Numerical investigation of hydrodynamics in submerged membrane bioreactor with aeration

V. Iliev, D. Moutafchieva*, R. Doukovski

University of Chemical Technology and Metallurgy, 8 Kl. Ohridski Blvd., 1756 Sofia, Bulgaria

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Submerged membrane bioreactors (SMBRs) are an established technology for wastewater treatment, but the efficient fouling reduction by air sparging remains an operating problem and the design rules are still of a purely empirical nature. Therefore, many modeling approaches have been proposed to solve these operating problems and increase the process efficiency. The design of SMBRs is affected by a combination of both hydrodynamic and biological conditions, CFD models and simulations should be performed considering both of these phenomena. The present study focuses on the design of a SMBRs and on the determining of the required aeration rate to achieve a minimum deformation rate of the material in the membrane boundary layer referred to as 0.8 s⁻¹. Following determination of the dimensions and operating parameters of the bioreactor and the membrane module with MATLAB, computer simulations of cell growth have been performed in the selected SMBR with the software ANSYS CFX. The rate of deformation in the boundary layer at inlet air velocities from 0.1 m/s to 0.8 m/s was calculated and dependences for the rate of deformation at the boundary layer on the outer side of the membrane were obtained. It was also found that in order to achieve the set minimum strain rate of 0.8 s^{-1} the minimum aeration velocity should be 0.55 m/s. CFD modeling of SMBRs allowed calculations of the appropriate shear on the membrane surface in order to control sludge filterability and fouling. The adequacy of the computer model used was confirmed by comparing the numerical results obtained by ANSYS CFX with those obtained by MATLAB. The results obtained could be used to clarify the effect of aeration on shear rate in order to achieve more intense turbulence in the reactor that could contribute to the higher efficiency of the membrane module.

Keywords: Submerged membrane bioreactor (SMBR); CFD; Shear stress; Bubble column

INTRODUCTION

Membrane reactors with submerged membrane (SMBR) and aeration of bubble or airlift columns with integrated membrane module use the favorable effect of the two-phase gas-liquid flow on the shear stresses around the membrane. The increasing of the shear stresses to the membrane is considered one of the most effective ways to control its blockage. Therefore, it is important to study the field of tangential stresses and its homogeneity near the surface of the membrane, for which there is no systematic information.

The design of SMBRs is mainly based on knowledge of biokinetics and the conditions under which membrane clogging occurs, although the hydrodynamics in SMBRs are crucial for the operation of these reactors. The influence of the flow regime in the process of design and operation of SMBRs is not sufficiently studied and analyzed. The current methods of designing the desired flow regime within the SMBRs are largely based on empirical techniques (for example: the specific mixing energy). It is difficult to predict how the scaling of the apparatus and the design of industrial installations (size and position of inlets, barriers or membrane orientation) will affect the hydrodynamics and therefore the overall performance of the membrane reactor. Recently, and more studies are more using CFD (Computational Fluid Dynamics) techniques for studying and modeling of the fluid flow through a membrane module and for studying the factors that cause membrane contamination. CFD is a widely used tool for studying membrane contamination and for studying the mechanisms and factors that influence this process. The computational dynamics of the fluids makes it possible to predict how the characteristics and geometrical operating parameters of the submerged membrane bubble reactor will affect the hydrodynamics and the choice of the optimal design and therefore the performance of the aerated membrane bioreactor.

In the present work a two-step algorithm of SMBR design - e.g. supported by MATLAB and CFD, was verified in a way as to ensure productivity at a reference deformation rate not allowing eventual cell death.

Controlling the hydrodynamic conditions near the membrane is extremely important for the stability of the flow, as well as for minimizing the required membrane surface, reducing the collected

^{*} To whom all correspondence should be sent: E-mail: dessislava_moutafchieva@yahoo.com

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sediment on the surface and increasing the transmembrane pressure (TMP) or constant permeate flow. The increasing of the shear stresses to the membrane is considered to be one of the most effective ways to control its blockage.

The shear forces are generated by pumps, by bubbling or by stirring devices to remove the layer formed on the membrane. Of course, care should be taken for possible deactivation of shear-sensitive components. In this sense, the hydrodynamic environment in the MBR (membrane bioreactor) is a compromise between the requirements of the separation process (the area around the membrane surface) and the biochemical reaction (in the reactor volume). From a computational point of view, this means studying the field of velocities and tangential stresses and its homogeneity in these two areas [1, 2].

