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Non-Newtonian Behavior Effect on Gas-liquid Mass Transfer using an Anchor Impeller for CSTR Bioreactors: A CFD Approach

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Abstract

Objectives: k_La mass transfer coefficient was predicted using CFD (computational fluid dynamics) for analyzing non-newtonian effects on gas liquid mass transfer in a 10 L bioreactor stirred with an Anchor Impeller. **Methods/Statistical Analysis:** The set up bioreactor configurations were defined by typical culturing conditions used for fungi organism. Bubble breakage frequency and coalescence rate were simulated using Luo - Colaloglou and Tavlarides models and PBM approaches, respectively. Simulated results from different shear rates due to non-newtonian behaviour are compared by analyzing its influences in bubble size and power input. **Findings:** A clear relationship between high levels of shear rates and small bubble sizes is found in this work. The later is also associated with the high values of k_La simulated (270 h-1) and compared to levels found at low shear rates (62 h-1). **Application/Improvements:** Impressed by these findings new design optimizations for non-newtonian bioprocessing applications would be improved using CFD.

Keywords: Anchor, Bubble Coalescence, Non-Newtonian, Sauter Diameter, CFD

1. Introduction

Mixing of non-Newtonian fluids is one of the most difficult constraining in Bioprocess engineering Field since viscosity exerts a resistance to fluid deformation. This problem increases in multiphase fluids related to bubble interactions because it must be broken for oxygen can be transfer to culture media. Because oxygen transfer controls reaction rates in a bioprocess, it is considered a limiting factor that significantly affects overall productivity[1].

The most common application occurs in the fungi cultivation at high viscosity levels[2]. The later affects the oxygen transfer rate and leads the process to gradients and poor mixed zones in a bioreactor. Consequently,mass transfer is proportional to biomass concentration, which means that constrains due to mass transfer and mixing are expected, leading the bioprocess to lots of productivity[3].

Often bioreactors are configured with stirring system to conserve homogeneous operating conditions. Anchor impellers are well known for its common application in non-newtonian fluids and its ability for avoiding stagnation at bioreactor walls zones[4]. CFD is a simulating tool used for predicting bubble behaviour in reactors by simulating coalescence and breakage phenomena focusing on inhomogeneous zones.

Nowadays, CFD is used for in device type Impellers, including from one phase models[5-7], to its implementation for modeling bubble size behaviours in gas - liquid systems[1,8,9].

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Although several works have been applied in understanding Anchor flow patterns, bubble size behaviour and rheological effects on mass transfer has not been studied so far. Based on the later there is weakness knowledge in gas liquid hydrodynamics for understanding Anchor device abilities. For this reason new design optimizations for non-Newtonian bioprocessing applications would be improved using CFD. Hence it is the main propose of this contribution to analyze bubble interactions caused by rheology in an Anchor Impeller using a Computational Simulation for mass transfer analysis.

2. Materials and Methods

An Anchor impeller for stirring 10 liters tank was simulated using CFD shown in Figure 1. The air dispersion does it by a ring sparger. The set up bioreactor configurations were defined by typical conditions used for filamentous cultures: N_i and vvm are set up at 200, 400 and 600 rpm and 1.0 vvm, respectively. Ansys Fluent 13.0 software was used for CFD calculation.

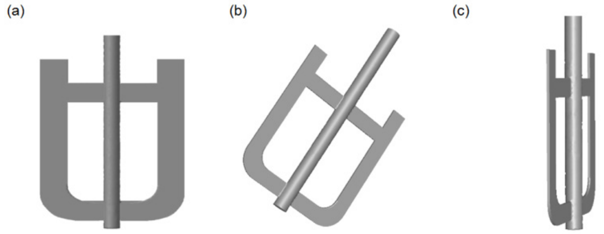

Figure 1. Helical Impeller. (a) Front View, (b) Diagonal View, (c) Cross section.

The finite volume method is used to discretize conservation equations in algebraic equations for all phases[10]. The Eulerian model was used to solve momentum and continuity equations. The Pressure-Velocity Method is used for coupling pressure and velocity via interfacial exchange coefficients. For modeling rotating zone the MRF (Multiple Reference Frame) model was applied.

Turbulence is modelled based on the dispersed turbulence $k-\varepsilon$ model and the power law model was used for simulating viscosity. Shear stress (shear rates range: 1-100s^{-1}) in 0.25% xanthan gum[11] was analyzed via viscometer to calculate rheological parameters (Figure 2) to be included in the CFD model. Results are k : 0.28 kg/ms and n : 0.37.

