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CFD Analysis of the Effect of Baffle Plates on the Fluid Flow in an Anaerobic Sequencing Batch Reactor

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With the development of agro-industrial processes, the waste generation has increased. Fermentation of organic wastes has attracted considerable attention, as it is an effective production route of hydrogen and it reduces environmental organic pollution.

In this work, a numerical study is presented, with the aim of optimizing an anaerobic sequencing batch reactor (ASBR) for biohydrogen production. The Computational Fluid Dynamics (CFD) technique was used to provide accurate results for the fluid flow, which directly influences the mass transfer, momentum, and hence the kinetics of the reactions involved. An Eulerian-Eulerian approach was applied to describe the flow of the phases, using the OpenFOAM code.

The inclusion of baffles in the bioreactor was studied, to verify the configuration which provides higher mixing. It was found that the inclusion of a baffle with length equal to ¼ of the bioreactor radius caused the largest increase in the turbulent kinetic energy, with little effect on the pressure drop.

1. Introduction

The use of alternative energy sources is a priority today, given the need to circumvent the problems caused by greenhouse gas emissions, which are generated by the combustion of fossil fuels. The current concern for pollution reduction and the energy crisis have spurred the global biofuels market. The demand for clean energy and renewable resources is continuously increasing (Bilgen et al., 2008). Many scientists point to hydrogen as the future fuel, due to its clean features and because it can be used in highly efficient fuel cells to generate electricity (Show et al., 2011).

The hydrogen producing microorganisms can metabolize substrate via photosynthetic or fermentative routes. The production by anaerobic fermentation of organic wastes appears as the most favorable method, combining high yields with reduced organic pollution (Show et al., 2011).

The anaerobic sequencing batch reactor (ASBR) is one of the most widely used reactors. This reactor allows higher process control when compared to continuous systems, thus demonstrating great potential for industrial scale use (Novaes et al., 2010).

Although hydrogen production is complex and multiphasic, involving physical, chemical and biological processes with numerous interactions among gas, liquid and solid phases, current research has devoted special attention to chemical and biological aspects. Moreover, the physical characteristics that affect the efficiency of the process have been neglected and many reactors are still scaled by empirical correlations (Wang et al., 2010). The understanding of the hydrodynamic phenomena involved in the production of hydrogen is a necessary precursor to its application on an industrial scale. Turbulence is an important factor to consider in the gas-liquid flow (Sanchez-Forero et al., 2013). It can promote mixing in the reactor, which enhances mass transfer and process efficiency.

With the use of CFD, industrial equipment can be simulated in real scale and processes can be studied prior to performing real scale experiments, which saves time and reduces costs (Wang et al., 2010).

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The contribution of the present work is a numerical study, using CFD methods for the analysis of the flow inside an ASBR in different scales. Based on the knowledge of fluid dynamic behavior, changes in their internal flow are evaluated in order to optimize the mixing, which directly influences the efficiency of the bioreactor. The Eulerian-Eulerian approach was used for the calculation of a two-phase, turbulent flow. Simulations were conducted with the computational code OpenFOAM 2.2.0.

2. Methodology

Three-dimensional, transient, turbulent simulations were performed to predict the fluid dynamics of the proposed cases. The Eulerian-Eulerian approach was applied to resolve the two-phase flow. The considered phases were a continuous liquid mixture, and dispersed gas bubbles. The formulation of Weller (2002) apud Rusche (2002) for two-phase incompressible flow was adopted. The Boussinesq hypothesis, in which the effective viscosity of the continuous phase has a contribution of molecular and eddy viscosities, was considered. The k-epsilon turbulence model was used to determine the effects of turbulence in the liquid phase.

The drag force dominates the flow in bubble columns. There are many correlations to estimate this force, and it is important to evaluate them properly. System conditions indicate that the bioreactor is in the homogeneous regime (Kantarci et al., 2005), thus the drag force can be considered as acting on spherical rigid spheres. The Schiller and Naumann correlation was then used to estimate the drag between the fluid and bubbles.