A large number of studies [4-7] show that the shear stress of the wall is a very important parameter that can be used to indicate the effectiveness of the membrane. It is known that particles accumulated on the surface of the membrane will be washed away when the shear stress increases, as it can increase the reverse transport of the particles away from the membrane. An earlier study of the relationship between membrane contamination and the relationship between permeate flow and wall shear stress was performed by Le Berre and Daufin in 1996 [4]. It shows that the ratio between the permeate flow and the shear stress of the wall can be a useful parameter for predicting the performance of the membrane under different operating conditions. In later studies [5-9], the effect of wall shear stress on membrane contamination during membrane filtration was investigated by digital simulation using CFD [5-8] or investigated experimentally [9].

There are studies that correlate each process resistance to a linear function of the shear stresses on the membrane surface created by the liquid and gas phases. It has been found that the size of the gas bubbles is of significant importance for the shear stresses of the membrane surface. Thus, the aeration of submerged MBR is one of the main topics studied.

The purpose of aeration is to generate small gas bubbles that are evenly distributed across the cross section of the apparatus, thus achieving better mixing of the liquid and more intensive mass transfer. The dispersion of the gas is obtained by passing it through openings, a porous medium or by mixing the gas with a rapid stream of liquid. The rising gas bubbles in contact with the surface of the membrane affect in the direction of reducing the concentration polarization and, respectively, the formation of a layer of sediment on it. The effect comes from the liquid phase, respectively, from higher actual velocities to the membrane (related to the volume part of the liquid phase in the reactor, 1- $\varepsilon_{\rm G}$), as well as the mechanical impact of the bubbles on the membrane, which washes away the sediment layer. In submerged MBRs, air dispersion not only delivers oxygen to the biomass, but also retains solids in suspension and is used to reduce membrane contamination by creating a shear stress. The efficient air distribution contributes to the permeability of the membrane, the stability of the applied flow and the reduction of pollution. The appearance of bypass jets and fluid channels, which lead to enhanced sludge removal and high transient shear patterns, is influenced by the interactions between the fluid and the structure. The efficiency parameter of gas bubbling depends on the gas velocity, the size of the nozzle and the concentration of the suspension; the efficiency of the module is affected due to changes in the local flow distribution and suction pressure of the module outlet. [1,16].

The membrane reactors with mechanical stirring combine the hydrodynamic picture created by a certain type of stirrer in the volume of the reactor with that around the surface of the membrane. The size and the direction of the velocity vectors of the fluids to the membrane strongly depend on the stirring rate. The specific design of the agitator and the location of the diaphragm relative to it significantly affect the velocity fields and shear stresses of the diaphragm. The submerged membrane bioreactor allows higher concentrations to be reached relative to the cells and makes it possible to retain the cell mass in the reactor. They are suitable solutions when the goal is to increase the concentration of cell mass in a biomass production reactor.

In the selected type of bioreactors with stirring and aeration, gas bubbles and mechanical stirring jointly affect the uniformity of distribution of velocities and shear stresses to the membrane surface.

The membrane module is placed in the aeration zone to use the beneficial effect of both factors (gas and mechanical stirring) on the reduction of membrane contamination [1, 2].

The optimal operation of the membrane reactor is related to:

• the position of the membrane module in the reactor;

- the gas / liquid ratio;
- the transmembrane pressure;
- the creation of sufficient shear stresses.

Relatively new and few are the attempts to model the process taking into account the dynamics of the relationship between the transmembrane pressure, the shear stresses of the membrane and the flow through the membrane.

EXPERIMENTAL

Description of the bioreactor

For the purpose of the study, based on the literature review, the bioreactor is composed of two chambers (1-outer chamber and 2-inner chamber). The substrate necessary for cell growth passes in the outer chamber through the lower opening (9). It then passes through the membrane surface (5) into the inner chamber, where the cell growth takes place. An agitator (4), driven by an electric motor (13), is mounted in the inner chamber. A toroidalshaped sparger (3) is placed in the lower part of the outer chamber, through which air for mixing the materials and cleaning the membrane module is introduced. The air required for aeration is introduced through the supply pipe (11), released on the free surface of the solution in chamber 1 and exits through a ventilation opening (12). The membrane module can be dismantled by predismantling the electric drive motor (13) and the gearbox (14) and separating the fastening elements (8) from the bed of the membrane unit (7).



Fig. 1. Submerged membrane bioreactor with stirring and aeration

Numerical experiment for determining the size of the membrane bioreactor

The required volume and height of the membrane bioreactor were determined by a numerical experiment in the programming environment MATLAB, to achieve the desired cell productivity of 6 g/h. To determine the height, the

following ratio H/d = 1.5 was taken for a laboratory reactor with standard geometry and the diameter was calculated from the volume obtained from the experiment. Figure 2 shows the dimensions of the components of the bioreactor.

