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Gas-Liquid Hydrodynamics Simulation using CFD in a Helical Ribbon Impeller Applied for Non-Newtonian Fluids

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Abstract

In the present study Computational Fluid Dynamics applied to non-newtonian fluids was developed in order to characterize the gas-liquid mass transfer in a 10 L bioreactor equipped with a helical ribbon impeller. Gas-liquid Hydrodynamics was estimated Based on CFD results. The operating conditions chosen were defined by typical settings used for culturing fungi organism. Turbulence, rotating flow, bubbles breakage and coalescence were simulated by using the k-e, MRF (Multiple Reference Frame) and PBM approaches, respectively. The numerical results from different operational conditions are compared by evaluating its effect on $k_L a$. Interested by these simulated results CFD simulations are qualified as a very promising tool not only for predicting gas-liquid hydrodynamics but also for finding design requirements that must be implemented to optimize an aerobic bioprocessing useful for non-newtonian applications which are characterized by the constrain of achieving relatively high stirring conditions and avoiding cellular damage due to hydrodynamic conditions.

Keywords: bioreactor, scale up, multiple reference frame (MRF), population balance model (PBM), spin filter

INTRODUCTION

Adequate supplying of oxygen for aerobic cell cultures in a bioreactor has been a very common problem in fermentation technology. This problem is increased when the bioreactor reaches a high cell density, in which the rate of oxygen transfer is insufficient, thus limiting cell growth and process productivity.

In the case of filamentous fungi, the mycelial suspensions are generally viscous and behave non-Newtonian [1]. The latter is often associated with poor bulk mixing, an inhomogeneous distribution of the various phases to be processed, and the presence of rheological complexities. Consequently, oxygen requirements are proportional to cell density, which means that limitations in gas-liquid mass transfer are expected, leading the process to anoxic conditions, cell damage and decreased cellular viability, which generates a reduction in the productivity of the process.

To respond to the needs of industrial processes, reactors are often equipped with conventional mechanical agitation devices. Helical Ribbon Impellers is well known for the high efficiency in terms of agitation of viscous fluids [2]. Computational Fluid Dynamics (CFD) is used for analyzing hydrodynamic phenomena in stirred tank bioreactors. The latter can simulate an aerobic process to consider breakup and coalescence phenomena by focusing on gradients causing poor gas-liquid mass transfer.

Currently, CFD is more and more extended to the study of reactor Impellers, including from fluid phase rotation models [3-7], and to the use of population balance models in gas - liquid agitation systems [8-25].

Although several research has focused on understanding flow patterns, gas-liquid mass transfer phenomena and hydrodynamics has not yet been studied. To the authors knowledge CFD simulations for gas-liquid hydrodynamics in Helical Ribbon Bioreactor had never been used previously for evaluating mass transfer prediction. For this reason, detailed understanding of hydrodynamic behavior can be useful not only for identifying mass transfer limitations but also for finding design requirements that must be implemented to optimize an aerobic non-newtonian bioprocessing. Hence it is the motivation of this work to simulate gas-liquid hydrodynamics in a Helical Ribbon bioreactor using a CFD approach for mass transfer.

METHODS

A. Bioreactor setup

A stirred tank bioreactor with 10 L working volume was used for dimensioning all evaluated geometries. The gas is supplied through a cylinder sparger. The operating conditions chosen were defined by typical settings used for culturing fungi organism: stirring velocity was simulated at 200, 400 and 600 rpm and aeration rate of 1.0 vvm. Based on Based geometrical dimensions, the design of the virtual geometry is performed using Ansys 13.0 software and shown in Figure 1.

