

# Using Computational Fluid Dynamics, an Analysis of the Interfacial Force Influence on a Bubble Column's Simulated Oxygen Transfer

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## Abstract

The usage of pneumatic bioreactors in bioprocesses is on the rise because they offer adequate heat and mass transmission, quick mixing, and effective solids suspension. In this study, oxygen transport from a bubble column bioreactor with a square cross section was studied numerically and experimentally using computational fluid dynamics (CFD), and the outcomes were compared to experimental data. In the numerical simulations employing the two-fluid Eulerian model, several specific air flow rates (1.0, 3.0, and 5.0 vvm) as well as drag and lift interfacial forces were taken into account. The simulations that took lift force into account produced results that were more in line with the experimental data, with the greatest values of  $k_L a$  being discovered for the higher specific air flow rate (5 vvm) that was examined in this work.

**Keywords:** Bubble column • Computational fluid dynamics (CFD) • Lift force • Oxygen transfer

## Introduction

Particle properties in a polydisperse system are strongly correlated with chemical engineering processes-related phenomena. One example is the bubble column bioreactor, which exhibits a gas-liquid flow in which the dispersed phase is formed by bubbles, defining the equipment's efficiency. Due to their geometric and operational simplicity, bubble column reactors have been widely used in aerobic bioprocesses to promote gas-liquid contact, adequate oxygen transfer, and low energy consumption. In order to analyze, design, implement, and improve industrial processes, it is essential to comprehend the equipment's hydrodynamic and transfer phenomena. Due to momentum transfer across the interface, interfacial forces can have a significant impact on the fluid dynamic patterns in multiphase flow simulations. Drag, lift, turbulent dispersion, and virtual mass forces stand out in bubble columns [1].

## Description

It is essential to the design, implementation, and optimization of numerous industrial processes to comprehend and model the internal behavior of bubble column bioreactors in relation to performance parameters. The gas-liquid systems are controlled by the interactions between the dispersed gas phase, which is made up of bubbles that interact with one another because of their chaotic movement in the heterogeneous regime, and the continuous liquid phase. In these instances, computational fluid dynamics (CFD) has been widely used in modeling and simulation for these reasons. Based on a few fundamental parameters, computational fluid dynamics makes it possible to simulate the momentum, heat, and mass transfers in bioreactors. Due to its

low computational cost, the Euler-Euler method is the one that is utilized the most frequently for modeling bubble column bioreactors. The steady-state simulation of a gas-liquid flow in an internally circulating airlift reactor, followed by verification and comparison with data from the literature. There was a comparison of several models for estimating the mass transfer coefficient, some of which do not work in real life. Along the bioreactor, theoretical spatial profiles of gas holdup were also discovered. The authors discovered that, in comparison to the other mass transfer models tested, the time model performed better and could be used for a wider range of bubbly flow than any other category model [2].

They proposed using the Eulerian formulation for both phases in the simulations to investigate the interfacial forces that influence the gas-liquid flow in a rectangular bubble column reactor with centralized aeration. The author looked into various models of lift, turbulent dispersion, virtual mass, and drag force. The best models were identified by comparing them to experimental values of global gas holdup. The author recommended including all other forces in simulations of systems that operate in conditions that are comparable to those studied because, out of the forces analyzed, only the virtual mass force had no significant effect, carried out a sensitivity analysis with the intention of confirming that the axial velocity profiles of liquid and gas were affected by the drag, lift, turbulent dispersion, and wall lubrication models. Water and air were used in a bubble column reactor with a square section. As a result, the authors came to the conclusion that the Ishii and Zuber (1979) model should be used to get better velocity profiles for the gas phase. The axial velocity profiles for both phases were accurately predicted by the drag and lift forces alone, and the velocity distribution was unaffected by the virtual mass and turbulent dispersion forces. On the other hand, these profiles were overestimated due to the wall lubrication force [3-5].

For Newtonian fluid-operating systems, the hydrodynamics of various pneumatic bioreactors (bubble column, concentric duct, and split cylinder airlifts) were evaluated experimentally and numerically. The authors ran additional tests with bubble diameters ranging from 3 to 7 mm at 3 vvm in the simulations to confirm the effect of bubble diameter. The bubble column bioreactor's air-water results demonstrated that was highly dependent on the bubble diameter, with the value of decreasing as the bubble diameter increased. The Euler-Euler multiphase model was used to evaluate oxygen transfer in bubble column bioreactors with a 0.15 m diameter and a 0.75 m initial liquid height in Open Foam-based computational fluid dynamics simulations. A superficial gas velocity of 0.1 m/s and an average and constant bubble diameter of 6 mm were utilized. For the numerical calculation of the convective oxygen transfer

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coefficient (kL), the authors used Higbie's penetration theory and found that the experimental and simulated data for the volumetric oxygen transfer coefficient were in good agreement. Adding the lift force to the model used in the simulations, computational fluid dynamics (CFD) was used to evaluate the volumetric oxygen transfer coefficient of a bubble column with a square cross-section experimentally and numerically. In order to better comprehend how lift force affects this mass transfer parameter, simulated values were compared to experimentally obtained values [6-8].

The analyzed bubble column had a liquid height of 510 mm, a total height of 755 mm, and a square cross-section with sides measuring 142 mm. Water was used as the liquid phase in both the simulations and the experiments, and atmospheric air was fed through a 180-orifice cross-type sparger at the bioreactor's base at specific airflow rates ranging from 1 to 5 vvm as the gas phase. The Ansys® package's Design Modeler and Meshing tools were utilized to create the computational mesh, sparger geometries, and bubble column geometries. The result was a structured mesh with hexahedral elements. The minimum node spacing was set at 4 mm along the column and 0.5 mm closer to the sparger region. The mesh had orthogonal quality values greater than 0.8 and skewness values below 0.5, indicating that it was of high quality. Additionally, the mesh used was of high quality because the aspect ratios of the mesh elements were less than 1.9 [9,10].

## Conclusion

Because it permits the association of numerical error values with various tested meshes, the Grid Convergence Index (GCI) was utilized for mesh independence analysis. As a result, it is possible to assess and quantify the mesh refinement required for a particular numerical solution. The Richardson Extrapolation method is the foundation of the approach, which is related to determining a more precise solution from the obtained domain discretization solutions. The bubble diameter, which was assumed to be constant in all of the cases examined, has an inverse relationship with the parameter "a," which represents the interfacial area of the bubbles. In addition to neglecting the size distribution, the equation used to calculate "a" is only applicable to perfectly spherical bubbles. Despite this, it is established that the water-air system exhibits a distribution of irregularly shaped bubble sizes, which may have contributed to the divergence between the experimental and CFD data. Additionally, given that bubbles with larger diameters have a smaller specific interfacial area, these findings may indicate that the actual average diameter of the bubbles is less than the diameter analyzed in this study.

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## Conflict of Interest

None.

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