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CFD Simulation of Hydrodynamic Behaviors and Gas-Liquid Mass Transfer in a Stirred Airlift Bioreactor

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Abstract**—**The speed profiles, gas holdup (ε_G) and global oxygen transfer coefficient (k_La) from a stirred airlift bioreactor using water as the fluid model, was investigated by computational fluid dynamics modeling. The parameters predicted by the computer model were validated with the experimental dates. The CFD results were very close to those obtained experimentally. During the simulation it was verified a prevalent impeller effect at low speeds, propelling a large volume of fluid against the walls of the vessel, which without recirculation, results in low values of ε_G and k_La; however, by increasing air velocity, the impeller effect is smaller with the air flow being greater, in the region of the riser, causing fluid recirculation, which explains the increase in ε_G and k_La.

Keywords**—**CFD, Hydrodynamics, Mass transfer, Stirred airlift bioreactor.

I. Introduction

BIOREACTORS are devices widely used in production lines, such as the production of antibiotics, enzymes, and amino acids; beverages and dairy products; in wastewater treatment, and recently in biodiesel production. Mechanically stirred airlift bioreactors have been studied by several authors [1]-[3]. Studies with mechanically stirred airlift bioreactors demonstrated a significant increase in gas holdup and global oxygen transfer coefficient, when compared with traditional airlift bioreactors [2], [3]. The acquisition and validation of experimental data through the computational fluid dynamics is an important tool that allows us to correlate laboratory experiments with simulated ones; thus, obtaining data and conclusions allowing for their scale up. Recently, several studies have been conducted on the effects of the mixture [4], mass transfer [5], and shear environment [6] in different types of bioreactors. All these studies demonstrate the CFD capability and reliability as a tool for the investigation of major hydrodynamic parameters, and analysis of the influence from operating conditions in the design and scales of bioreactors.

In this work, a three-dimensional hydrodynamic simulation of a stirred airlift bioreactor, in laboratory scale, was performed using the commercial software ANSYS CFX 12.0. The simulation results were used to calculate the velocity profile within the bioreactor, originated by the action of a Rushton impeller and different inflows of gas. We also evaluated the gas holdup, and the gas-liquid mass transfer coefficient. The parameters predicted by the computer model were validated with the experimental results.

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II. Materials and Methods

A. Bioreactor and Fluid

Measurements were made in a concentric draft-tube stirred airlift bioreactor (Fig. 1) agitated with a Rusthon impeller of 0.040m in diameter with six blades. The bioreactor vessel was 0.12m in diameter with overall height of 0.40m. The draft-tube, 0.09m in internal diameter and 0.30m tall, was located at 0.05m above the bottom of the tank. Air was sparged in the internal zone through a porous plate the 0.05m diameter, with 90 holes with a diameter of 0.001m. To avoid the formation of vortex, four baffles were added above the draft-tube location. A dissolved oxygen electrode (O2-sensor InPro6800/12/220 Mettler Toledo, Switzerland), and pH probe (405-DPAS-SC-K8S/225 Mettler Toledo, Switzerland) were positioned at a centerline of the vessel, and 0.15m above the bottom of the tank.

The reactor was sparged with oxygen or nitrogen. Distilled water was used as the fluid model. The superficial oxygen velocity in the riser (U_{GR}) was set within the range of 0.0105 to 0.0209m.s^{-1}.The agitation speed was of 200rpm. All experimental runs were carried out at normal atmospheric pressure and temperature of 25^{0}C.

B. Gas Holdup

The total gas holdup (ε_G) was measured by the volume expansion method as follows [7]:

$$\varepsilon_G = \frac{h_D - h_L}{h_D} \quad (1)$$

where h_D is the height of gas-liquid dispersion, and h_L is the height of gas free liquid.

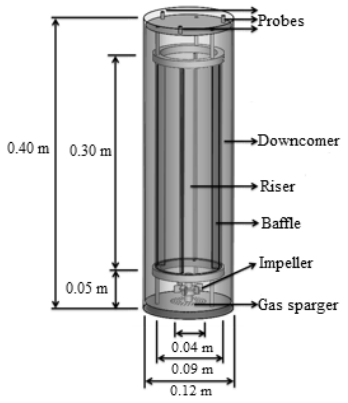


Fig. 1 The schematic diagram of experimental bioreactor system

C. Volumetric Oxygen Transfer Coefficient

The volumetric oxygen transfer coefficient (k_La) was measured with the dynamic gassing-in method [8]. For each test, the fluid was purged by bubbling nitrogen until reaching a dissolved oxygen concentration lower than 5% of air saturation. Later, the nitrogen flow was suspended, the outflow of its bubbles was allowed, and the airflow was established to the required condition. The increase in dissolved oxygen concentration was followed with time until the fluid became nearly saturated with oxygen (>90%). The k_La was calculated as the slope of the linear equation:

$$-\ln(1-E) = k_L a(t - t_0) \tag{2}$$

where E, is the fractional approach to equilibrium [7] and can be estimated by:

$$E = \frac{C - C_0}{C^* - C} \tag{3}$$

where C^* is the dissolved oxygen saturation concentration, C_0 is the dissolved oxygen initial concentration at time t_0 when a hydrodynamic steady-state has been reestablished (≤ 60 s) upon the beginning of aeration, and C is the dissolved oxygen concentration at any time t.

D. Computational Models

In the present work, the Eulerian two-phase model was used for the gas–liquid flow in the stirred bioreactor. The governing equations in this approach can be derived by assembling the averages of the fundamental conservation equations for each phase to describe the motion of liquid and gas in the reactor. For three-dimensional, incompressible fluid, the Navier-Stokes equations for phase i can be expressed by using a uniform equation [9]:

$$\begin{aligned}&\frac{\partial \alpha_i \phi}{\partial t} + \frac{\partial(\alpha_i r U\phi)}{r.\partial\theta} + \frac{\partial(\alpha_i V\phi)}{r.\partial\theta} + \frac{\partial(\alpha_i W\phi)}{\partial z} \\ &= S_\phi + \frac{\partial}{r.\partial r}\left(\frac{\alpha_i r \Gamma \partial\phi}{\partial r}\right) + \frac{\partial}{r.\partial\theta}\left(\frac{\alpha_i \Gamma \partial\phi}{r.\partial\theta}\right) + \frac{\partial}{\partial z}\left(\frac{\alpha_i \Gamma \partial\phi}{\partial z}\right)\end{aligned} \tag{4}$$

where α_i is volume fraction of phase i; ϕ stands for different variable of different equation; r, θ, z are the three cylindrical coordinates. Γ *denotes* an effective turbulent exchange coefficient for ϕ, and S_ϕ denotes source item of ϕ. The corresponding Γ and S_ϕ for different ϕ can be found in Table I in Ranade's work [9], [10]. And the equations were enclosed by adding the following equation [9]:

$$\sum_i \alpha_i = 1 \tag{5}$$

For the CFD modeling, the commercial CFD finite volume solver Fluent (version 12.0, ANSYS) was utilized to solve the Navier-Stokes equations. CFX-Mesh was used to generate the mesh of the models. Two meshes were created for the simulation: (i) the stationary domain consisting of the stationary bulk of the tank including the baffles; (ii) the rotational domain consisting of the Rushton impeller. The Frozen-rotor approach was chosen for modeling the stationary and rotational domains. Fig. 2 depicts the meshes obtained for each domain.

The interim estimate of the impeller Reynolds number in this work was calculated as $Re = \rho N D^2/\mu = 31665$, which indicated that the bioreactor was operated under turbulent flow regime. Along with the Eulerian two-phase model the dispersed multiphase k-ε turbulent model was also included.

The simulation and the experimental study used the same airflow rates. Due to the presence of baffles in the bioreactor, the vortex formation in the liquid surface was not considered in the simulation; instead this surface was defined by the degassing boundary condition, allowing the gas to escape the domain, while the liquid is retained by the non-friction condition on this surface. The shaft and impeller speed were set at 200 rpm. The liquid and gas phases were defined as water and air at 25°C, respectively.

It is assumed that there is no coalescence or breakage of bubbles, and a constant bubble diameter (1mm).

The governing equations are solved using the advanced coupled multi grid solver technology of ANSYS CFX 12.0. The convergence criteria used in all the simulations is 1×10^{-4}, which is a factor by which the initial mass flow residual is reduced with the simulation progress. The simulations are carried out on the Intel Xeon X5675 3.06 GHz processor, and 16 GB memory.

E. Gas–Liquid Mass Transfer Model

A theoretical mass transfer model is used for the prediction of gas-liquid volumetric mass transfer coefficient. Based on Higbie's penetration theory, that is widely used to describe gas–liquid transfers, as follows [11]:

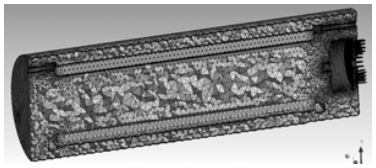
$$k_L a = \frac{12\alpha_g}{d_B}\sqrt{\frac{D_L U_{slip}}{\pi d_B}} \tag{6}$$

where D_L is the molecular diffusivity of gas in liquid, for water $D_L = 2.10 \times 10^{-9}$ m^2s^{-1} [12]; U_{slip} is the slip velocity

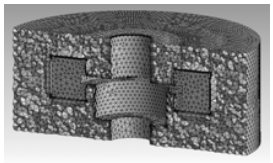
$\left(U_{slip} = \sqrt{\sum (u_g - u_l)^2}\right)$, u is the velocity.

