Chemical Engineering Science 64 (2009) 501 – 508

Contents lists available at ScienceDirect

Chemical Engineering Science

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

Analysis of breakage kernels for population balance modelling

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ARTICLE INFO

Article history:
Received 14 April 2008
Received in revised form 24 September 2008
Accepted 27 September 2008
Available online 17 October 2008

Keywords:
Population balance
Breakage kernel
Least squares method

ABSTRACT

The accurate prediction of droplet sizes is fundamental in many industrial applications. In order to be able to simulate the evolution of a size distribution, suitable kernels should be used in the population balance. In this paper we make use of four different breakage kernels in order to predict a size distribution and compare the results among them as well as with experimental data. Two breakage kernels are derived from inverse problems and the other two are derived from physical or empirical interpretations.
The Sauter mean diameter, a moments-based error and Gaussian shape factors were used to compare between the resulting distributions.

1. Introduction

The production of oil and gas plays a major role in the economy of many countries. Since the presence of a dispersed phase in multiflow separators, transport pipings, rotating equipment or down steam separation processes can provoke break down or create erosion or degradation, a close to 100% phase separation is of major concern. The physics of this separation process involves different phenomena such as entrainment, deposition, coalescence and breakage of the disperse phase resulting in complex polydisperse multiphase systems.

The dispersed phase can be described statistically in terms of the governing phenomena controlling the size distribution evolution regardless of whether it consists of droplets in a gas, bubbles in a liquid or other similar systems.

The complexity in the processes and phenomena governing the changes of such systems makes the derivation of the corresponding models a significant challenge. For that reason, practical approaches often end up in using semi-empirical correlations which are problem and system specific. As an example of this, Ueda (1979) approximated the size distribution of droplets in the core of a pipe dispersed flow with a gamma distribution function, and then proposed empirical equations for the mean diameter to find the flow rate of the entrained droplets. On the other hand, Lucas et al. (2001) presented a study on bubble size distribution, in which simple models for breakage and coalescence were used.

When enough experimental information is available, an inverse problem technique could present one alternative to improve the existing models as well as to derive new ones. The population balance approach is found suitable in this type of problems since it allows us to describe a dispersed phase by means of a density function. The accurate prediction of the evolution of the density function relies on the adequate modelling for the initial condition and the physical model used for describing the interactions between the particles.

In the present article we focus only on breakage-dominant flows. The breakage process can be described in terms of a breakage rate function ($b(\xi,t)$) and a redistribution function ($h(\zeta \rightarrow \xi)$). The breakage rate gives the frequency for the splitting of particles to occur and the redistribution function describes the outcome of a split as particles with property ξ produced in the breakage of particles with internal coordinate ζ.

Despite the fact that significant modelling work has been carried out during the last decades, the capability of most of the derived models is limited to particular given cases (Dorao et al., 2007; Maaß et al., 2007; Hinze, 1955; Kolmogorov, 1949). The adaptation of a model to new cases will then demand its re-tuning usually leading to the need for a completely new model. In this respect, one of the simplest approaches is to apply an inverse problem analysis to the data. A self-similarity approach to solve an inverse problem is shown in the book by Ramkrishna (2000), and the use of the least squares method on inverse population balance problems can be found in Patruno et al. (2008).

The main goal of this work is to show the evolution of a density function predicted with different breakage kernels and to compare the modelling results with experimental data. Four intrinsically different breakage kernels are tested and the results are compared by the shape of the size distribution and the mean diameter.

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doi:10.1016/j.ces.2008.09.029

Section 2 introduces the population balance equation (PBE) in its breakage-dominant formulation and describes the breakage and redistribution models used in this work. Section 3 briefly describes the least squares method (LSM) used to solve the PBEs. Section 4 presents the results for the comparisons and finally Section 5 sums up the main conclusions drawn from this work.

2. The PBE

Given a two phase system, we can consider it as homogeneous at a certain level if enough stirring is provided. The system can then be described only as two dimensional, taking one dimension in time and another one in the internal property of the dispersed phase. The property can be assumed to be represented by a continuous density function $f(\xi,t)$ with ξ being any property characterizing the dispersed phase (e.g. droplet diameter, volume, mass, etc.) and t the time coordinate. A detailed discussion of the population balance in general can be found in Jakobsen et al. (2005). For this particular work we choose ξ to represent the droplet diameter.

2.1. Breakage-dominant formulation

Considering only the breakage process and the redistribution of daughter droplets, the mathematical description of the problem is

$$\begin{cases} \dfrac{\partial f(\xi,t)}{\partial t} = -b(\xi,t)f(\xi,t) + \int_{\zeta=\xi}^{\zeta=\xi_{\max}} h(\zeta\to\xi)b(\zeta,t)f(\zeta,t)\,\mathrm{d}\zeta + g(\xi,t) & \text{in } \Omega=[\xi_{\min},\xi_{\max}]\times[0,t_{\max}] \\ f(\xi,t)=f_0(\xi) & \text{on } \Gamma_0=\Omega(t=0) \end{cases} \quad (1)$$

with $b(\xi,t)$ being the breakage kernel, $h(\zeta\to\xi)$ the redistribution probability, $g(\xi,t)$ the source (or sink) term which can include entrainment (or deposition) and $f_0(\xi)$ the initial droplet distribution.

