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CFD simulation of industrial bubble columns: Numerical challenges and model validation successes☆

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ABSTRACT

Although bubble columns are widely used in many industrial situations, there are very few studies of such devices operating at high superficial velocities. Numerical simulations using an Euler–Euler methodology are reported here across a wide range of operating conditions, where we discuss model assumptions and model validation. Key to obtaining physically correct results is the choice of closure assumptions. Particular emphasis is placed on the various solution methods that can be employed. In particular, we show that massive speed-up is possible using the new Eulerian multiphase NITA solver in ANSYS Fluent 16. Comparison of results from ANSYS CFX and ANSYS Fluent show that both do a good job of capturing the main features of the flow, the mixing time and the oxygen transfer rate.

1. Introduction

Bubble columns are widely used as gas–liquid contactors in the chemical and bioprocessing industries due to their good heat and mass transfer characteristics [1]. It is for this reason that we have embarked on a major project to understand industrial bubble columns used in the fermentation industry.

Despite their relatively simple structure, the hydrodynamics occurring inside bubble columns is very complex. Hence, the simulation of such processes using Computational Fluid Dynamics (CFD) presents a considerable challenge, particularly given that the model must be able to predict hold-up, oxygen transfer rate, mixing times and the impact of these factors on the kinetics of micro-organisms. Generally speaking the Euler–Euler framework is used to model such systems [2–4], hence selection of appropriate closure models to describe the transfer of momentum and turbulence between phases is a key challenge. Other issues in the development of such models include the need to adequately describe the fermentation media (containing a range of surface active compounds), the decision whether to use a single bubble size model or account for a distribution of sizes, and ensuring that the model is both robust and computationally efficient given the need to perform transient averaging over a relatively long period of time to obtain meaningful results.

Over the last four years, we have embarked on a major project to examine these issues, with the aim of developing a model of industrial-scale bubble column fermenters. In addition to the issues involved in such a modelling exercise, another challenge of central importance was the extension of the existing experimental database and models to high superficial velocities, for which the available literature is largely empirical [1,5,6]. By using a staged approach in which CFD simulations

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have been progressively validated using data from bench-top experiments [7–9] and a pilot-scale plant [10–15], we have made considerable progress.

Four mechanisms of inter-phase momentum transfer have been proposed in the literature, namely drag, lift, added mass and turbulent dispersion [3]. Of these four, drag is generally held to be the most significant, and there is extensive experimental data describing the drag coefficient for a single bubble in relatively pure liquids [16,17]. At higher volume fractions (i.e. at higher superficial velocities), it is generally necessary to include a term in the drag model to account for the interaction between bubbles [2,18]. In our previous work, we found that including a modified version of the term developed by Simonnet et al. [19] gave good agreement with experimental results.

Of the remaining inter-phase momentum transfer terms, added mass is generally regarded as having minimal impact [2,3]. In our previous work [7], we have also found that inclusion of the lift force did not result in any improved agreement with experimental data, whilst incorporation of turbulent-dispersion (using the model developed by Burns et al. [20]) led to good agreement between model predictions and our experimental data.

A range of authors have proposed models to account for the transfer of turbulence from the gas to the liquid phase [21–23]. Such models account for bubble-induced turbulence via the inclusion of additional source terms in the transport equations for turbulence kinetic energy and turbulence energy dissipation. In our previous work, we found that the inclusion of bubble-induced turbulence production proved essential to obtaining meaningful results, as without it both volume fraction and velocity predictions were very poor [7].

A range of approaches exist to account for the fact that a distribution of bubble sizes will invariably exist. The simplest approach is obviously to assume a constant bubble size; such an assumption has indeed been shown to be reasonable in our previous work [7,15]. This approach has the considerable advantages of simplicity and computational efficiency, whilst also being a reasonable approximation for industrial fermenters where the high levels of surface-active compounds present in the liquid phase tend to inhibit bubble coalescence, thus leading to a relatively narrow size distribution [15]. More complex approaches exist, including making the bubble diameter a function of the turbulence energy dissipation [24], as well as MUSIG [25,26] and Quadrature Method of Moments (QMOM) methods [27]. These approaches introduce considerable additional model complexity, as there is a need to include closures which account for both bubble break-up and coalescence. Work in this area has been reviewed by Liao and Lucas [28,29], however to the best of our knowledge no generally applicable set of closure relations exists in the open literature; indeed work in this area is an active area of research [30].

As previously discussed, robustness and computational efficiency are key considerations in the development of any model. Our initial work was carried out in ANSYS CFX version 15 which proved to be very robust and to allow easy extension of the in-built models using the expression language. However, with the release of ANSYS 16, we have recently migrated this model to ANSYS Fluent, using its User Defined Function (UDF) capability. The prime motivation here was to evaluate the recently released non-iterative (NITA) Eulerian multiphase solver in Fluent which has the potential to speed up computations to the point where industrial-scale bubble column simulations become practical. Therefore, the objectives of this paper are as follows:

1. To provide a complete description of the bubble column model developed;
2. Discuss the choice of closure relationships and numerical schemes;
3. Compare the results obtained using ANSYS Fluent against our experimental data and previously published results from ANSYS CFX;
4. Draw insightful conclusions on the optimum solution approach to employ for the software considered.

2. Model description

The model is based on the standard shared pressure formulation of the Eulerian multiphase flow equations. As discussed in Section 1, we have used a single bubble size based on our measurements of bubble size distributions and the need to keep the simulations manageable in terms of computational cost.

2.1. Conservation equations

The conservation equations for mass, momentum and species for the gas and liquid phases are as follows:

$$\frac{\partial(\rho_G\alpha_G)}{\partial t} + \nabla\cdot(\rho_G\alpha_G\boldsymbol{U}_G) = -\Gamma_{GL}, \tag{1}$$

$$\frac{\partial(\rho_L\alpha_L)}{\partial t} + \nabla\cdot(\rho_L\alpha_L\boldsymbol{U}_L) = \Gamma_{GL}, \tag{2}$$

$$\frac{\partial(\rho_G\alpha_G\boldsymbol{U}_G)}{\partial t} + \nabla\cdot(\rho_G\alpha_G\boldsymbol{U}_G\otimes\boldsymbol{U}_G) = -\alpha_G\nabla p + \nabla\cdot\left(\alpha_G\mu_{G,\,eff}\left[\nabla\boldsymbol{U}_G + (\nabla\boldsymbol{U}_G)^T - \frac{2}{3}\boldsymbol{\delta}\nabla.\boldsymbol{U}_G\right]\right) + \alpha_G\rho_G\boldsymbol{g} + \boldsymbol{M}_{GL} - \Gamma_{GL}\boldsymbol{U}_G, \tag{3}$$

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