Three-dimensional geometries were used to represent two ASBRs with different sizes. One had an internal diameter of 0.604 m, height of 3.8 m and a total capacity of 1 m³. The other had half these sizes, and a total capacity of 0.125 m³. The recirculation pipe of the larger and smaller reactors had internal diameters of 0.04 m and 0.02 m respectively. Several configurations with the inclusion of baffles were considered, in order to evaluate how they affect the mixing in the reactor. A schematic diagram of the geometries elaborated is shown in Figure 1.

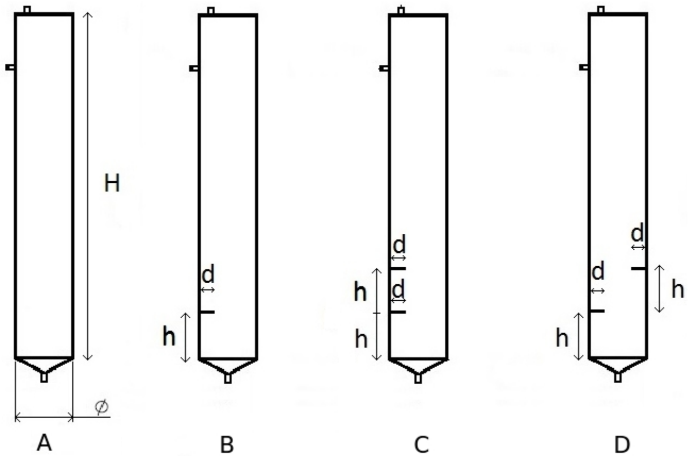

Figure 1: Representation of the modifications applied in (A) the original bioreactor, including (B) one or (C and D) two baffles at different positions.

In Figure 1, d represents the length of each baffle, which had the values of ½ and ¼ of the reactor diameter, h is the height of placement, which is 1 m in the larger reactor, and 0.5 m in the smaller one. Table 1 presents the properties of the baffles included in each case considered in this study.

Mesh independence tests were performed with mesh sizes ranging from 60,000 to 210,000 control volumes, simulated considering the gas-liquid two-phase model. Results shown that the mesh containing 130,000 control volumes provided values close to those obtained with finer meshes, requiring less computational time (Maurina et al., 2013). This mesh has y^+ values (dimensionless measure of the boundary layer) equal to 32.5, which is suitable for the simulation of turbulent cases. Its “grid convergence index” (Roache, 1997) was 2.34 %. Details of the meshes with this refinement for different configurations of the bioreactor are shown in Figure 2.

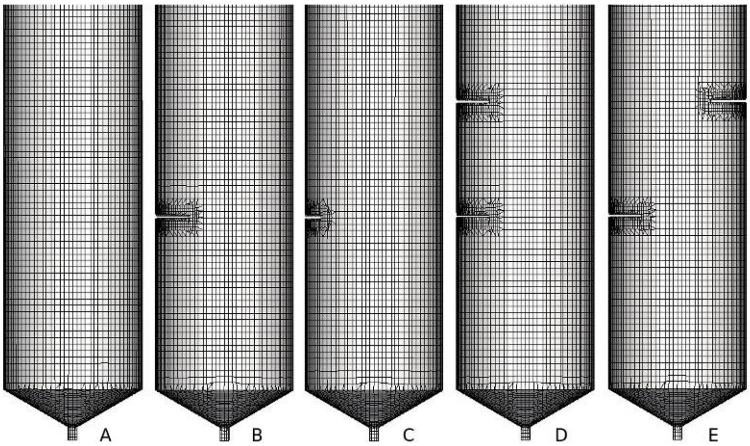

Figure 2: Computational mesh of bioreactor (A), with baffles of 0.151 m (B), 0.075 m (C), and of different positions (D and E) respectively.

Table 1: Properties of the baffles included in each simulated case.