For the Newtonian viscous and incompressible fluids in both phases, the densities of the liquid and gas are constant, and the closure relation of phase holdup is:

$$\alpha_l + \alpha_g = 1 \quad (7)$$



(a)



(b)

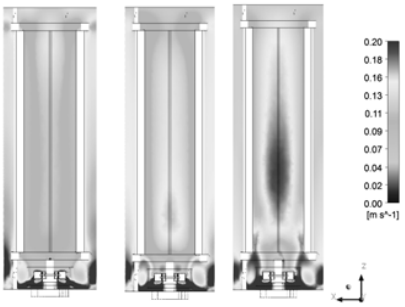
Fig. 2 Illustration of computational mesh: (a) stationary domain, and (b) rotational domain

III. Results and Discussions

A. Velocity Profiles

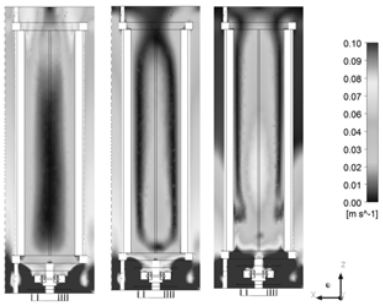
Figs. 3 and 4 show the velocity profiles resulting from the simulation in steady state for the gas and liquid phases.

The presence of the Rushton impeller demonstrates that the radial gas flow is driving the volume of fluid against the walls of the tank; at low gas flow rates (Fig. 3 (a)) the main task of the impeller is to propel the gas-liquid mass against the wall of the reaction vessel; thus, forcing the air to circulate mainly in the downcomer region. The impeller effect is quite dominant in this step, with the increasing the airflow rate (Fig. 3 (b)) a small volume of fluid begins to move in the region of the riser. However, most of the gas is directed into the vessel wall, with the increasing air velocity, part of the fluid and air moves to the riser, the rotation from the impeller produces an intense flow in the radial direction, dividing the wall into two distinct recirculations, one above and one below the impeller, the impeller geometry is also responsible for creating two very strong vortexes behind each blade. These high turbulence areas are responsible for breaking up the bubbles. There is a proportional increase in the displacement of the liquid volume and the air flow in the reactor (Fig. 4), with greater recirculation of liquid from the riser to the downcomer causing higher gas holdup; thereby, increasing the volumetric gas-liquid mass transfer coefficient.



(a) (b) (c)

Fig. 3 Distribution of gas velocity in the bioreactor under different superficial gas velocities: (a) U_{GR} = 0.003 ms^{-1}, (b) U_{GR} = 0.010 ms^{-1}, (c) U_{GR} = 0.018 ms^{-1}



(a) (b) (c)

Fig. 4 Simulated liquid phase velocity profiles under different superficial gas velocities: (a) U_{GR} = 0.003 ms^{-1}, (b) U_{GR} = 0.010 ms^{-1}, (c) U_{GR} = 0.018 ms^{-1}

B. Gas Holdup

The gas holdup (ε_G) was determined experimentally, and by computer simulation (CFD). Fig. 5 shows the distribution of gas holdup obtained by both the CFD simulation and experimentally. In both cases, there was an increased gas holdup, as the air velocity in the riser increases. The CFD simulation results were approximately 10% higher than the experimental values, one of the key reason for the observed over prediction of gas holdup may be due to the inaccurate estimation of inter-phase drag force [13].

Both results (experimental and computational) were adjusted using the equation proposed by Chisti and Moo-Young [14] for airlift bioreactors, which are defined by:

$$\varepsilon_G = aU_{GR}^b \quad (8)$$

The equations for the two cases were expressed by:

$$\varepsilon_G = 1.67U_{GR}^{0.81} \ (r^2 = 0.995) - \text{experimental} \quad (9)$$

$$\varepsilon_G = 1.64U_{GR}^{0.79} \ (r^2 = 0.998) - \text{CFD simulation} \quad (10)$$

The adjustment of the obtained data showed equations with coefficients *a* and *b* in close proximity, according to Chisti

and Moo-Young [14] for the water the *b* value should be closer or equal to 1.00. The agitation has a strong impact on the increase of gas holdup; studies with a stirred airlift bioreactor revealed that the presence of agitation increased gas holdup to up 300% [3]. The stirring system causes the breakage of the bubbles; thus, increasing its retention. Comparative studies with traditional and stirred airlift bioreactors found that the higher the rotational speed of the impeller, the greater the gas retention in the column; however, this increase results in a higher shear rate, decreasing the yield of the processes, especially the ones with non-Newtonian viscous medium [1], [3], [15], in addition to the high power consumption, especially, when they are agitated with radial impellers [16].

