Simulation of Bubbly Flow and Mass Transfer in a Turbulent Gas-Liquid Stirred Tank with CFD-PBM solver in OpenFOAM: Study of Impeller Rotational Speed and Volumetric Mass Transfer Coefficient

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Abstract

In the present paper, the oxygen dispersion in a laboratory scale (3 litres) bioreactor is modelled using open source Computational Fluid Dynamic (CFD) package OpenFOAM (Open Source Operation and Manipulation). The combined effect of the bubble breakup and coalescence in the tank is accounted by a novel method of Population Balance Model (PBM) called Extended Quadrature Method of Moments (EQMOM). The three dimensional simulation is made within a Multiple Reference Frame (MRF), which is a well established method for the modelling of mixers. Dispersed gas and bubbles dynamics in the turbulent flow are modelled using Eulerian-Eulerian (E-E) approach with mixture k-ϵ turbulent model. A modified Tomiyama drag coefficient was used for the momentum exchange, as well. Parallel computing is employed to make efficient use of computational power to predict the spatial distribution of gas phase fraction, Sauter mean bubble diameter (d32), Number Density Function (NDF), oxygen mass fraction in water and flow structure. The numerical results are compared with experimental data, and good agreement is achieved. The result are discussed based on four impeller rotational speeds with different volumetric mass transfer coefficients. However, the discussion in extended abstract is limited to one case using one mass transfer coefficient.

1 INTRODUCTION

Modelling of the complex flow in a chemical or bioprocessing reactor in the presence of a rotating impeller, is a formidable computational challenge. The scientific and technical literature on the subject has rapidly evolved from single-phase rotating impeller systems (G. Holzinger [1]; G. Lane [2]) to population balance methods aiming at the prediction of the disperse phase bubble sizes (Kerdouss et al.[3, 4]; Lane et al. [5, 6]; Gimbun et al. [7]; G. Holzinger [1]). Gimbun et al. [7] applied a CFD mass transfer model to simulate gas-liquid stirred tanks agitated by Rushton impeller using Quadrature Method of Moments (QMOM) method. Their model was established for a high speed of impeller which leads to remove the convective and diffusion terms in mass transfer equation of oxygen. Hence, their comparison was based on overall two-phase mass transfer coefficient. Kerdouss et al. [4] reported the same approach but in different stirred tank reactor named "laboratory scale New Brunswick BioFlo " using Method of Classes (CM). These two studies confirm monodispersity of the bubbles is not a good choice in gas-liquid stirred tanks and Population Balance Model (PBM) gives better accuracy. The most used PBMs are CM (Kumar Krishna [8, 9]), QMOM (McGraw [10]), and Direct Quadrature Method of Moments (DQMOM)(D. Marchisio and R. Fox [11]). In spite of the fact that the CM is intuitive and accurate, it is computationally heavy due to a large number of required bins to discretize Number Density Function (NDF), properly. Additionally, this way requires a bubble size range to solve the Population Balance Equation (PBE). Compared to CM, QMOM can consider a broad range of bubble size with reduced number of equations. However, in some evaporation and combustion problems (Fox et al. [12]; Yuan et al. [13]) the value of the NDF is needed to be known for null internal coordinates, which is not the case if the QMOM method is used (E. Madadi-Kandjani and A. Passaloacqua [14]). Another most severe restrictions of QMOM is the implicit use of a discontinuous reconstructed NDF which is assumed to be the summation of Dirac delta functions. This limitation can be an obstacle through the simulation of combustion problems, as well as processes involving oxygen dissolution due to mass transfer. DQMOM solves the equations for weights and abscissae directly. Shortcomings related to the conservation of moments affect the DQMOM approach due to the fact that weights and abscissas are not conserved quantities (Yuan et al. [13]). To overcome these limitations, Yuan et al. [13] introduced an Extended Quadrature Method of Moments (EQMOM) which enables the shape of NDF to be reconstructed from a moment set using continuous kernel density functions instead of Dirac delta