Case	Number of baffles	d	Position
A	none	–	–
B	one	0.151 m	1 m from the bottom
C	one	0.075 m	1 m from the bottom
D	two	0.151 m	same side
E	two	0.151 m	opposite sides
F	two	0.075 m	same side
G	two	0.075 m	opposite sides
H	none	–	–
I	one	0.075 m	0.5 m from the bottom
J	one	0.037 m	0.5 m from the bottom
K	two	0.075 m	same side
L	two	0.075 m	opposite sides
M	two	0.037 m	same side
N	two	0.037 m	opposite sides

Both phases were considered incompressible. The continuous phase was characterized as a Newtonian fluid, with rheological properties similar to the mixture between the microbial culture and substrate, composed by vinasse and glycerin. For the dispersed phase, the properties of biogas were applied. The simulations disregarded fermentation reactions. Thus, the dispersed phase was characterized according to Ding et al. (2010), as spherical bubbles with a uniform diameter of 0.001 m. Both phases are injected at the pipe located in the bottom of the reactor. An upward flow rate of 0.00159 m³/s was applied to the large bioreactor. A flow rate of 0.00079 m³/s was applied to the smaller reactor, to maintain the same retention time. An amount of approximately 5.8 % of these flow rates are composed of bubbles, which corresponds to the gas production in the reactor. A total simulation time of 300 s was considered, of which 200 s is necessary to establish a pseudo-steady state flow in the bioreactor, and 100 s are used to calculate the average values of transient results. Table 2 shows the boundary conditions and physical properties used in the cases proposed.

The system of linear algebraic equations is partially solved at each iteration. Thus, several iterations are necessary until convergence is achieved. As convergence criterion, the total residue was set to 10^{-5}, and as stability criterion, the number of Courant-Friedrichs-Lewy (CFL) was kept below 1 when performing the calculations.

$$\mathrm{CFL} = U\frac{\Delta t}{\Delta x} \tag{1}$$

where U is the mixture velocity (m s^{-1}), t is the time step (s) and x is the control volume size (m).

Table 2: Operational conditions and physical properties used in the numerical simulations.

Operational Conditions		
Inlet	Total flow rates of 0.00159 and 0.00079 m³/s	
Outlet	Pressure of 101,325 Pa	
Walls	Smooth surface, non-slipping condition for both phases	
Physical Properties		
Phase	Density	Kinematic Viscosity
Disperse (gas)	0.089 kg/m³	$8.4\text{x}10^{-6}$ m²/s
Continuous (liquid)	1,009.7 kg/m³	$1.0\text{x}10^{-6}$ m²/s
Bubbles Diameter	0.001 m	

Although most of the gas bubbles leave the bioreactor exit located on the top, a small amount can pass through the side outlet, along with the liquid. Thus, the amount of liquid leaving the system varies. To maintain a constant total quantity of liquid inside the bioreactor, a new boundary condition was established to determine the liquid flow in the bioreactor, and adjust the inlet condition according as expected in a recycle duct:

$$\alpha_{g,in} = 1 - \frac{U_{l,out}\, A_{out}\, \left(1-\alpha_{g,out}\right)}{U_{l,in}\, A_{in}} \tag{2}$$

where U_l is the liquid velocity (m s^{-1}), α_g is the gas volume fraction (m^3 m^{-3}) and A represents the boundary area (m^2). With this new boundary condition, the liquid volume was maintained constant in the simulation, even after a long flow time simulation (300 s).

3. Results and Discussion

Average values were calculated, using simulated results between 200 and 300 s of flow. Figure 3 shows the vector field of the liquid phase obtained in the simulation of the larger bioreactor, collected at a transversal section along its height, and Figure 4 presents the respective turbulent kinetic energy.

Large vortices were observed in the unobstructed flow (Figure 3A). Even without baffles, the flow presents asymmetries. With the inclusion of one baffle, the flow is partially obstructed, thereby following a preferred path. In Case B, with includes a baffle with 0.151 m of length, or half the radius (Figure 3B), it is noted that even though the flow followed a preferred path, there are still vortices in the bioreactor. The adoption of one baffle with length equal to 0.075 m or ¼ of the radius (Figure 3C), was sufficient to equalize the flow. Such behavior is also observed in Figure 3G, which shows the flow in the presence of two baffles with a length of 0.075 m, positioned on opposite sides. In this case, there is only one large vortex positioned near the outlet of the reactor.