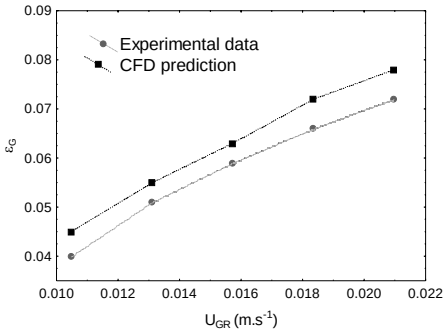


Fig. 5 Comparison of predicted average gas holdup (ε_G) with experimental data

C. Volumetric Oxygen Transfer Coefficient

The gas-liquid transfer coefficient (k_La) was experimentally determined by the dynamic method regardless the electrode response time, and by CFD simulations. The k_La values obtained by the simulation were close to those obtained experimentally, although these values were somewhat lower. Fig. 6 shows the increase in the k_La with the increasing superficial gas velocity. The simulated results were about 5-10% lower. Although this was relatively small error, it is noteworthy that the experimental methodology used for the determination of k_La, did not consider the delay time of the electrode response [3]; some studies have also reported that the dynamic method shows k_La values 10% higher than the pressure variation method [17], [18]. Another important factor relates to the model used for calculating the k_La by CFD, which considers the diameter of the gas bubble in the reactor to be constant and of the same diameter as the gas sparger, and the effects of breakage and coalescence of bubbles were not considered in the models used for simulation. Comparative studies conducted with experimental data from Kawase and Hashimoto [19] using an airlift reactor, and CFD simulation has shown that a model with constant bubble diameter resulted in higher values of ε_G and k_La; however, when considering the effects of breakage and coalescence of the bubbles, the simulated data showed good fit with the experimental one [20].

Shah et al. [21] suggested a correlation where the superficial gas velocity (U_{GR}) is the only variable for estimating the k_La in bubble column bioreactors. This correlation is given by:

$$k_La = cU_{GR}^{d} \quad (11)$$

where: the two constants *c* and *d* depend on the operating scale, the dimensions of the system, and the physical properties of the gas-liquid mixture.

The correlations between the k_La experimental and computational data as a function of U_{GR} are given by:

$$k_La = 0.086U_{GR}^{0.45} \ (r^2 = 0.973) - \text{experimental} \quad (12)$$

$$k_La = 0.063U_{GR}^{0.39} \ (r^2 = 0.971) - \text{computational} \quad (13)$$

Although this correlation does not take into account the dependence of the stirring speed, the results showed that the differences between the experimental and simulated values were very small. The constant *d* of the obtained models showed a discrepancy of ± 15%, and the superficial gas velocity in the riser has a greater contribution in the simulated model.

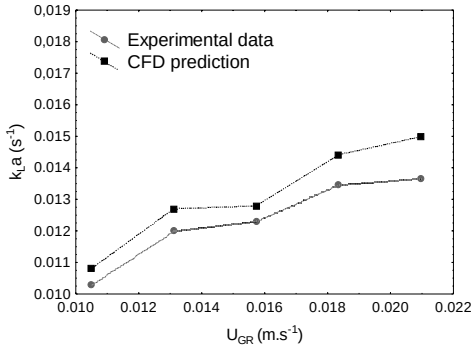


Fig. 6 Comparison of predicted average mass transfer coefficient (k_La) with experimental data

IV. Conclusion

The prediction for hydrodynamic data, such as gas holdup and mass transfer in stirred airlift bioreactors can be performed using computational fluid dynamics simulations, the choice of equations and mathematical method used involves the fitting quality of the simulated and experimental data. Although the model used in the simulations did not consider the breakage and coalescence of the bubbles, the predictive results differed in approximately 10% of the experimental values. We also observed by simulation that the bioreactor used in the experiments has a high directional flow in the region of the riser, where there is an increased gas velocity causing the gas to detach at the top of the column, and the partially de-gasified liquid goes through the downcomer, while the liquid recirculation will become more

effective with the increased air flow. The impeller effect is prevalent at low gas flow rates, and it propels the liquid against the walls of the vessel, without recirculation, resulting in low values of gas holdup and volumetric oxygen transfer coefficient.

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