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# Investigation of gas dispersion characteristics in stirred tank and flotation cell using a corrected CFD-PBM quadrature-based moment method approach

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ABSTRACT

In this study, the population balance model (PBM) is coupled with computational fluid dynamics (CFD) to investigate the steady-state bubble size distribution in two types of process equipment namely, a standard Rushton turbine stirred tank reactor and a generic lab-scale flotation cell. The coupling is realized using Fluent 15.07 software, and the numerical model is validated for the stirred tank reactor. The population balance equation (PBE) is solved using the quadrature method of moments (QMOM) technique along with a correction procedure implemented to check and correct invalid moment sets. The breakage and coalescence of bubbles due to turbulence are considered. The breakage rate and daughter size distribution models proposed by Laakkonen et al. (2007) are considered. For modeling coalescence rate, models proposed by Coulaloglou and Tavlarides (1977) are considered. The interaction between the phases is handled by considering the drag model proposed by Lane et al. (2005) while ignoring the other interphase forces. The correction algorithm has been successfully implemented, and improved predictions of gas volume fraction and Sauter mean diameter (SMD, $d_{32}$) have been observed with a good match between the predictions and experimental measurements. The local SMD predictions are compared against predictions from the past studies and the superiority of the current approach for moderate gassing rates is established. The CFD-PBM approach is then used to study and characterize different flow regimes occurring in a generic mechanical flotation cell at different aeration rates and impeller rotation speeds. Also, power numbers are calculated from torque data and are found to drop considerably with an increase in aeration rate and impeller rotation speed as the flow regime approaches recirculating flow. The predicted SMD for flotation cell indicates that smaller bubbles are concentrated near the high turbulence impeller stream, the lower recirculation region, and close to the tank walls. On the other hand, large bubbles are formed in the upper tank region and are concentrated around the shaft during the flooding, loading, and transition flow regimes. In the future, the corrected QMOM approach will be further extended by implementing kinetic models capable of predicting the flotation rate constant using local bubble size information obtained from CFD-PBM simulations.



## 1. Introduction

Multiphase flows in flotation cells are highly turbulent and polydisperse in nature (Evans et al., 2008; Karimi et al., 2014a; Lane et al., 2005; Schwarz et al., 2016). The presence of all the three phases, namely the continuous phase (water) and the two dispersed phases (air bubbles and solid particles), and their complex interactions make studying the flotation process a challenging task (Koh et al., 2009; Koh and Schwarz, 2006, 2008; Schwarz et al., 2016). Furthermore, the presence of many chemical reagents and their tendency to adsorb on the surface of dispersed phases (bubbles and particles) severely alters the behavior and dynamics of the dispersed phases in comparison to pure systems (Karimi et al., 2014a; Miskovic, 2011; Schwarz et al., 2016). Information about the local bubble size distribution (BSD) is necessary to facilitate an accurate prediction of the flotation rate constant and valuables recovery (Koh and Schwarz, 2007, 2008; Miskovic, 2011). Recent comprehensive experimental investigation of gas dispersion behavior and properties of various flotation cells have shown that BSD can differ significantly in different regions of the cell (Miskovic, 2011). Similar observations have been made by other researchers in both lab and pilot scale flotation cells (Grau and

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Heiskanen, 2003, 2005; Koh and Schwarz, 2008). Smaller bubbles are found in the region of high turbulence close to the impeller while larger bubbles, generated due to bubble coalescence and incomplete gas dispersion, are concentrated in the bulk region above the impeller.

The number of numerical studies focusing on fluid flow modeling and simulation in different type of process equipment have increased in recent years owing to the availability of improved models and inexpensive computational resources (Evans et al., 2008; Laakkonen et al., 2007; Lane et al., 2005; Petitti et al., 2013; Schwarz et al., 2016). The computational fluid dynamics (CFD) simulations have been used in the past to study single-phase and multiphase flow behavior in stirred tanks and flotation cells (Basavarajappa et al., 2015; Karimi et al., 2014b; Koh et al., 2003; Szczygieł et al., 2013). Table 1 gives a summary of the relevant gas-liquid CFD simulation work conducted in stirred tanks and mechanical flotation cells published over the last 15 years. In more recent papers, models describing specific flotation sub-processes have been implemented in two-phase CFD model to facilitate the prediction of flotation rate constant (Karimi et al., 2014a,b; Koh and Schwarz, 2003, 2006; Koh and Smith, 2011; Schwarz et al., 2016). However, in majority of the mentioned studies, a single bubble size or a single scalar equation solving the bubble number density is considered to simplify the calculations and make the computational time tractable (Alopaeus et al., 1999; Karimi et al., 2014a; Koh and Schwarz, 2006). For instance, (Evans et al., 2008) investigated mixing and gas dispersion behaviors in flotation cells where the authors used a single bubble number density equation to predict BSD in the cell, which was not validated experimentally. These simplifications can lead to inaccurate predictions of flow phenomena (Buffo et al., 2012; Petitti et al., 2010, 2013) and implementation of wrong fitting constants in flotation kinetic models (Koh and Schwarz, 2008). More recently, the population balance model (PBM) has been successfully coupled with CFD to obtain reasonably accurate bubble sizes in process equipment such as stirred tanks (Buffo et al., 2012; Laakkonen et al., 2007; Petitti et al., 2010). The application of the CFD-PBM approach to simulate bubble size distribution in a flotation cell was demonstrated for the first time by Koh and Schwarz (2008). Experimental validation of the numerical solution was not offered in this work, but the authors conclude that the bubble size distribution has a significant effect on the predicted flotation rate constant; higher flotation rate constant values are observed when a full bubble size distribution range is considered compared to the assumption of mono-sized bubbles.

