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Discrete bubble modeling for a micro-structured bubble column

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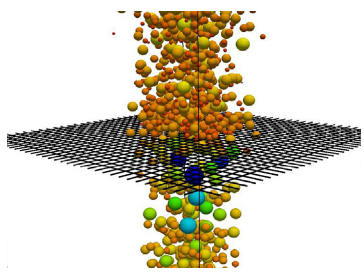
HIGHLIGHTS

- A discrete bubble model is used to model a micro-structured bubble column.
- Wires present in the column cut the bubbles into smaller ones.
- Compartmentalized liquid flow indicates possibility of plug flow kind of behavior.
- Reduced mesh opening leads to reduced bubble size.

GRAPHICAL ABSTRACT



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ABSTRACT

Gas–liquid flows with solid catalyst particles are encountered in many applications in the chemical, petrochemical, pharmaceutical industries, etc. Most commonly, two reactor types are applied for large scale in the industry. They are slurry bubble column and trickle bed reactors. Both of these types of reactors have some disadvantages limiting their efficiencies. To overcome these disadvantages, a novel reactor type, micro-structured bubble column (MSBC), is proposed. In the MSBC, the micro-structuring of catalytic material is realized by introducing a static mesh of thin wires coated with catalyst inside the column. Wires also serve the purpose of cutting the bubbles, which in turn results in high interfacial area and enhanced interface dynamics. The static catalytic mesh also ensures lower cost by avoiding filtration of catalyst particles. Numerical formulation of the described reactor is based on the 3-D discrete bubble model (DBM) presented in the previous works of Darmana et al. (2005, 2007). The extended version of DBM presented here introduces wires in the existing model and studies their effect on liquid and bubble dynamics. Bubbles and wires are represented by spherical and cylindrical markers, respectively; and the liquid flow-field is solved in the Eulerian gird cells. An improved drag correlation for bubbles in dense (up to 50%) swarm flow is also incorporated in the model. The model implementation and results are verified for a wide spectrum of parameters from the data available from the previous studies, analytical results and experimental findings. Our results show that the model is able to predict the hydrodynamic behavior and bubble dynamics, including the cutting of bubbles through wire mesh, very well.

1. Introduction

Many processes in the chemical, petrochemical and/or biological industries involve three phase gas–liquid–solid flows. Usually the solid material acts as a catalyst, whereas the gas phase supplies the reactants for the (bio)chemical transformations and the liquid phase carries the product. Example processes are hydrogenations, oxygenations and Fischer–Tropsch synthesis. In these processes, the performance of the reactor is mostly constrained by the interfacial mass transfer rate and the achievable in situ heat removal rate. To improve upon these drawbacks, a novel reactor type is proposed

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here. It is computationally investigated here with a model based on first principles, in a Eulerian–Lagrangian framework. This new reactor type comprises a micro-structured bubble column (MSBC).

In this reactor, micro-structuring of the catalytic material is realized by the introduction of a static mesh of thin wires (coated with catalyst material) placed inside the bubble column. The wire mesh serves a number of purposes including cutting bubbles into smaller pieces (resulting in high interfacial area), enhancing interface dynamics (increasing mass transfer coefficient), avoiding filtration of catalyst particles (lowering costs). Cooling pipes can also be introduced so as to facilitate the heat removal process.

Since the past few decades, efforts have been made to understand and demonstrate the working of bubble columns through various empirical correlations, theoretical models and computational fluid dynamics (CFD) modeling. Extensive review of such studies is presented in Shah et al. (1982) and Deen et al. (2010). Various modifications in bubble columns have been proposed from time to time, often equipped with sieve trays, structured packing or vertical shafts, in combination with static mixers. All these modifications are suggested to reduce gas/liquid backmixing and achieve uniform bubble distribution. Chen and Yang (1989) have studied the characteristics of a mubrous catalyst material (Höller et al., 2000, 2001b; Kiwi-Minsker et al., 2004). These studies provide design and modeling information for multistaged bubble columns, with and without reaction. Höller et al. (2000) studied the hydrodynamics in a non-reactive system by considering the effect of superficial gas velocity on various flow regimes. In a later study, the observed mass transfer coefficient was reported 10 times higher than that of a column without stages (Höller et al., 2001a). The proposed MSBC reactor resembles these staged columns and hence it can be inferred that gas redistribution and high mass transfer can be obtained in it.

Measurement of bubble size distribution (BSD) is of paramount importance to quantify the column performance. Various techniques have been used to measure BSD, including wire mesh sensors. Therefore, intrusive effect of wires on bubbles has been investigated by several authors. Prasser et al. (2001, 2005) demonstrated the cutting of a single large bubble through wire mesh sensors by using high speed imaging and stated that slugs tend to distort as they pass through the wires. Ito et al. (2011) also concluded the effect of the wires on bubble dynamics in column. So, it can be concluded that the study of the effect of wires on bubble dynamics is important while modeling the MSBC reactor.