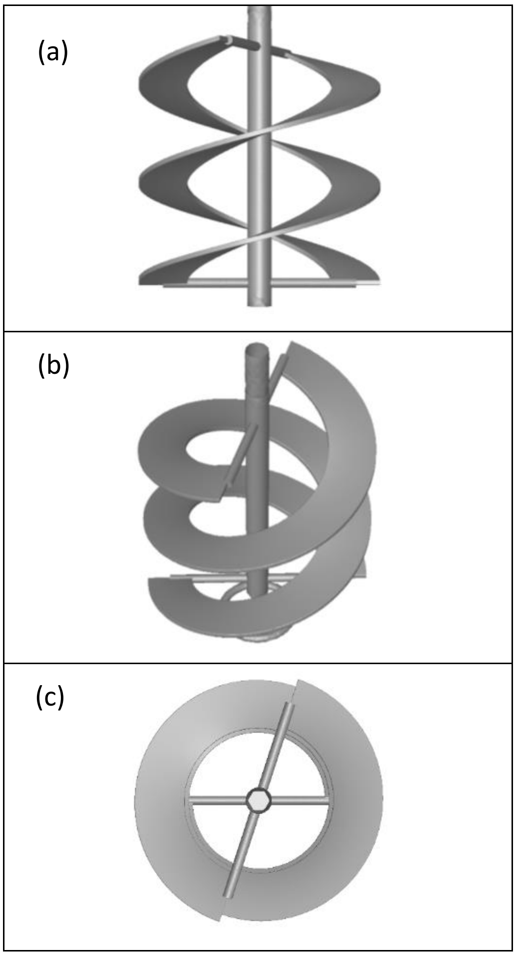

Figure 1. Helical Impeller. (a) Front View. (b) Diagonal View. (c) Cross section.

B. Computational Fluid Dynamic Model

The conservation equations for each phase are derived to obtain a set of equations, which have similar structure for all phases [15]. The Eulerian model was used in this work. It solves a system of *n*-momentum and continuity equations for each phase. The coupling is achieved through pressure and interfacial exchange coefficients. Interfacial momentum exchange, Coriolis and centrifugal forces were also included expressed in the MRF (Multiple Reference Frame) model for rotating flows.

Drag forces depends on friction, pressure, cohesion, and other hydrodynamic effects. To calculate the drag coefficient the standard correlation [26] was applied.

The dispersed turbulence $k - \varepsilon$ model can be considered as the multiphase standard turbulence approach. Previous studies [27] have shown that mycelium organism in highly viscous fluids behave like a viscosity power law model for non-Newtonian fluid. For estimating experimentally the rheological parameters to be included in the CFD model, a DV-E Brookfield Viscometer was used to calculate shear stress applying different shear rates (1-100 s^{-1}) in 0.25% xanthan gum.

The discrete method [28-29] is used herein to solve the population balance equations. The bubble population is discretized into a finite number of intervals of bubble diameters. The bubble breakup is analyzed in terms of bubbles interaction with turbulent eddies. These turbulent eddies increase the bubble surface energy to cause deformation. The breakup occurs if the increase in the surface energy reaches a critical value. The break up rate is defined as [4]. The bubble coalescence is modeled by considering the bubble collision due to turbulence, buoyancy and laminar shear [30].

C. Mesh processing and numerical technique

A fine 3D mesh is composed for hybrid cells with 1000 computational k cells [31]. The finite volume technique implemented in the CFD code Ansys Fluent 13.0 Software was used to convert the Navier- Stokes equations into algebraic equations which can be solved numerically. Tank walls, stirrer surfaces and baffles are treated with no slip conditions and standard wall functions.

RESULTS

The purpose of this research to study the gas-liquid mass transfer hydrodynamics using a Helical Ribbon Impeller. Special emphasis of $k_L a$ simulations is also presented using computational fluid dynamics to identify the influence of different stirring velocities on gas-liquid hydrodynamics. For that reason, understanding of gas liquid hydrodynamics can be useful not only for identifying mass transfer limitations but also for finding design requirements that must be implemented to optimize an aerobic non-newtonian bioprocessing.

Figures 2-4 show the air volume fraction dispersion.

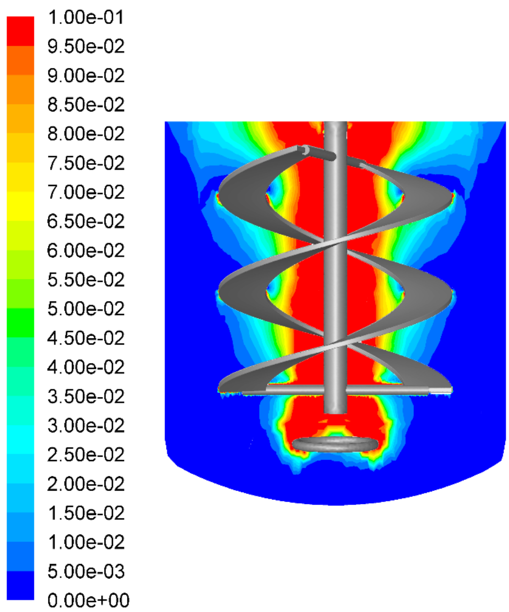

Figure 2. Air volume fraction contours [-]. Helical Ribbon. N_i: 200 rpm.

