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Estimation of turbulent fragmenting forces in a high-pressure homogenizer from computational fluid dynamics

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ABSTRACT

The aim of this study was to find models for turbulent fragmenting forces in the high-pressure homogeniser from data available in Computational Fluid Dynamics (CFD) simulations with Reynolds Averaged Navier Stokes (RANS) turbulence models. In addition to the more common RANS k–ε turbulence models, a Multi-scale k–ε model was tested since experimental investigations of the geometry imply large differences in behaviour between turbulent eddies of different length-scales.

Empiric models for the driving hydrodynamic factors for turbulent fragmentation using the extra information given by multi-scale simulations were developed. These models are shown to give a more reasonable approximation of local fragmentation than models based on the previously used RANS k–ε models when comparing to hydrodynamic measurements in an experimental model.

1. Introduction

The high-pressure homogeniser (HPH) is used for emulsification in industrial scale for various applications. The fragmentation of emulsion drops in the HPH valve is caused by hydrodynamic forces, mainly turbulence and/or cavitation (Walstra and Smulders, 1998; Kurzhals, 1977). During the last couple of years, there has been a growing interest in dynamic modelling of emulsification in homogenisers (Soon et al., 2001; Vankova et al., 2007; Håkansson et al., 2009a,b; Raikar et al., 2009, 2010, 2011; Casoli et al., 2010; Tcholakova et al., 2007). The models are often based on population balance frameworks (see e.g., Ramkrishna, 2000) allowing the prediction of drop size distributions from rate expressions for fragmentation and coalescence. Predicting fragmentation rates require accurate estimation of the fragmenting forces. Furthermore, models describing the fragmentation process in the HPH locally (Håkansson et al., 2009a,b; Casoli et al., 2010) are of special interest for a deeper understanding of the link between geometry and efficiency of emulsification. These models require methods for estimating fragmenting forces locally.

Turbulent fragmentation is often described using the Kolmogorov–Hinze theory (Kolmogorov, 1949; Hinze, 1955), where a fragmenting force due to pressure fluctuations (in the Turbulent Inertial regime) and velocity gradients (in the Turbulent Viscous regime) is set against the stabilizing Laplace pressure in order to predict a resulting drop size. However, making predictions based on the Kolmogorov–Hinze theory requires estimation of the driving factors in the two regimes; fluctuations of turbulent eddies smaller than the drops, $\langle uu \rangle_D$, in the inertial regime and gradients of turbulent eddies larger than the drops, G_D, in the viscous regime. The traditional method for obtaining these is by using scaling laws and model spectra (Kolmogorov, 1949; Hinze, 1955). Furthermore, most studies use global mean effective values of the modelled fragmenting forces, since local measurements are rare.

Based on high resolution Particle Image Velocimetry (PIV), Håkansson et al. (2011), described a method for obtaining $\langle uu \rangle_D$ and G_D experimentally in a scale model of the HPH valve. However, performing these experimental measurements are highly time consuming and requires the construction of scaling models for each geometry to be investigated.

Computational Fluid Dynamics (CFD) offers an alternative method for rapidly and inexpensively obtaining flow fields and turbulence characteristics locally in the homogeniser. A large number of CFD studies have been conducted on HPH valves (e.g., Casoli et al., 2010; Stevenson and Chen, 1997; Floury et al., 2004; Kleinig and Middelberg, 1997; Raikar et al., 2009; Steiner et al., 2006). Recently, Håkansson et al. (2012) compared the CFD models used in the previous studies with experimental measurements in a

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HPH valve geometry. The focus was how well velocity fields and turbulent kinetic energy could be predicted. It was concluded that CFD (with the right choice of turbulence model) was able to describe the flow upstream and inside the gap accurately. The highly turbulent region downstream of the gap, however, was not well described by the CFD models, most probably due to an inability of the utilised Reynolds Averaged Navier Stokes (RANS) k–ε turbulence models to handle the recirculation zone between the exiting jet and the wall of jet attachment.

The turbulence models used in all the previous CFD studies on HPH valves are based on a number of simplifications and model assumptions, one of these is the assumption of all turbulent eddy length-scales being described by one set of turbulent variables (i.e., one turbulent kinetic energy, k, and one dissipation rate of turbulent kinetic energy, ε). The experimental measurement, on the other hand, show large differences in behaviour between turbulent eddies of different eddy length-scales. (Håkansson et al., 2011) Thus, it is reasonable to assume that a CFD model including this multi-scale effect could improve models of turbulent fragmentation. In addition, this would also enable estimation of small scale turbulent fluctuations and gradients which was not possible using the more common RANS models as in Håkansson et al. (2012).

A RANS CFD turbulence model with multi eddy length-scale support was first proposed by Hanjalic et al. (1979) and a number of different forms have been suggested (e.g., Kim and Chen, 1987, 1989; Ko and Rhode, 1990). Especially the method according to Kim and Chen (1989) has been widely utilised (Kim, 1989; Kim, 1990; Kim and Benson, 1992).

The aim of this paper is to examine how well the small scale turbulent energy and velocity gradients can be estimated locally in a HPH outlet chamber using data from CFD with RANS turbulence models by comparison to experimental measurements. Of special interest is if a Multi-scale turbulence model could improve the estimations.