A 3-D Discrete Bubble model (DBM) or Euler–Lagrange model is used in this study. It adopts a continuum description for the liquid phase, and tracks each individual bubble using Newtonian equations off motion following Darmana et al. (2005, 2007). Use of bubble coalescence model (Darmana et al., 2006) and bubble breakup model (Lau et al., 2010) have been validated in the previous studies. Modifications have been made here to include the additional drag induced on liquid and cutting of bigger bubbles due to the presence of wires.

The outline of this paper is as follows: first a description of the model is given. Subsequently, numerical implementation and specific modifications in the DBM are detailed. Subsequently, the verification and validation of the method is presented, followed by discussion and conclusions.

2. Governing equations

The simulation model used here is an extension of the discrete bubble model (DBM), which is based on the Euler–Lagrange approach. It adopts a continuum description of the liquid phase and a Lagrangian description for the bubbles. The effect of wires (i.e. fluid–structure interaction) is also incorporated using a source term in the fluid phase momentum equation. This allows for a direct consideration of additional effects related to bubble–bubble, bubble–wire, wire–liquid and bubble–liquid interactions. The hydrodynamic model can be extended for bubble breakup with the model of Lau et al. (2010), though this has not been considered in the current study. A new bubble cutting algorithm is proposed and its implementation in the model has been described as well.

2.1. Liquid phase hydrodynamics

The liquid phase is described by the volume-averaged Navier–Stokes equation consisting of the continuity and momentum equations. The presence of bubbles and wires is reflected by the liquid phase volume fraction ε_l, the source term that accounts for the inter-phase mass transfer $\dot{M}$, and inter-phase momentum transfer $\mathbf{\Phi}$:

$$\frac{\partial(\varepsilon_l \rho_l)}{\partial t} + (\nabla \cdot \varepsilon_l \rho_l \mathbf{u}) = (\dot{M}_{b\to l} - \dot{M}_{l\to b}) \tag{1}$$

$$\frac{\partial(\varepsilon_l \rho_l \mathbf{u})}{\partial t} + (\nabla \cdot \varepsilon_l \rho_l \mathbf{uu}) = -\varepsilon_l \nabla p - (\nabla \cdot \varepsilon_l \tau_l) + \varepsilon_l \rho_l \mathbf{g} - \mathbf{\Phi}_{l\to b} - \mathbf{\Phi}_{l\to w} \tag{2}$$

where $\mathbf{g}$ is the gravity constant, ρ_l, u and p, respectively, are the density, velocity and pressure for the liquid phase. All three phases are assumed to be incompressible, which is a reasonable assumption considering the limited height of the simulated systems. It is to be noted here that in the absence of mass transfer, $\dot{M}$ is zero. $\mathbf{\Phi}_{l\to b}$ and $\mathbf{\Phi}_{l\to w}$ represent the momentum transfer from liquid phase to bubbles and wires, respectively. The subgrid-scale model of Vreman (2004) is employed for the turbulence modeling.

2.2. Bubble dynamics

2.2.1. Bubble tracking

The motion for each individual bubble is computed from Newton's second law while accounting for bubble–bubble and bubble–wall interactions via an encounter model of Hoomans et al. (1996). The liquid phase contributions are taken into account via the inter-phase mass transfer rate $\dot{m}$ and the net force experienced by each individual bubble. For an incompressible bubble, the equations can be written as

$$\rho_b \frac{d(V_b)}{dt} = (\dot{m}_{l\to b} - \dot{m}_{b\to l}) \tag{3}$$

$$\rho_b V_b \frac{d(\mathbf{v})}{dt} = \mathbf{F}_G + \mathbf{F}_P + \mathbf{F}_D + \mathbf{F}_L + \mathbf{F}_{VM} + \mathbf{F}_W \tag{4}$$

where ρ, V_b, and $\mathbf{v}$, respectively are the density, volume and velocity of the bubble. The net force acting on each individual bubble is calculated by considering all the relevant forces. It is composed of separate, uncoupled contributions such as gravity, pressure, drag, lift, virtual mass and wall forces. Expressions for each of these forces can be found in Table 1. Detailed discussion about these forces can be found in Darmana et al. (2007). Note that the drag, lift and wall force closures used in the present study are obtained from Tomiyama et al. (1995, 2002). In recent studies by Roghair et al. (2011), a correction for the drag force to account for swarm effects has been proposed:

$$\frac{C_D}{C_{D,\infty}(1-\alpha)} = 1 + \left(\frac{18}{E\ddot{o}}\right)\alpha \tag{5}$$

where α is the gas fraction. The drag coefficient used for this closure does not take effects of contaminations into account (i.e. pure liquid). Therefore in this study, this correction closure of Roghair et al. is used with the single bubble drag coefficient ($C_{D,\infty}$) proposed by Tomiyama et al. for contaminated liquid. Also, the above closure being defined for two-phase systems needs to be