The cell growth in the inner chamber, as well as the amount of substrate in both chambers was calculated using the ode23 function in the programming environment MATLAB, which allows up to three differential equations to be calculated. The balance equations used are the following (perfect mixing is assumed):

• for the substrate (S₁) in the outer chamber:

$$\frac{dS_1}{dt}V_1 = \dot{v}S_0 - \dot{v}S_1 - Per(S_1 - S_2)$$
(1)

• for the substrate (S₂) in the inner chamber:

$$\frac{dS_2}{dt}V_{12} = Per(S_1 - S_2) - \frac{1}{Yx/s}\mu XV_2$$
(2)

• for the cells (X):

$$\frac{dX}{dt}V_2 = \mu X V_2 \tag{3}$$

For the parameters of this model we used experimental data from the literature review (cell growth) [1]: mono kinetics with parameters: $\mu_{max}=0.5$ h⁻¹; Ks=0.12 g/l; Y_{x/s}=0.52; initial substrate concentration S₀= 2 g/l; flow rate on the outer chamber $\dot{v}=$ 2 l/h and membrane data: Per=0.52 dm/h and A=5.29 dm².



Fig. 2. The bioreactor dimensions. $V1 - 0.0014 \text{ [m^3]}$; $V2 - 0.0014 \text{ [m^3]}$; D1 - 0.067 [m]; D2 - 0.053 [m]; H1 - 0.201 [m]; H2 - 0.159 [m]; d1 - 0.002 [m]; d2 - 0.116 [m]; h1 - 0.021 [m]; h2 - 0.035 [m]; h3 - 0.056 [m]; h4 - 0.03 [m]; $\emptyset1 - 0.01 \text{ [m]}$; $\emptyset2 - 0.005 \text{ [m]}$; $\emptyset3 - 0.01 \text{ [m]}$; $\emptyset4 - 0.01 \text{ [m]}$; $\emptyset5 - 0.01 \text{ [m]}$.

From the obtained results it was determined that for achieving the required productivity of 6 g/h, the volume of the membrane module must be 1.4 dm^3 (Fig. 5). Figure 2 shows the dimensions of the components of the bioreactor. The influence of the aeration in the outer chamber and the agitation in the inner chamber were not taken into account during the sizing with MATLAB. These factors were included in the calculation procedure with the program environment ANSYS.

Experiment for determining the minimum aeration velocity

The computer simulation was performed on the working volume of the reactor shown on Figure 3. The immersed membrane is placed at a distance of A = 0.021 m from the base of the reactor and has a height of H = 0.159 m and a diameter of D = 0.053 m. The toroidal sparger, with a diameter of D = 0.01 m and a ring radius of R = 0.058 m, is located at the lower end of the reactor at a distance of B=0.01 m from the base. The agitator is located at a distance of C= 0.056 m from the base of the reactor and the distance between the two propellers is E= 0.03 m. This size also corresponds to their height, and the length is the same for both.



Fig. 3. Schematic representation of the experimental reactor

The inclusion of a sparger in the reactor design increases the turbulence and affects the rate of deformation along the length of the membrane module. The aeration process tends to be highly turbulent, which requires an appropriate model of turbulence. In a computer simulation, the turbulence model k- ε is used to correctly determine the rate of deformation around the membrane wall. This turbulence model is commonly used to model bubble columns, as it is a trade-off between computational accuracy and efficiency [17]. The distribution of the strain rate along the membrane is more homogeneous in the presence of gas. Rising gas bubbles in contact with the membrane surface affect the direction of reducing the concentration polarization and respectively, the formation of a layer of sediment on it [1]. For the purposes of the present work, it is accepted that the minimum strain rate, at which cake layer formation and membrane clogging is prevented, is 0.8 s^{-1}

The complete modeling of the two-phase flow in the ANSYS programming environment was performed according to the methodology, which includes creating a geometric model of the object, crosslinking the studied object, setting the variables describing the physicochemical behavior of the fluid in the reactor and setting the initial and boundary conditions of the process.

Experimental conditions

Initial conditions of the numerical experiments:

• the amount of air supplied by the sparger is equal to 0.05 volume fractions, which at the specific dimensions of the sparger corresponds to 100 openings, creating bubbles with a diameter of 6 mm;

• the amount of the mixture which includes two solutions - Mixture and Cells, at the entrance, is equal to 0.95 volume fractions;

• the degassing function, which is provided by the software product ANSYS CFX, is used for the gas output;

• the equations 1-3 are used for the calculation of the growth of the cells in the membrane module;

• the water concentration is set to Constant.