Since the experimental hydrodynamic investigations were obtained in a one phase flow, without disperse phase and/or cavitation, this study only considers one phase flow.

2. Modelling turbulent fragmenting forces in the HPH

Originally, Kolmogorov (1949) derived expressions for the maximum stable drop size in a turbulent flow. Depending on drop size in comparison to Kolmogorov length-scale, η, the turbulent fragmentation was divided into different regimes based on dimensional analysis; Turbulent Inertial (TI) regime for drops smaller than η and Turbulent Viscous (TV) regime for larger drops. The fragmenting stress in the TI regime, σ_{TI}, can be written

$$\sigma_{\mathrm{TI}} = \frac{\rho_C \langle uu \rangle_D}{2} \tag{1}$$

where ρ_C is the continuous phase density and $\langle uu \rangle_D$ is the velocity fluctuations of turbulent eddies of length-scales smaller than or equal to the drop diameter D. In the TV regime, the fragmenting stress, σ_{TV}, is

$$\sigma_{\mathrm{TV}} = \mu_C \cdot G_D \tag{2}$$

where μ_C is the continuous phase (dynamic) viscosity and G_D is the turbulent velocity gradients of eddies with length-scales larger than or equal to the drop diameter D.

Predicting local fragmentation using the Kolmogorov–Hinze theory thus requires information on how the driving factors, $\langle uu \rangle_D$ and G_D, varies with drop diameter and over the homogeniser geometry. From definition, $\langle uu \rangle_D$, could be calculated if the one dimensional spectrum of turbulent kinetic energy, $E_{11}(\kappa)$, is known as a function of wave number, κ:

$$\langle uu \rangle_D = \int_{\kappa = 2\pi/d}^{\infty} E_{11}(\kappa)\mathrm{d}\kappa \tag{3}$$

Similarly, G_D, can be obtained if the velocity gradients as functions of eddy length-scales are known. In a two dimensional flow,

$$G_D = \max_{l_e > D} \left(\left|\frac{\partial U}{\partial x}(l_e)\right|, \quad \left|\frac{\partial U}{\partial y}(l_e)\right|, \quad \left|\frac{\partial V}{\partial x}(l_e)\right|, \quad \left|\frac{\partial V}{\partial y}(l_e)\right| \right) \tag{4}$$

where U,V are mean velocities, x,y are spatial coordinates and l_e is an eddy length-scale.

The one dimensional spectra of turbulent kinetic energy and eddy length-scale dependent mean velocity gradient are, however, not easily accessible. CFD simulations with RANS turbulence modelling are insufficient for directly obtaining these measures and simplistic scaling law based models are therefore often used (Hinze , 1955). Assuming E_{11} following a Kolmogorov model spectrum and drop diameters small enough to be inside the inertial subrange yields

$$\langle uu \rangle_D = C_1 \cdot \varepsilon^{2/3} D^{2/3} \tag{5}$$

with constant C_1 equal to 0.44 according to Pope (2000).

Similarly, G_D is often estimated by combing the model spectrum with scaling in order to obtain:

$$G_D = C_2 \cdot \varepsilon^{1/3} D^{-2/3} \tag{6}$$

with C_2 equal to 0.66 (Pope, 2000). The expressions in Eqs. (5) and (6) are based on approximations and assumptions such as sufficiently high Reynolds number, no wall effects and isotropy of turbulent eddies. Especially Eq. 6 is an unreasonable description of eddies with length-scales larger than the drop since it is based on information of smaller length-scales (see discussion in Håkansson et al., 2011). On the other hand, a practical advantage with Eqs. (5) and (6) is that they only include variables that are directly accessible from a RANS CFD simulation which is the standard method for hydrodynamic analysis of the HPH valve (Casoli et al., 2010; Stevenson and Chen, 1997; Floury et al., 2004; Kleinig and Middelberg, 1997; Raikar et al., 2009; Steiner et al., 2006). Thus, Eqs. (5) and (6) together with RANS-CFD would allow for local evaluation of the fragmenting forces in the HPH valve geometry.

Experimental validation of Eqs. (5) and (6) locally is scarce and due to the assumptions used in their derivation it is not clear to what extent these models are suitable for assessing local turbulent fragmenting forces in the HPH. In this paper, the ability of Eqs. (5) and (6) to predict the fragmenting factors is compared to empiric models.

3. Models and methods

3.1. CFD modelling of the HPH valve

The previous CFD studies of HPH valve turbulence all use various RANS k–ε models (see an overview in Håkansson et al., 2012). The traditional RANS k–ε models do not give information on the distribution of turbulent kinetic energy over different length-scales. This is a clear disadvantage of the method since the distribution of turbulent kinetic energy on different length-scales is decisive for its effect in fragmentation, c.f. Eqs. (3) and (4).

An alternative to using the RANS approach would be CFD simulations using either Direct Numerical Simulation (DNS) or Large Eddy Simulation (LES) where turbulence is either completely resolved (DNS) or resolved for eddies of large length-scales (LES). DNS on high Reynolds number flows (Re $\approx$ 30 000 in the