functions. Additionally, E. Madadi-Kandjani and A. Passaloacqua [14] reported EQMOM procedures ensure the reconstructed NDF preserves all the moments used for its reconstruction. The formulation of EQMOM equations involves transport by convection and source/sink terms for the coalescence or breakup. In present work, we simulate gas-liquid flow and oxygen transfer from air to water in a laboratory scale (3 litres) New Brunswick bioreactor. The experimental set-up corresponds to the one used by Kerdouss et al. [4]. We employ CFD-PBM solver using EQMOM to reconstruct the bubble size distribution in water zone (liquid phase). In this study, EQMOM was for the first time implemented in the CFD code OpenFOAM to simulate coalescence and breakage of gas-liquid systems in stirred tanks. Moreover, we solved the equation of oxygen mass fraction by our CFD-PBM OpenFOAM solver to achieve the concentration distribution of oxygen as a dissolved component in water. The implementation and use of EQMOM with a log-normal NDF in a two phase CFD solver based on open source CFD code OpenFOAM and validation of dissolved oxygen evolution are the main novelties of this work.

2 Numerical model

The flow model is based on solving Navier-Stokes equations for The Eulerian-Eulerian (E-E) multiphase model along with mixture k-ϵ turbulent model [15]. Tomiyama drag coefficient has been selected in the model [16]. Other forces such as lift and added mass force have not been included in this paper. We applied the EQMOM method using log-normal kernel density function with two primary nodes and six secondary nodes which is implemented in the CFD program. The breakup model of Luo and Svendsen [17] and coalescence model of Hagesather et al. [18], were used in population balance library. Dissolved oxygen concentration equation is added to the system regarding mass concentration fraction. The saturation concentration fraction is calculated by Henry's law and four different volumetric mass transfer coefficients relied on four different theories (Frossling, Higbie, Penetration and Surface Renewal), were applied to model oxygen transfer between gas and liquid.

3 Tank specifications and numerical technique

The solution domain for experimental system investigated in this work, is shown in Fig. 1. The Salome and snappyHexMesh as open source tools are used as geometry and mesh generator, respectively. Figs.1.b-c show essential features of the 482'422 cells generated for the tank consisting of hexahedral, prisms, tetrahedral and polyhedral. The final mesh resolution is based on Kerdouss et al. [4] which allows us to consider 2-3 bubbles per each computational cell. The domain of tank is discretized by an unstructured finite volume method obtained using CFD-PBM OpenFOAM solver to convert the governing equations to algebraic equations that can be solved numerically. In this work, reactinhTwoPhaseEulerFoam solver of the Open source CFD code OpenFOAM-4.0 was added to simulate the gas-liquid dispersion. The solver was integrated and fully coupled with open-source implementation of Quadrature-Based Moment Methods (OpenQBMM) [19].