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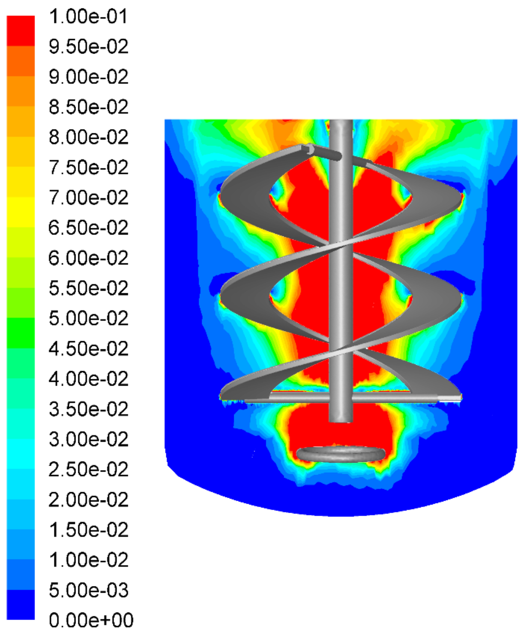

Figure 3. Air volume fraction contours [-]. Helical Ribbon. N_i: 400 rpm.

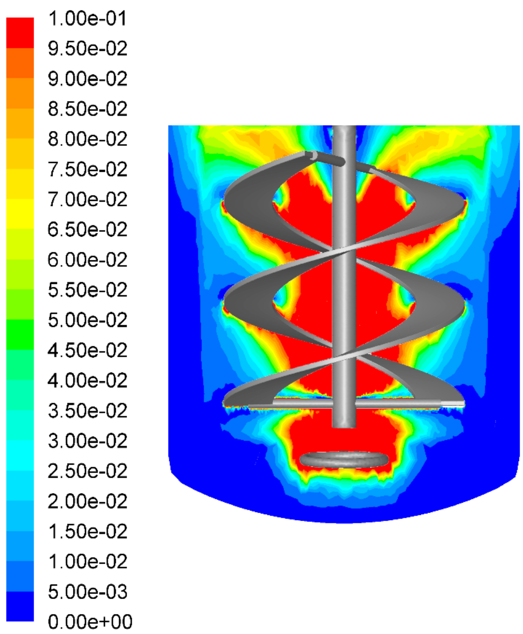

Figure 4. Air volume fraction contours [-]. Helical Ribbon. N_i: 600 rpm.

The bioreactor was operated under different agitation conditions commonly used in fungal culturing (200, 400 and 600 rpm). For all cases, the simulations were performed at an aeration rate of 1.0 vvm.

Figure 2 shows a poor air dispersion in areas closed to Helical Ribbon and bioreactor walls, which is not overcome with the increase in stirring speed (Figures 3-4). Although centrifugal forces prevent air buoyancy at high stirring levels, the latter are not enough to disperse gasses in the bioreactor. These discrepancies can be explained by the velocity magnitude contour (Figure 5-7).

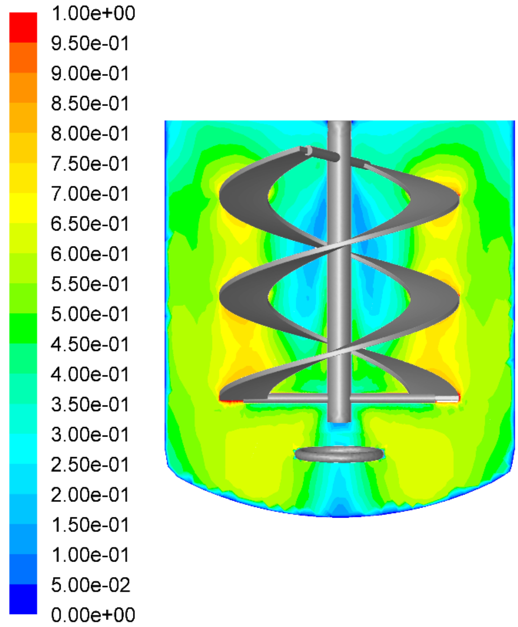

Figure 5. Velocity Magnitude contours v/vt_{ip} [-]. Helical Ribbon. N_i: 200 rpm.

