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Modelling and simulation of extensional-flow units in emulsion formation

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ABSTRACT

Here we studied the emulsification process carried out in an extensional-flow unit. By means of rigorous population and momentum balances we captured the phenomenological description of the first principles occurring in such unit. The strong feature of our model approach resides in the fully mechanistic description of the governing phenomena. A population balance equation was formulated and solved to account for the disappearance and appearance of droplets at each size class. Coalescence mechanism was included to account for the instability of newly created droplets. We validated the accuracy of the results obtained from our equation-based model with experimental data obtained at pilot-plant scale. The results obtained by simulation showed that at a given set of operational conditions and pre-emulsion properties the product obtained was within the desired and narrow specifications space. As a concluding remark we suggest further exploring the design and development of extensional-flow units for structured emulsions.

1. Introduction

Every day we are in direct contact with emulsions and dispersions. Many food products do not form homogeneous mixtures but are composed of at least one component in the form of solids or droplets. This microstructure is responsible for key sensory attributes in food products, such as mouth-feel, colour, aroma and spreadability. Reaching a desired microstructure involves not only the close marriage between product composition and processing, but also the development of a process synthesis methodologies embracing both (see, e.g. Bongers, 2009; Bongers & Almeida-Rivera, 2009). A model-based approach is a fundamental building block of such design methodologies.

Current technologies for the production of emulsion-type foods include, among others, static mixers (Grace, 1982), stirred tanks (Nienow, 2004), rotator-stator devices (Calabrese, Francis, Mishra, & Phongikaroon, 2000; Wieringa, Janssen, & Agterof, 1996), and high-pressure and ultrasonic homogenisers (Karbstein, 1994). The governing droplet break-up mechanism in each device is highly dependent on the physical properties of the system (e.g. viscosities of continuous and dispersed phases), and on the flow conditions. The type of flow profile that the droplets experience depends on the mechanical configuration and operational regime of the unit and can be characterized by the flow parameter $\alpha \in [-1, 1]$ (Stork, 2005). For instance, stirred tanks are basically featuring simple shear in the laminar regime, whereas turbulent inertial and cavitation mechanisms are responsible for droplet break-up in high-pressure homogenisers. Despite the sound expertise generated over the last decades regarding droplet disruption and coalescence mechanisms (Nienow, 2004; Saboni, Alexandrova, Gourdon, & Cheesters, 2002; Tjaberinga, Boon, & Cheesters, 1993), the effort has been exclusively channelled to those units where either single shear flow ($\alpha = 0$) or rotational flow ($-1 < \alpha < 0$) is dominating. Contrary to that research focus, both single shear flow and rotational flow are rarely the dominant droplet break-up mechanisms in commercial emulsion technologies. As a result, little (or rather non-existing) attention has been paid to explore units based on, for instance, extensional flow ($0 < \alpha \leq 1$). In this regard, this contribution intends to broaden the spectrum of current emulsification devices to this flow pattern.

2. Modelling framework

We address here the modelling and simulation aspects of a unit characterised by the extensional flow of material. In this type of flow regime, normally referred to as 'shear-free' flow, a preferred molecular orientation occurs in the direction of the flow field. Moreover, it is characterised by the absence of competing forces to cause rotation, resulting in a maximum stretching of molecules and

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Nomenclature

A	Hamaker constant (=1.059×10^{-20} J for a oil-in-water emulsion)
$B(v, v', z)$	droplet size distribution of daughter droplets of volume v produced by breakage of parent droplets of volume v' at location z
F	frictional force
$N(v', z)$	number of daughter droplets produced by breakage from parent droplets of volume v' at location z
N_i	number of droplets in the size class i with mean diameter d_i
P_L	capillary pressure (or Laplace pressure)
P	pressure
R	nozzle outlet diameter
R_b	nozzle inlet diameter
Re_p	droplet-related Reynolds number
Re_{HB}	generalised Reynolds number for HB fluids
$S(v, z)$	break-up frequency (or rate) of droplets of volume v at location z
W	work exerted on the system
We^{cr}	Weber critical value
We	Weber number of droplets in a given size class
c	variable related to yield stress and shear stress,
d_h	hydraulic diameter
d^{max}	maximum unbreakable droplet size in the inertial regime
d_{32}	radius of the droplet, Sauter mean droplet diameter
$d_{32-init}$	initial Sauter diameter
f	friction factor
g	gravity acceleration
h^{cr}	critical rupture thickness
k_{col}	constant =0.43
k_f	friction coefficient for accessories
l	element length
l_k	length of Kolmogorov energy dissipating eddies
m	power law index for extensional stress
n_c	number of size classes
$n(v, z, t)dv$	number of droplets per unit volume of the dispersion at time t and location z with volumes between v and $v+dv$
q	volumetric flowrate
$r(y)$	radius at axial position y
t_b	break-up time
t_r	residence time
t_b^*	model constant
$\overline{u}$	averaged local fluid velocity
x_{oil}	oil content
y	axial location of the volume element
z	location within the unit, position with respect to a reference plane