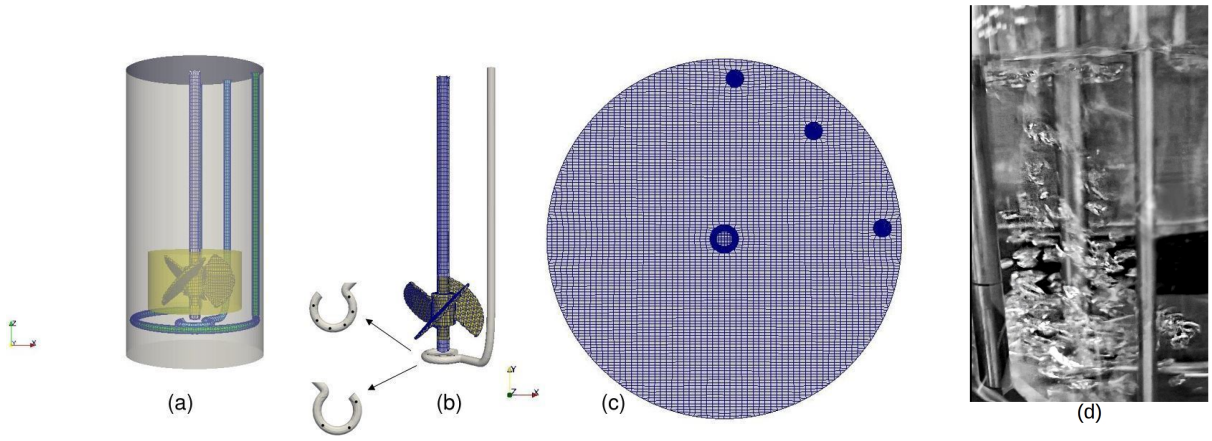

Figure 1: From left to right: (a) solution domain and MRF zone, (b) unstructured mesh in impeller and shaft with sparger location and (c) front view of unstructured mesh and (d) experimental image in the reactor for 50 rpm

4 Discussion and results

The result of 50 rpm using one volume mass transfer coefficient is selected to show in the current abstract. In the first case (50 rpm), the flooding behaviour has been observed in the experiment (Fig.1.d) and simulation (Fig.2.c) concerning gas phase fraction. This similarity verifies the CFD-PBM solver, qualitatively. For quantitative validation, the evolution of the dissolved oxygen concentration ([DO]) calculated using Danckwerts volumetric mass transfer coefficient (surface renewal theory) was tracked versus time and compared with experimental measurements. Fig.2.c shows predicted oxygen concentration profile is in good agreement with our experimental data.

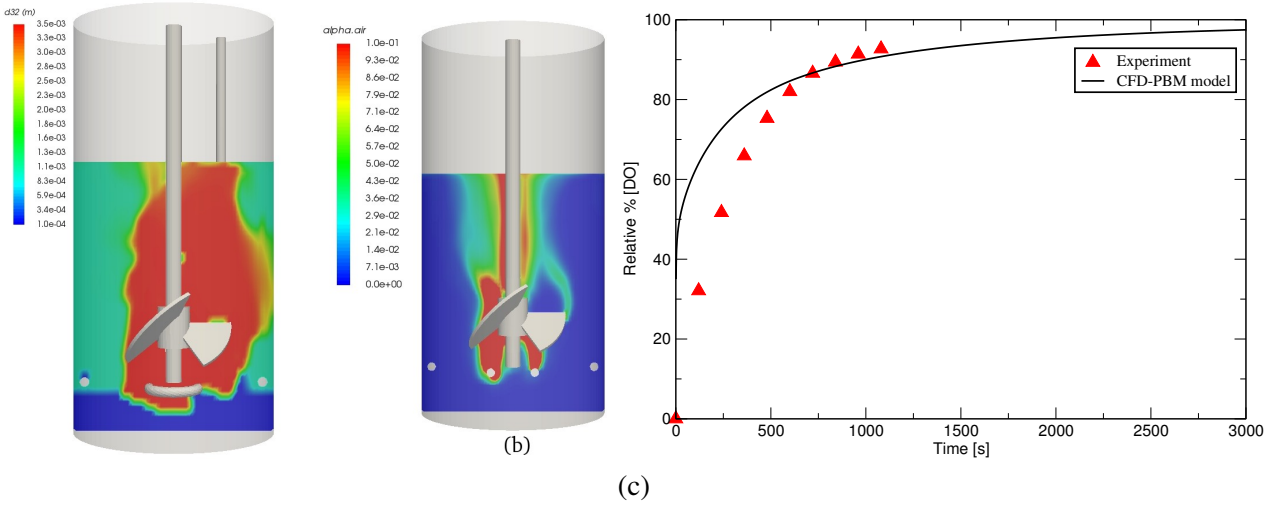

Figure 2: From left to right: (a) contour of Sauter mean diameter (b) contour of gas phase fraction and (c) Prediction of the evolution of the dissolved oxygen [DO]

The results obtained in Fig.2.a, local Sauter mean bubble diameter (d32) is reduced along the axial direction. When bubbles move upward and pass the impeller zone, the vortex caused by rotation of impeller affects the bubbles. The strong eddies decrease the bubble size in impeller region due to breakage event.