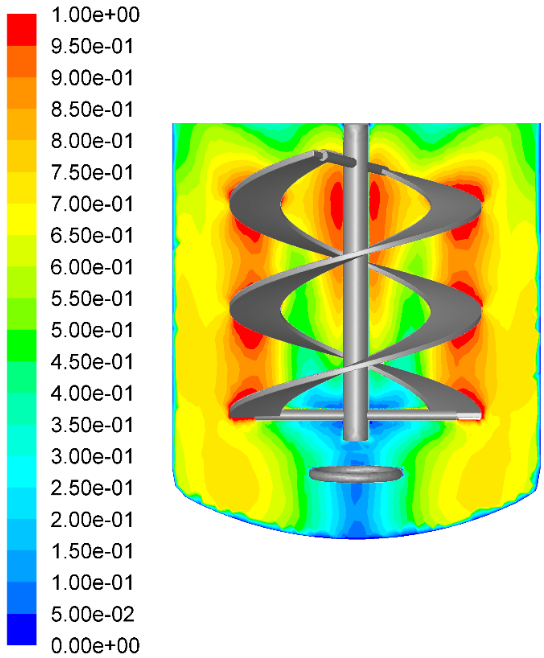

Figure 6. Velocity Magnitude contours v/vt_{ip} [-]. Helical Ribbon. N_i: 400 rpm.

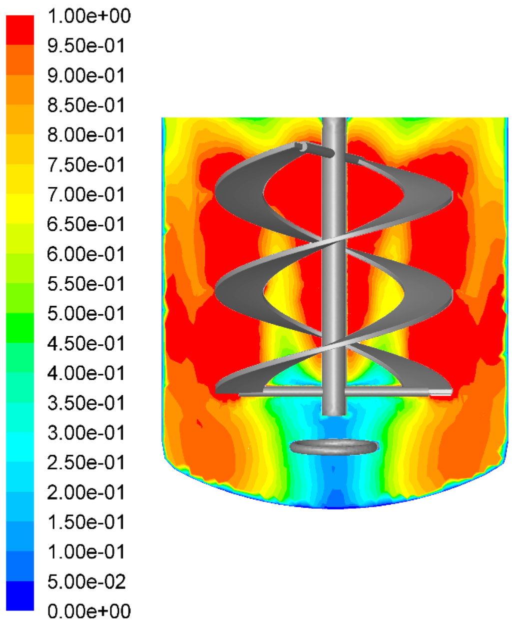

Figure 7. Velocity Magnitude contours v/vt_{ip} [-]. Helical Ribbon. N_i: 600 rpm.

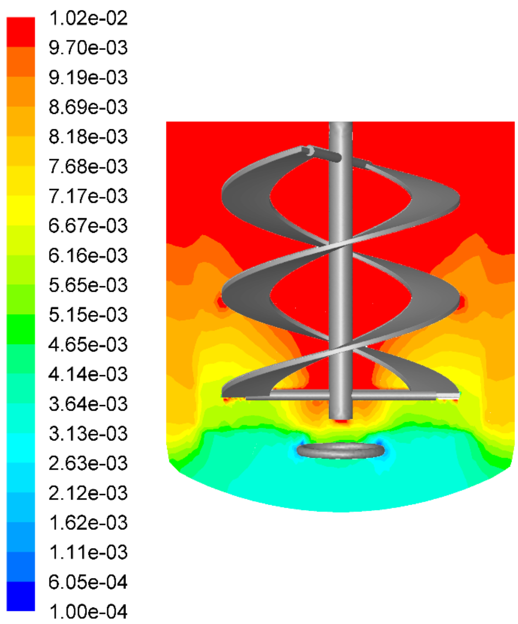

Figure 8. Sauter mean diameter contours. Helical Ribbon. N_i: 200 rpm.

Velocity magnitude is a very important design parameter in gas-liquid mass transfer. The latter is directly related to turbulence kinetic energy dissipation. For all cases, highest velocities occur in areas closed to blades. According to the results, axial upwards pumping velocities govern the gas-liquid hydrodynamics in Helical Ribbon device. As a consequence of its flow pattern air dispersion is adversely affected and may induce an increase in bubble coalescence, generating heterogeneous zones in the bioreactor, characterized by inability to transport air to the walls of the bioreactor. Figures 8-10 show the simulations of bubble mean diameter (Sauter diameter) generated by the breakup and coalescence phenomenon. Maximum bubble sizes are observed at rotation center with values of 10 mm in diameter. The latter due to air accumulation caused by the limitation of disperse efficiently bubbles as explained before. This phenomenon is according to [31].