Greek symbols

ΔP_{in}	total pressure drop at the nozzle's inlet
$\Delta P_{in,S}$	shear-flow contribution to pressure drop at the nozzle's inlet
$\Delta P_{in,E}$	extensional-flow contribution to pressure drop at the nozzle's inlet
Γ	coalescence efficiency
Ω	capillary number
Ψ	auxiliary variable
α	flow parameter
$\hat{\alpha}$	kinetic correction factor
η_E	extensional viscosity of fluid
η_e	viscosity of the emulsion
ϵ	total specific power dissipation
$\dot{\gamma}$	shear rate
$\dot{\gamma}_w$	apparent wall shear rate in the nozzle
λ_η	ratio of viscosities the disperse and continuos phases ($\lambda_\eta=\eta_d/\eta_c$)
λ_{col}	collision efficiency
v	mean volume of class
$\phi(v, z, t)$	convective flow of droplets of volume v
ρ_e	density of the emulsion
ρ_d	density of the disperse phase
ρ_c	density of the continuous phase
σ	deformation stress
σ_s	interfacial surface tension
θ	angle of the conical nozzle
φ_{col}	coalescence frequency
$\dot{\varepsilon}(y)_E$	extensional shear rate at position y

large resistance to deformation (Steffe, 1996). As turbulent flow is responsible for droplet break-up in high stress emulsification units, we focus here on this flow regime. Note that from an industrial perspective, production of emulsions in the laminar regime ($Re_p < 10^{-2} - 10^{-6}$) (Grace, 1982) is a highly energy-demanding operation for systems where the ratio of viscosities of the disperse and continuos phases, η_d/η_c, is less than 0.1 and even impossible for systems where $\eta_d/\eta_c > 4$ (Fig. 1). Under single shear conditions, the droplets are not able to deform as fast as the flow regime induces deformation (Walstra, 1993).

From a mechanical point of view, an extensional-flow unit is materialised, for instance, in a converging element of the nozzle-type (Fig. 2).

The dynamic modelling of the production process of an oil-in-water structured emulsion involves the description of all first principle phenomena together with a reliable estimation of relevant physical properties.

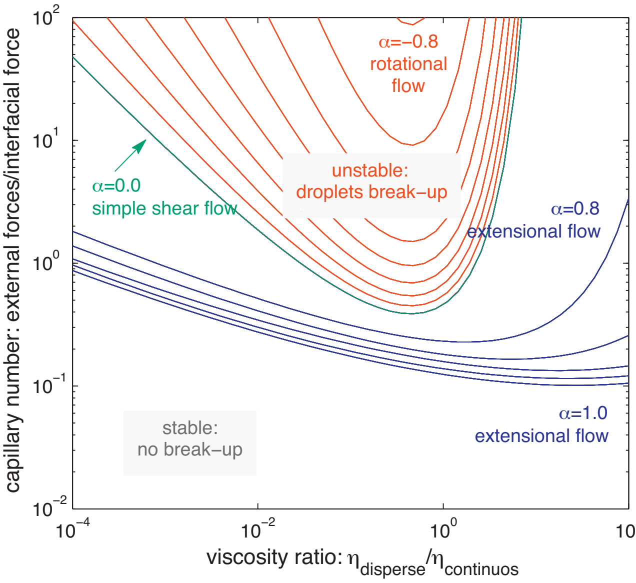

Fig. 1. Critical capillary number for droplets break-up in single shear, extensional flow and only rotational flow; α represents the flow type. Modelling parameters are those reported in Grace (1982) and De Bruijn (1989).