EQMOM is capable of reconstructing continuous NDF and provide more detailed information about dispersed phase and bubble particles. Fig. 3 indicates the shape of NDF in the liquid phase for a five- second period. The reason behind of using of PBM is to capture the physics of the problem accurately. Even from the size distribution, it can be observed that there are bubbles with different mean values. The mean bubble diameter nearly ranges from 0.1mm-4 mm and thus the monodispersity is not a good approximation.

5 Conclusion

In this work, E-E model coupled with EQMOM to simulate turbulent gas-liquid flow in a stirred tank reactor and concentration distribution of dissolved oxygen in the water. In the extended abstract, the lowest speed of impeller (50 rpm) was selected to discuss in which was operated under flooding regime condition. The comparison between CFD result and the experimental observations indicated the flooding regime is well-predicted by CFD-PBM solver in terms of gas phase fraction and dissolved oxygen evolution. The solver is able to extract the continuous bubble NDF for each arbitrary zone of the domain because of the capability of EQMOM approach in capturing the mean values along with the deviation from the mean. It is seen when gas bubbles pass impeller, their size is reduced.

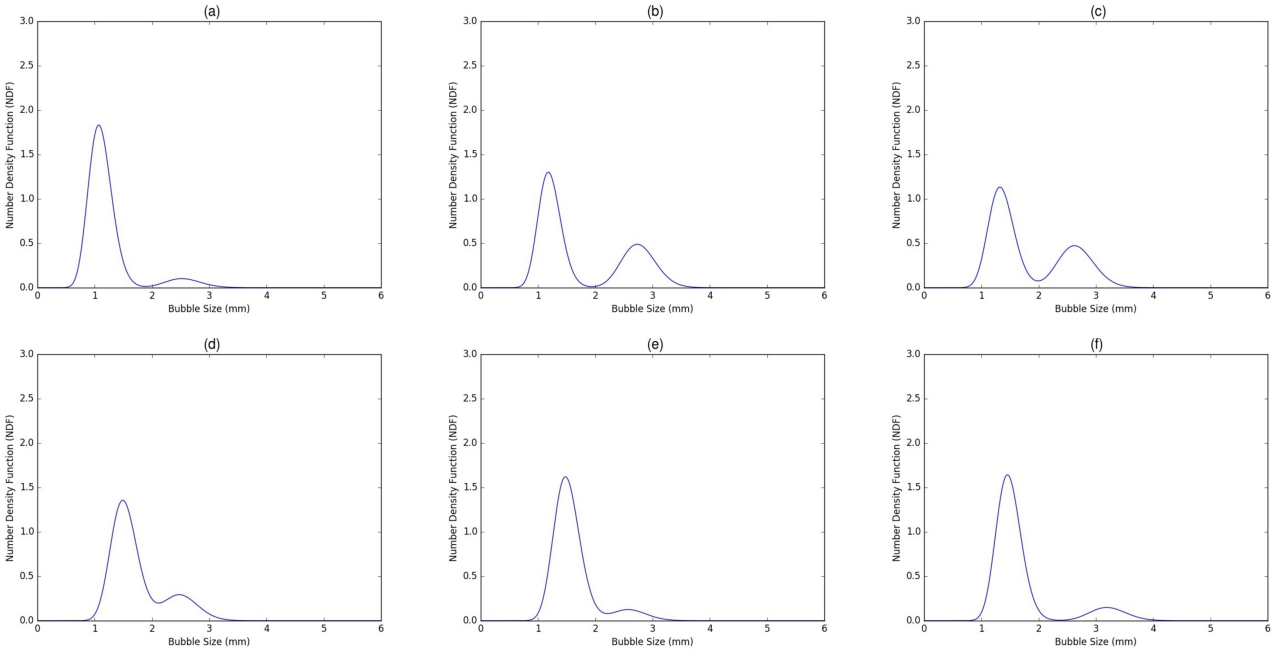

Figure 3: Number Density Function (NDF) in water at time= (a) 10s, (b) 11s, (c) 12s, (d) 13s, (e) 14s and (f) 15s

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