The population balance equation (PBE) is an integro-partial differential equation describing the evolution of some selected property of the dispersed phase, such as size or composition (Petitti et al., 2010; Ramkrisha, 2000). The solution of the continuous form of PBE is possible only for a few simple cases (Laakkonen et al., 2007; McGraw, 1997; Petitti et al., 2010; Ramkrisha, 2000). A large number of numerical techniques have been proposed over the past two decades, many of which have found wide acceptance for the multiphase flow applications (Buffo et al., 2012; Kerdouss et al., 2006; Laakkonen et al., 2007; Petitti et al., 2010). Of the many proposed PBE numerical solution techniques, the techniques based on the method of classes (MC) and the method of moments (e.g. QMOM, DQMOM, CQMOM) techniques have been reported to be the most suitable for multiphase gas-liquid flows (Kerdouss et al., 2006; Koh and Schwarz, 2008; Laakkonen et al., 2007; Petitti et al., 2010; Selma et al., 2010).

In the MC technique, the BSD is discretized into a sufficient number of finite size classes or bins, and a transport equation is solved for each size class with the appropriate sink and source terms depending on the physics of the problem (Koh and Schwarz, 2008; Ramkrisha, 2000). In the QMOM technique, the PBE is transformed into a moment transport equation using the concept of mathematical moment for density function, where each moment represents a unique intrinsic property of a distribution (Marchisio et al., 2003; McGraw, 1997). (Gimbun et al., 2009; Petitti et al., 2010) reported that considering the first six moments is sufficient to obtain meaningful results and good predictions for flows dominated by both breakage and coalescence when using the QMOM approach for gas-liquid flows.

In chemical engineering, coupled CFD-PBM simulations have been carried out for various reactor types, such as bubble columns and stirred tank reactors, and a good match with experimental measurements have been reported in the literature (Laakkonen et al., 2007; Petitti et al., 2010; Selma et al., 2010; Wang and Wang, 2007). (Laakkonen et al., 2006, 2007) performed experimental measurement of BSD in stirred tanks using three different experimental techniques. The local BSD measurements were compared with the numerical solutions obtained using the coupled CFD-PBM approach based on the MC approach. The BSD and air holdup predictions using the CFD-PBM model was found to match the experimental measurements reasonably well based on the fitted parameters for breakage and coalescence kernels (Laakkonen et al., 2007). Recently, (Gimbun et al., 2009 and Petitti et al., 2010) studied gas-liquid flows in a stirred tank identical to the design used by Laakkonen et al. (2007) by coupling the CFD and QMOM techniques. Both the papers reported a good match between predictions and measurements of the Sauter mean diameter ($d_{32}$) and overall holdup. Though the MC approach is reported to provide an accurate description of BSD and is computationally robust, it is computationally intensive and usually requires a large number of size classes (~80) for accurate predictions (Selma et al., 2010). For instance, (Selma et al., 2010) compared the MC and direct quadrature method of moments (DQMOM) approaches and found the MC technique to be over ten times computationally expensive in comparison to the DQMOM. In the DQMOM approach, the values of weights and abscissas are obtained directly by solving the transport equations for weights and abscissas resulting from the Gaussian quadrature approximation (Marchisio and Fox, 2005). However, the DQMOM approach requires an unsteady solution of the governing equations and can suffer from moment corruption issues when coupled with CFD for complex flows such as stirred tanks (Buffo et al., 2012). Therefore, there is a great need for the development of an improved steady state numerical approach based on the QMOM approach, which, with the integration of a suitable moment correction step, could be used to solve industrially relevant problems accurately and in a tractable time frame, i.e. within a few days as opposed to weeks. A comprehensive review of the literature dealing with flotation modeling and gas-liquid flow in stirred tanks using radial impellers is compiled in Table 1. It is clear from the review of the recent literature that benefits of the QMOM and related methods (DQMOM and CQMOM), which have proven to be highly accurate for stirred tank flow at low gassing rates, could be further extended for multiphase flows in stirred tanks and flotation cells at moderately high gassing rates and holdup values (>3%).

One of the main advantages of the QMOM technique over the MC technique is the reduction in the number of equations that need to be solved to facilitate accurate prediction of the dispersed phase properties such as SMD and local holdup. However, the QMOM predictions are prone to error due to decoupling and independent advection of moments that can often give rise to a moment sequence not belonging to any physical distribution (Wright, 2007) – such a moment sequence is called an invalid or a corrupted moment sequence/set. This issue and many causes of the moment corruption have been explained in greater detail by Wright (2007) and McGraw (2012), and useful checks and solutions are proposed to remedy the problems occurring as a result