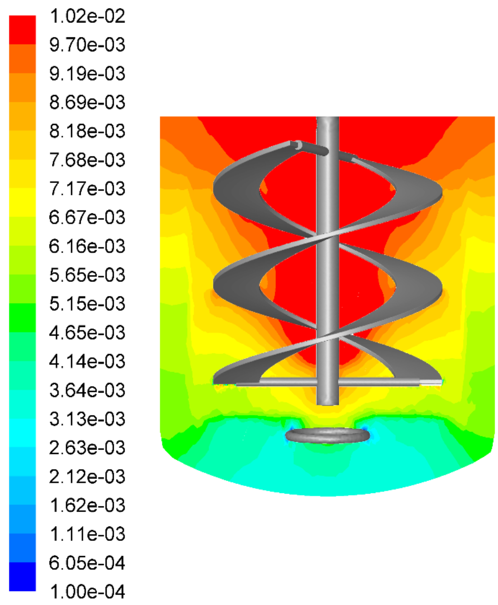

Figure 9. Sauter mean diameter contours. Helical Ribbon. N_i: 400 rpm.

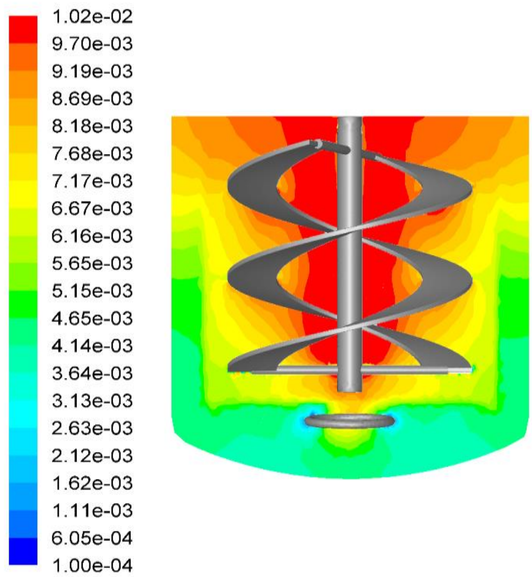

Figure 10. Sauter mean diameter contours. Helical Ribbon. N_i: 600 rpm.

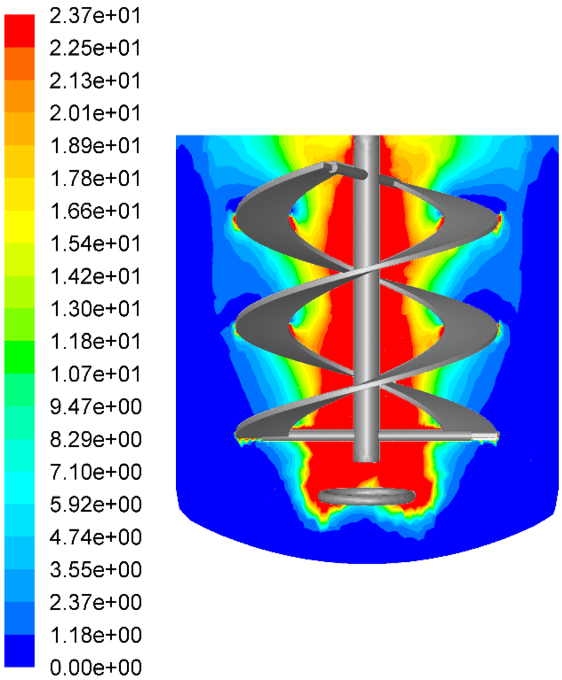

Figure 11. $k_L a$ mass transfer simulation. Helical Ribbon..N_i: 200 rpm.

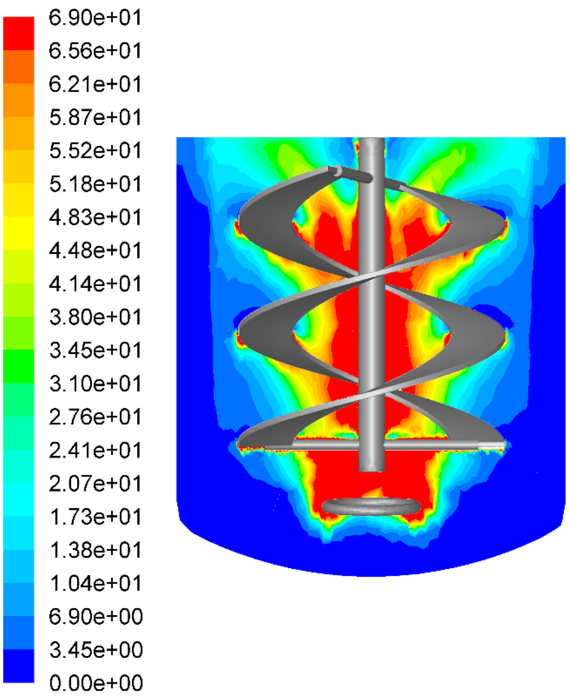

Figure 12. $k_L a$ mass transfer simulation. Helical Ribbon..N_i: 400 rpm.