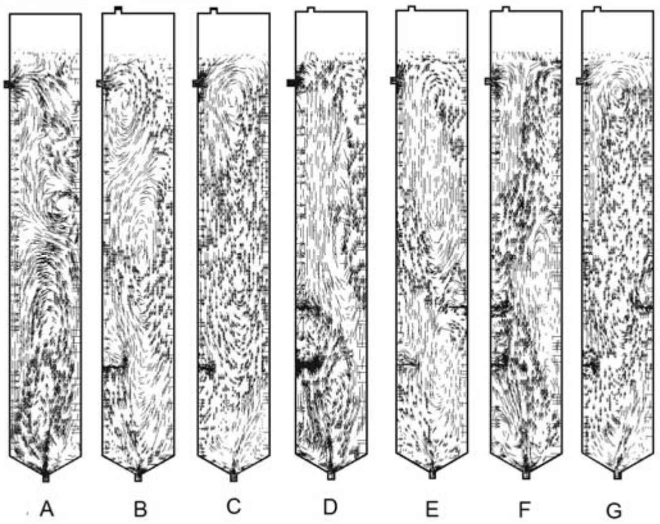

Figure 3: Vector field of liquid phase for Cases A, B, C, D, E, F and G.

The turbulent kinetic energy (k) can be used as an indirect measure of mixing within the reactor, since this energy is defined as the instantaneous velocity deviation. In Figure 4, it is noted that the turbulent kinetic energy is strongly influenced by the inclusion of baffles. In the base case (Figure 4A), there are small values of k in most regions of the bioreactor, except in regions close to the inlet and outlet. In the remaining cases, the inclusion of obstructions to flow resulted in an increase of the turbulence throughout the reactor, as well as a considerable reduction of "dead zones", or regions with little movement. The simulation of a reactor with one baffle of length equal to ¼ of the radius provided the highest increase in the turbulent kinetic energy (Figure 4C). In this case, the dead zones are diminished and a better mixing is achieved.

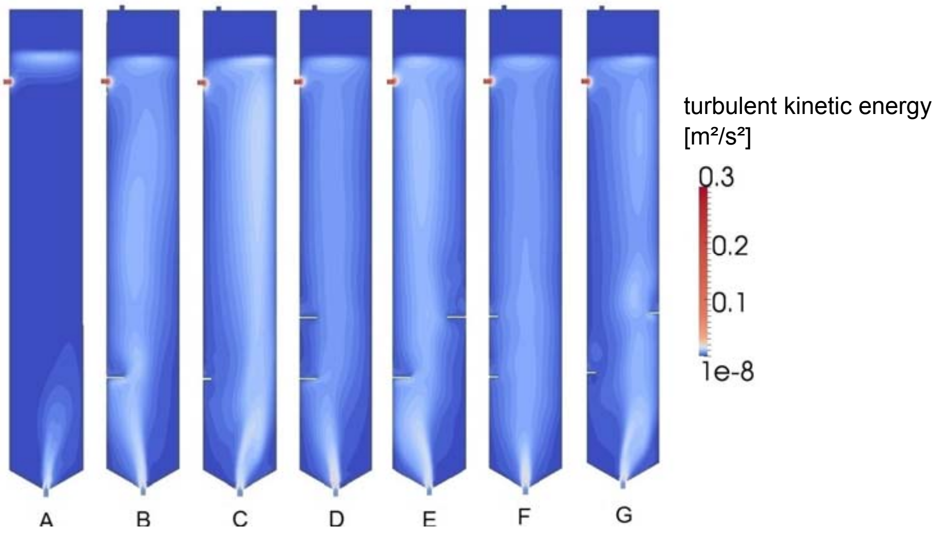

Figure 4: Turbulent kinetic energy obtained in Cases A, B, C, D, E, F and G.