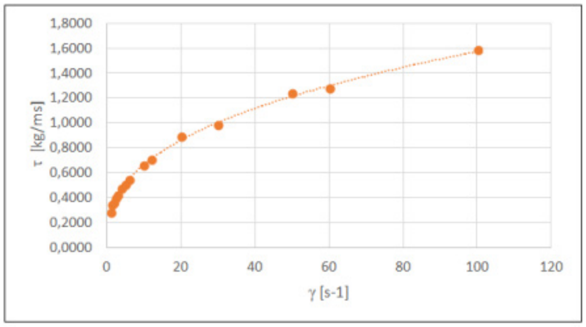

Figure 2. Rheogram for Parameter estimation (0.25 % xanthan gum).

For CFD model verification Impeller Power input P was calculated as[1]:

$$P = N_p \rho N_i^3 D_i^5 \qquad (1)$$

With N_P The power number, ρ density, N_i Stirring velocity, and D_i Impeller diameter.

Bubbles are discretized using the discrete method[11,12]. Eddies increase the particle surface energy for causing breakage. The increase in bubble surface energy to a critical value causes the breakup[13]. The Coalescence model[14] was used to simulate coalescence by considering bubble collision due to buoyancy, turbulence and laminar shear.

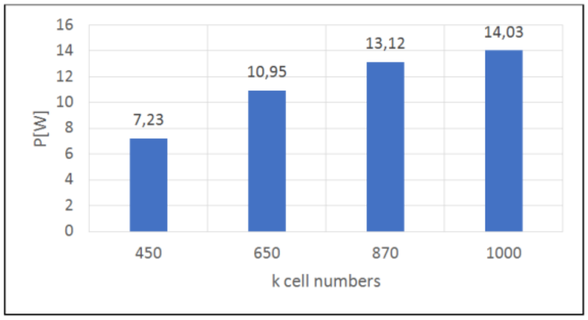

Figure 3. Mesh sensibility analysis.

Different grid sizes meshed were estimated for a sensitivity study (Figure 3): 450, 650, 870 and 1000 k cells. A grid-independent solution was reached at 1000 k cells.

3. Results

The main goal of this research is to simulate bubble size interactions caused by rheology in an Anchor Impeller using a CFD for mass transfer analysis. Special focus of $k_L a$ simulations is also showed using fluid dynamics to identify the influence of different mixing velocities on gas-liquid hydrodynamics for non-Newtonian fluids. Figure 4 shows the air volume fraction.

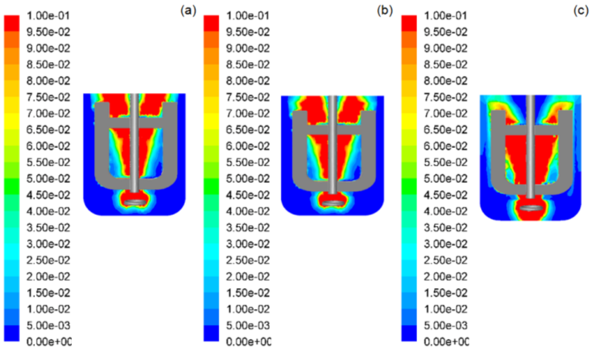

Figure 4. Air volume fraction [-]. Anchor Impeller. (a) N_i : 200 rpm; (b) N_i : 400 rpm; (c) N_i : 600 rpm.

Figure 3 shows an inhomogeneous air dispersion in regions closed to Anchor device and reactor walls, which is not released by increasing mixing speed.

Shear rate in non-Newtonian fluid can be defined as the rate at which a fluid deforms. Figure 5 shows shear rate calculations from different stirring velocities. It was found in this research that shear rate, positively influences bubble size and the $k_L a$ values, respectively (Figures 6-7). The latter are main criteria for being considered during a design optimization stage for a stirring-aeration device, since it generates important information to determine how resistance due to viscosity in non-Newtonian fluids can be overcome. The latter is also a clear evidence of viscosity resistance affecting the mixing process.

Figure 6 shows the simulations of bubble mean diameter (Sauter diameter) generated by the breakup and coalescence phenomenon. Interestingly, low values of ~ 2.0 mm are found closed to Impeller blades in the transverse areas of pumping direction. Also, for all cases, the smallest Sauter diameter is calculated in the bottom of bioreactor. These regions reflect relatively high rates of bubble breakage due to high levels of: turbulent dissipation energy and shear rate in areas closed to Anchor Impeller and walls.

