Chemical Engineering Science 117 (2014) 376–388

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

Population balances combined with Computational Fluid Dynamics: A modeling approach for dispersive mixing in a high pressure homogenizer

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HIGHLIGHTS

- The pressure drop and the number of passes were examined in a homogenizer.
- Population balances combined with CFD were used to model the droplet sizes.
- Four compartments were defined around the high speed jet.
- One set of parameters was found covering all hydrodynamic conditions.
- The model predictions have improved by 65% compared to a single compartment model.

ARTICLE INFO

Article history:
Received 7 April 2014
Received in revised form
26 June 2014
Accepted 30 June 2014
Available online 8 July 2014

Keywords:
Emulsification
High pressure homogenizer
Population balance equations
Computational Fluid Dynamics
Turbulence

ABSTRACT

High pressure homogenization is at the heart of many emulsification processes in the food, personal care and pharmaceutical industry. The droplet size distribution is an important property for product quality and is aimed to be controlled in the process. Therefore a population balance model was built in order to predict the droplet size distribution subject to various hydrodynamic conditions found in a high pressure homogenizer. The hydrodynamics were simulated using Computational Fluid Dynamics and the turbulence was modeled with a RANS k–ε model. The high energy zone in the high pressure homogenizer was divided into four compartments. The compartments had to be small enough to secure nearly homogeneous turbulent dissipation rates but large enough to hold a population of droplets. A population balance equation describing breakage and coalescence of oil droplets in turbulent flow was solved for every compartment. One set of parameters was found which could describe the development of the droplet size distribution in the high pressure homogenizer with varying pressure drop. An improvement of 65% was found compared to the same model containing just one compartment. The compartment approach may provide an alternative to direct coupling of CFD and population balances.

1. Introduction

Many emulsified consumer products contain micron or even submicron sized droplets, for example mayonnaise, cream liquors, margarine and lotions. The droplet size is important for many product properties like appearance, stability (McClements and Chanamai, 2002), rheology (Luckham and Michael, 1999; Scheffold et al., 2013) and controlled release of substances (McClements and Yan, 2010). It is therefore of interest to control the droplet size during the production process. A typical production process consists of two steps: in the first step oil and water phases are mixed, possibly with other ingredients, forming a coarse emulsion; then, in the second step the droplet size of the dispersed phase is further reduced to a desired value. High pressure homogenization valves are often applied in the second step where they are able to generate submicron droplet sizes (Karbstein and Schubert, 1995; Schultz et al., 2004). A high pressure homogenizer consists of a pump and a homogenizing nozzle (Schuchmann and Schubert, 2001). The coarse emulsion is entering from the bottom along the main axis. The emulsion hits a solid impact head and spreads out through the narrow gap in the radial direction (Fig. 1). This type of homogenizing valve is

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http://dx.doi.org/10.1016/j.ces.2014.06.047
0009-2509/

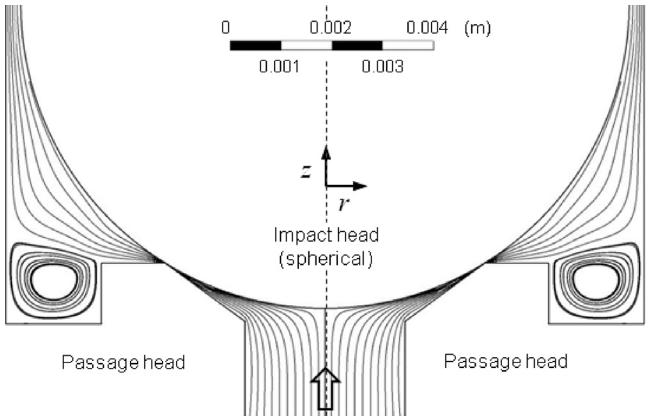

Fig. 1. The geometry of the high pressure homogenzier.

commonly referred to as a radial diffuser (Phipps, 1975; Schultz et al., 2004).

Although high pressure homogenizers are already utilized in industry for over a century, they remain a topic for scientific study. In the last decade, many researchers have tried to simulate the emulsification process inside the homogenizer valve, each using a different approach. For example, population balance equations (PBE) were developed to track the change of the droplet size distribution inside a homogenizer (Håkansson et al., 2009; Maindarkar et al., 2012; Raikar et al., 2009, 2010, 2011). The PBE models described the breakage and coalescence of droplets and the adsorption of emulsifier molecules (Håkansson et al., 2013b; Maindarkar et al., 2013). The advantage of using this approach is that the complete droplet size distribution could be retained. One drawback is that often 4–6 parameters are necessary to obtain a proper fit of the experimental data. These approaches are mainly based on the average energy dissipation over the valve. This means that no homogenizer geometry characteristics could be included and the fit parameters are equipment dependent and even pressure dependent for the same equipment (Maindarkar et al., 2012; Raikar et al., 2011). To allow predictions of the droplet size distribution it is necessary to have a single set of parameters describing the change in the droplet size distribution experiencing different pressures for one type of equipment and even for various geometries this would be desirable.