The first term in Eq. (1) on the right-hand side represents the change in the population due to the loss of individuals by the breakage processes, where $b(\xi,t)$ is the *breakage rate* of the droplets of type ξ. The second term on the right-hand side gives the change in the population due to the arrival of new individuals with property ξ. In the case of a breakage process, the breakage of particles of type ζ will produce new particles according to the *breakage yield or redistribution probability*, $h(\zeta\to\xi)$. The third term is the droplets source (entrainment) or sink (deposition).

To simplify the notation, we can define $\mathscr{L}$ as the population balance operator such that

$$\mathscr{L}f(\xi,t) \equiv \frac{\partial f(\xi,t)}{\partial t} + b(\xi,t)f(\xi,t) - \int_{\zeta=\xi}^{\zeta=\xi_{\max}} h(\zeta\to\xi)b(\zeta,t)f(\zeta,t)\,\mathrm{d}\zeta \quad (2)$$

Then the mathematical problem is simplified to

$$\begin{cases} \mathscr{L}f(\xi,t)=g(\xi,t) & \text{in } \Omega=[\xi_{\min},\xi_{\max}]\times[0,t_{\max}] \\ \mathscr{B}_0 f(\xi,t)=f_0(\xi) & \text{on } \Gamma_0=\Omega(t=0) \end{cases} \quad (3)$$

with $\mathscr{B}_0$ being the identity operator. Since we are considering a closed system (without any source or sink term) we take $g=0$.

It is also possible to define the moments of the distribution, being the nth moment operator defined as

$$\mathscr{M}^n f(\xi,t) \equiv \int_{\xi'=\xi_{\min}}^{\xi'=\xi} \xi^n f(\xi',t)\,\mathrm{d}\xi' \quad (4)$$

2.2. Models for the breakage kernel

Many attempts to model the breakage kernel have been made over the last years. Martínez-Bazán et al. (2002) give a meticulous review of available models for particle breakup. It is important to distinguish between kernels derived from physical models which can reproduce the evolution of a particular system's probability density function (PDF) (such is the case of Coulaloglou and Tavlarides, 1977; Martínez-Bazán et al., 1999 or Luo and Svendsen, 1996), and those derived from inverse problems (e.g. Sathyagal and Ramkrishna, 1996 or Patruno et al., 2008) which will simulate adequately the evolution of a system only under the same physical properties and operating conditions from which it was derived.

This work does not deal with Luo and Svendsen (1996) breakage kernel because it can only be used in the moment formulation of the PBE, and not in its particle size distribution form. A detailed description of the two forms of writing the PBE is given in Jakobsen (2008).

Even though the formalism shown in earlier literature for the PBE can describe systems with time-dependent breakage, in the majority of the breakage models already present in the literature we found that the breakage kernel does not depend explicitly on the time variable. Hence $b(\xi,t)=b(\xi)$, although $b(\xi)$ might depend on t through a coupling with the hydrodynamic variables.

2.2.1. Coulaloglou and Tavlarides model

Coulaloglou and Tavlarides (1977) defined the breakage frequency as the fraction of particles breaking divided by a characteristic time, mathematically

$$b(\xi) = \left(\frac{1}{\text{breakage time}}\right)\left(\begin{matrix}\text{fraction of}\\ \text{droplets breaking}\end{matrix}\right) = \frac{1}{t_b}\frac{\Delta F(\xi)}{F(\xi)} \quad (5)$$

the fraction of droplets breaking was modelled as

$$\frac{\Delta F(\xi)}{F(\xi)} = \exp\left(-\frac{E_c}{\overline{E}}\right) \quad (6)$$

with $E_c=c_1\sigma\xi^2$ being the surface energy and $\overline{E}=c_2\rho\varepsilon^{2/3}\xi^{11/3}$ the mean turbulent kinetic energy. They also assumed that the breakage time was given by a turbulent turnover time

$$t_b \propto \xi^{2/3}\varepsilon^{-1/3} \quad (7)$$

Combining Eqs. (5)–(7), they obtained the following expression

$$b\,(\xi) = \frac{k_1}{\xi^{2/3}}\exp\left(-\frac{k_2}{\xi^{5/3}}\right) \quad (8)$$

in which k_1 and k_2 are empirical constants. Given these parameters are known, this breakage kernel can be used to model the evolution of a dispersed phase. In this paper we tuned the values of k_1 and k_2 in such a way that the difference between experimental data and simulations was minimized.

2.2.2. Martínez-Bazán model

Martínez-Bazán et al. (1999) proposed a breakage model for bubbles based on kinematic ideas (energy balance). The basic idea is that for a droplet to be split, the turbulent stresses should overcome the deformation energy to modify the surface. If viscous forces are neglected, the confinement stress is defined as

$$\tau_s = \frac{E_c}{\text{Volume}} = \frac{6E_c}{\pi\xi^3} = 6\frac{\sigma}{\xi} \quad (9)$$