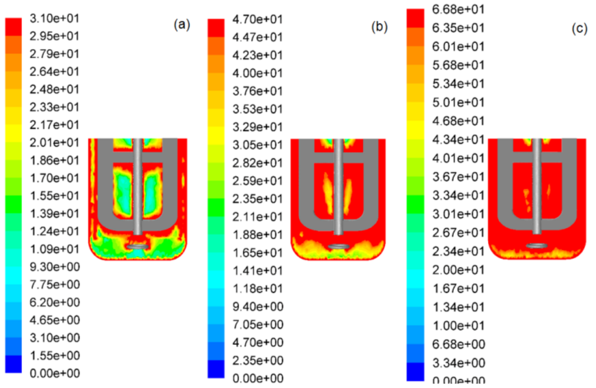

Figure 5. γ Shear rate [s^{-1}]. (a) N_i: 200 rpm; (b) N_i: 400 rpm; (c) N_i: 600 rpm.

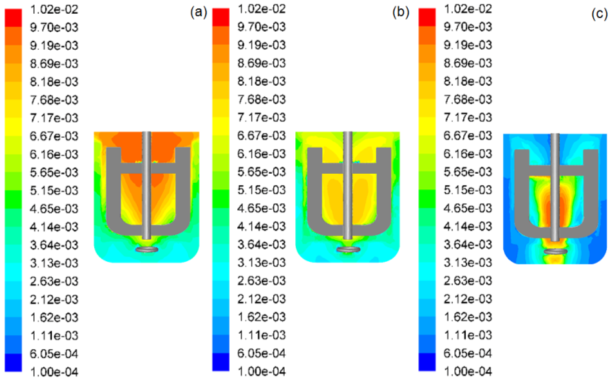

Figure 6. Sauter Diameter [m]. Anchor Impeller. (a) N_i : 200 rpm, (b) N_i : 400 rpm, (c) N_i : 600 rpm.

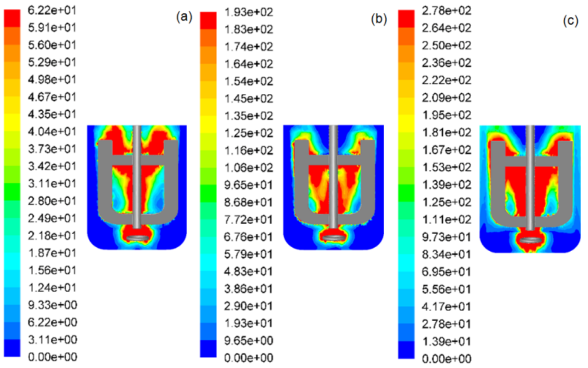

Figure 7. $k_L a$ [1/h]. Anchor Impeller. (a) N_i: 200 rpm, (b) N_i: 400 rpm, (c) : N_i 600 rpm.

They $k_L a$ calculations are designed as a main factor for analyzing bubble interactions. For interacting $k_L a$ to hydrodynamics the Higbies penetration theory was implemented[15] the interfacial area is limited by gas local fraction and mean local Sauter diameter. It is found is a clear dependence of bubble size on $k_L a$ values showing high values of $k_L a$ at the smallest level of bubble size.

CFD model verification is performed from Power Input P calculations from CFD and compared it with a common correlation (1) useful for mixing applications as shown in Table 1. Calculated values from correlation (1) identified integral P values of 13.97, 111.80 and 377.33 W for 200, 400 and 600 rpm, respectively, that fit very well to the simulations. The accurate of these results related to P calculation verifications is and evidence for the potential applicability of the CFD for future optimizations.

Table 1. CFD model verification from power input P[W] determinations

200 rpm		400 rpm		600 rpm	
P[W] CFD	P[W] Eq. (1)	P[W] CFD	P[W] Eq. (1)	P[W] CFD	P[W] Eq. (1)
14,03	13,97	103,04	111,80	326,73	377,33

Different scenarios are observed for $k_L a$ values. From 62 h^{-1} to levels above 270 h^{-1} are observed (Figure 7), depending on the agitation conditions evaluated. Results found here are clear evidence of shear rate on the $k_L a$ mass transfer coefficient.

4. Conclusions

The bubble size interaction from gas liquid mass transfer in an Anchor Impeller is analyzed using CFD. Impressed by these findings new design optimizations for non-newtonian bioprocessing applications would be improved using CFD. Shear rate and bubble size interactions can be treated as main starting point for improvement of operating conditions in non-newtonian fluids due to its influence on hydrodynamics.

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