Figure 5 shows the turbulent kinetic energy fields, obtained in the simulation of the 0.125 m³ reactor. Unlike the previous cases (Figure 4), the inclusion of obstructions to flow not always provided an increase in turbulence: for the cases with two baffles on opposite sides (Figures 5L and 5N), it was actually decreased. With the inclusion of a baffle with a length equal to half the radius (Figure 5I) or two at the same side of the reactor (Figure 5K), there is an intensification of turbulent kinetic energy along the feed stream of the reactor. This is also verified in the simulation considering two baffles with length equal to ¼ of the radius (Figure 5M). In this condition, the higher turbulent kinetic energy is transported throughout the reactor, which resulted in the optimal mixing.

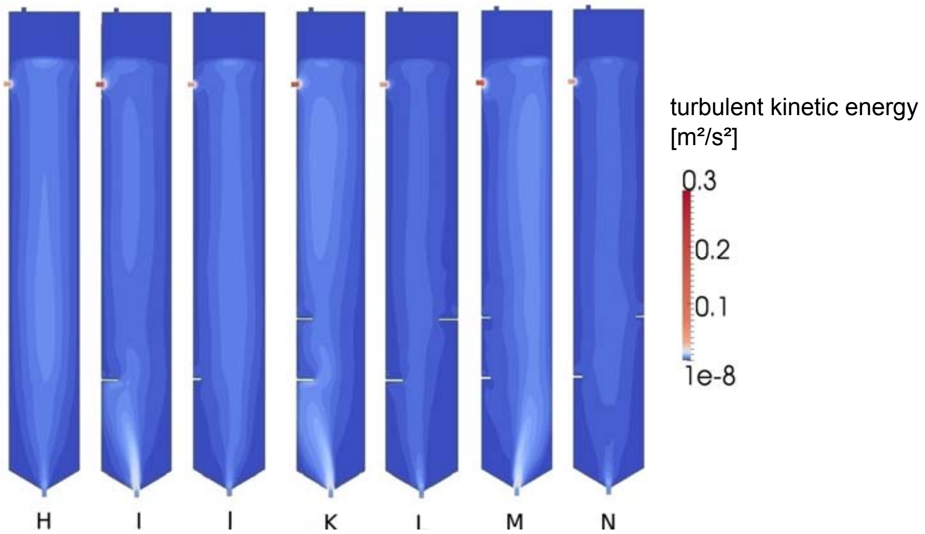

Figure 5: Turbulent kinetic energy obtained in Cases H, I, J, K, L, M and N.

The analysis of the turbulent kinetic energy showed the mixing conditions for each reactor. However, the resulting pressure after each change in the reactor must be analyzed. Since the bioreactor runs in batches of 24 h, the energy imposed to the flow recirculation can be a limiting factor for the operation of the process. Table 3 shows the calculated values for the difference between the pressure measured at the inlet and outlet of the bioreactor, in all simulated cases. Only small differences were observed, because the low recirculation flow resulted in a pressure drop far below the hydraulic pressure, which is incorporated in the calculated values. The highest value is observed for the case without baffles (Case A), which was attributed to the energy dissipated by excessive shear stress in flows without a preferred path. The inclusion of small baffles (Cases C and L) resulted in low pressure differences, when compared to other cases.

Table 3: Pressure difference resulting with the inclusion of baffles in the bioreactors.

Case	A	B	C	D	E	F	G
Pressure difference (Pa)	35,204	35,045	35,090	35,179	35,099	35,134	35,084
Case	H	I	J	K	L	M	N
Pressure difference (Pa)	17,225	18,218	17,204	18,164	17,216	18,190	17,214

4. Conclusions

Numerical simulations were applied to evaluate the influence of obstructions, with different sizes and positioned at different heights, in the flow of a bioreactor. It was found that the inclusion of certain baffles can provide a gain in the turbulent kinetic energy, due to the presence of preferred paths. Higher turbulence provides better mixing, and thus a better efficiency in the bioreactor. The best configuration among the evaluated variations was the inclusion of only one obstruction with size equal to ¼ of the radius of the reactor, as it resulted in an increase of the turbulent kinetic energy and little changes in pressure drop. This result is important for industrial-sized bioreactors, which are concerned with energy demand.

Acknowledgments

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