. On the other hand Andersson and Andersson (2006a) and Han et al. (2011) argue that eddies whose size is approximately equal to and up to three times larger than drop are responsible for breakage. According to Hinze (1955) only eddies of the size of drop diameter disperse the drop as larger eddies just convey the drop, while smaller ones are not active enough to break the drop. Hesketh et al. (1991) observed that the amplitude of small deformations did not grow, but the deformation was eliminated by stabilizing forces, preventing drop breakage to occur. Both, the small scale of deformations and their duration prove that they are brought about by eddies smaller than the droplet. Only large deformations caused by eddies of the size comparable to that of the droplet can lead to breakage.

Models based on classical Kolmogorov theory are often sufficient and allow to predict maximum stable drop size as well as DSD changes. They fail, however, to predict the correct exponent of the Weber number, when it is much smaller than −0.6, as observed after long agitation times or under scale effects (i.e. faster breakage in geometrically similar tanks when the mean energy dissipation rate is maintained the same). To explain these effects in stirred tanks, Konno et al. (1983) proposed to divide the tank into two breakage zones: one characterized by isotropic turbulence, and the second one characterized by large turbulence anisotropy. Another explanation was proposed by Bałdyga and Bourne (1995). According to them the observed effects can result from internal intermittency, which can be described using the multifractal formalism proposed by Parisi and Frisch (1985). As underlined by Frisch (1995) the multifractal description of turbulence is probabilistic and does not relate to the geometry of fine scales. This formalism was used by Bałdyga and Podgórska (1998) to derive a multifractal breakage model, which explains observed scale effects and the drift of the exponent on the Weber number. Intermittency has a profound effect on short duration processes such as drop breakage, but to some extent influences also the ones characterized by longer durations, such as coalescence.