For this reason, the probability of occurrence of undesired coalescence in these areas is high, since the mathematical model to simulate the coalescence phenomenon in this research [30] depends drastically on bubble contact time. The latter is also increased due to resistance influenced the viscosity in non-Newtonian fluids. Therefore, it is imminent that the contact time between the bubbles is increased [31].

Mass transfer oxygen in biotechnological process is one of the most important factors to take into account during the design of a device. Oxygen is essential for the generation of ATP as it functions as a substrate in oxidative phosphorylation. There is a wide variety of effects of dissolved oxygen levels on the metabolism of fungal cultures, for example, oxygen can affect cell growth, cell morphology, nutrient absorption and production of the metabolite of interest. In Figures 11-13 results of the $k_L a$ mass transfer coefficient contours are presented.

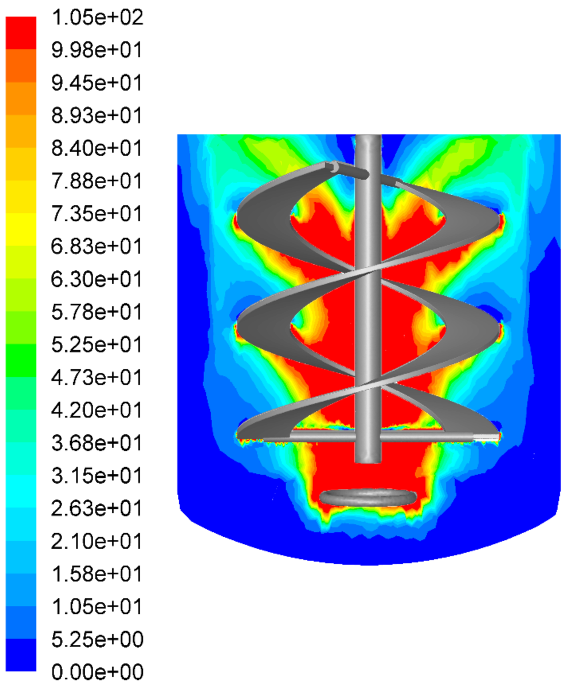

Figure 13. $k_L a$ mass transfer simulation. Helical Ribbon..N_i: 600 rpm.

The $k_L a$ values are considered as a main criterion for grading gas-liquid mass transfer. The Higbies penetration theory was used to calculate values from CFD simulations. These values are obtained as the product of the liquid phase mass transfer coefficient and the gas phase interfacial area [32]. The interfacial area is expressed as a function of gas local fraction and mean local Sauter diameter. The oxygen transfer rate (OTR) indicates the proportionality to increase the oxygen transfer either by increasing the dissolved oxygen gradient or by improving the values from $k_L a$ [2].

Values from 23 h^{-1} to levels above 100 h^{-1} are observed, depending on the agitation conditions evaluated. In all cases, the values are maximum in the rotating center areas. The latter can be explained by the characteristic circulation loop of the Helical Ribborn: fluid is upwards pumping by the blades and then it returns from surface to bottom in zones closet to rotating center. These latter turbulent area is govern by high axial downwards pumping velocities that enhance the k_L liquid coefficient mass transfer. So that $k_L a$ is also increased.

CONCLUSIONS

The information obtained in this phase of the work, which consisted in evaluating the effect of operating conditions for non - Newtonian fluids from CFD, allowed to elucidate the key criteria for the design of a stirring - aeration device, being axial downwards pumping velocities one of the most important parameters to consider in order to maximize the values of $k_L a$. According to the information from this work, the high axial upward pumping velocities adversely affect the air dispersion, and may induce an increase in bubble coalescence, generating heterogeneous zones in the bioreactor, characterized by inability to transport air to the walls of the bioreactor. That is why another key criterion in the design of a stirring-aeration system is the average bubble diameter.

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