Improvements can be made when more hydrodynamic features are incorporated. This could be achieved with tools like Computational Fluid Dynamics (CFD), where locally, inside the apparatus, shear rates and turbulent energy dissipation rates can be calculated. Many studies have focused on the flow patterns inside high pressure homogenizers, and predicted average stable droplet sizes from CFD-simulations (Casoli et al., 2010; Floury et al., 2004a, 2004b; Steiner et al., 2006). Some laboratories compared the CFD simulations with Particle Image Velocimetry (PIV) measurements (Blonski et al., 2007; Håkansson et al., 2013a; Innings and Trägårdh, 2007). It remains practically impossible to measure the velocity field inside real homogenizers because of the tiny geometry and high velocities. Therefore scaled model homogenizers were fabricated (Blonski et al., 2007; Innings and Trägårdh, 2007). The main conclusions from comparing simulations to measurements of the scaled homogenizer were that the Reynolds Averaged Navier Stokes (RANS) k–ε models are able to describe the flow in the turbulent region qualitatively (Håkansson et al., 2012).

Solving PBEs and CFD simulations take up a lot of computing power. Integration of the two techniques requires even more computing power. Advancing towards more detailed modeling of emulsification processes has resulted in a number of publications focusing on the coupling between the two techniques (Agterof et al., 2003; Becker et al., 2013; Drumm et al., 2009; Fathi Roudsari et al., 2012). To limit the calculation times, the moments of the particle size distribution were linked to CFD simulations for droplet size predictions (Agterof et al., 2003). The Direct Quadrature Method of Moments (DQMOM) solution of the population balance equation was implemented in CFD codes without increasing the computational costs too much (Drumm et al., 2009; Silva et al., 2008). Current versions of Fluent ANSYS are now equipped with DQMOM and QMOM and up to eight moments of the particle size distribution can be calculated. Algorithms have been developed to reconstruct any particle size distribution based on a finite number of moments (de Souza et al., 2010; John et al., 2007). Using these advanced algorithms in combination with CFD-QMOM could allow us to model the droplet size distribution for different hydrodynamic conditions. The accuracy of such an approach is yet to be investigated and the computational effort is expected to be high. Also, fully discretized PBEs coupled to CFD have been reported for emulsification systems (Becker et al., 2013; Fathi Roudsari et al., 2012). Fathi Roudsari et al. (2012) have been looking at the cumulative droplet size distribution for different hydrodynamic conditions in a stirred tank, i.e. the impeller speed was varied. Becker et al. (2013) have looked into a coupled PBE-CFD modeling framework for a high pressure homogenizer which runs only at a constant pressure drop. For systems where the geometry is confined to a space comparable to the droplet size it is physically not realistic to solve a balance for the whole population of droplets. Then one has to define compartments which are physically large enough to contain a population of droplets but small enough to ensure a low variation in the turbulent energy dissipation. This approach has been used in the past for stirred tanks, where the tank has been divided up into two (Alexopoulos et al., 2002; Almeida-Rivera and Bongers, 2010) or 11 (Alopaeus et al., 1999) zones based on the distribution of energy dissipation rates. The compartment approach has not yet been encountered in the literature for emulsification in high pressure homogenization valves under varying hydrodynamic conditions.

The aim of the work described in this paper was to construct a compartment model of a high pressure homogenizer, which enables predictions of droplet size distributions without the need to fit all the experiments separately. The experiments were performed with varying hydrodynamic conditions. The hydrodynamic conditions in the valve changed when the pressure drop was varied. To be predictive, the model should work outside the experimentally verified ranges. Therefore one set of parameters is needed to describe the evolution of the droplet size distribution over the whole pressure range of the apparatus. To accomplish this, a population balance model was built describing breakage and coalescence of oil droplets in an aqueous dispersion. A lot of models have been suggested in the past to describe the breakage and coalescence of droplets and bubbles; see for example the review papers of Liao and Lucas (2009, 2010). There are models available which do not include experimentally tunable parameters. The breakage rate model from Luo and Svendsen (1996) has been tested for a radial diffuser type homogenizer, these results were not satisfying (see Becker et al., 2013). Instead the breakage and coalescence functions from Coulaloglou and Tavlarides (1977) were used. They form the backbone of most breakage and coalescence models for turbulent flow (Liao and Lucas, 2009, 2010). The free parameters in the breakage and coalescence functions were optimized so that the modeled size distributions matched the experimentally obtained droplet size distributions. The experiments were carried out by changing the pressure drop for a single emulsion formulation. Four different compartments were defined inside the device to account for the large turbulent inhomogeneities. The compartments sizes were based on the jet length. The jet length was approximated with an algebraic model based on a free shear flow assumption, see Section 3. The average energy dissipation rates in the compartments were