The experiment was performed at an air velocity ranging from 0.1 m/s to 0.8 m/s with a step of 0.1 m/s. After each experiment, the average angular strain rate on the surface of the membrane on the side of the outer chamber was calculated using the built-in calculator. Additional cutting planes were constructed to monitor process characteristics as flow rate and reactor pressure.

Experiment for determining the maximum agitator velocity

This experiment was performed under the same conditions as the experiment to determine the minimum aeration velocity. The observations are concentrated on the inner chamber, where the cell growth takes place. The main parameter in this experiment is the angular velocity of the agitator, which varies in the range from 5 rev/min to 35 rev/min with a step of 5 rev/min. To observe the hydrodynamic characteristics of the process, the built-in program calculator and additional intersecting planes were used, as in the previous experiment.

RESULTS AND DISCUSSION

Determining the required reactor volume to achieve the desired cell productivity

Numerical experiments were performed in the MATLAB software environment to determine the operating parameters of the membrane module and the size of the entire reactor, varying the volume of the membrane module from 0.55 dm³ to 1.6 dm³ in steps of 0.1 dm³. A computer simulation with different reactor volumes was performed to monitor cell growth and the results are presented in Figure 4.



Fig. 4. Cell growth: S1 - concentration of substrate at the outlet of the reactor; S - concentration of substrate necessary for cell growth; X - concentration of cells.

The graph of the figure above shows that as the reactor volume increases, the growth rate of the microorganisms decreases (the slope of the graph lines decreases). The highest concentration of cells is at a membrane module volume of 0.55 dm^3 , however, the productivity relative to the reactor volume at this size is too low, which is explained by the smaller volume of the membrane module.

From the graph on Figure 5 it is reported that the set productivity of 6 g/h is achieved at a volume of 1.4 dm^3 . The two chambers of the reactor have the same volume, therefore the inner and outer chambers are 1.4 dm^3 and for the volume of the whole reactor we get a volume of 2.8 dm^3 .

Determining the rate of deformation by different aeration velocities

Aeration has a significant effect on the shear rate, by increasing the degree of aeration more intense turbulence is achieved inside the bubble column. In addition, aeration contributes to the higher efficiency of the membrane module by reducing the formation of sediment on the membrane surface. The presented results on Figure 5 show the dependence of the deformation rate at the boundary layer on the outer side of the membrane. The software environment ANSYS CFX is used to calculate the deformation rate at the boundary layer at different velocities of the introduced air from 0.1 m/s to 0.8 m/s.



Fig. 5. Performance curve for membrane size between 1.2 dm^3 and 1.6 dm^3





From the graph of Figure 6 it is seen that as the air velocity increases, the strain rate also increases. On one hand, this tendency prevents contamination of the membrane module, but may have a negative effect on the cells that are being developed in the reactor. For the set minimum strain rate of 0.8 s⁻¹, the graph shows a minimum air velocity of 0.55 m/s.

ANSYS CFX allows the obtained numerical results for the strain rate in the outer chamber of the reactor to be presented in vector form, as well as in the form of color contours (Fig. 7).

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Fig. 7. Shear rate in the outer chamber: at an aeration speed of 0.2 m/s (a); at an aeration speed of 0.4 m/s (b); at an aeration speed of 0.6 m/s (c)

Determination of shear stresses at different agitator speeds

Figure 8 shows the results for the distribution of the shear rate in the inner chamber of the reactor, caused by the agitator at different speeds from 5 rev/min to 30 rev/min.



Fig. 8. Deformation rate caused by the agitator



Fig. 9. Deformation rate caused by the agitator: at a stirring speed of 20 rev/min (a); at a stirring speed of 25 rev/min.



Fig. 10. Deformation rate caused by the agitator at a stirring speed of 10 rev/min (a); at a stirring speed of 15 rev/min (b); at a stirring speed of 20 rev/min (c); at a stirring speed of 25 rev/min (d).

From the graph in Figure 8 it can be seen that in order to reach the set maximum deformation speed of 15 s⁻¹ the maximum speed of the agitator must be 22 rev/min.

It can be seen from Figures 9 and 10 that as the stirrer speed increases, the strain rate also increases, which leads to better mixing, but can also lead to the destruction of living cells in the inner chamber of the reactor. The strain rate shown in Figure 10d, when rotating at a fast speed of 25 rpm, is the most pronounced with the highest achieved strain rate being colored in red and the lowest in blue.

Comparison between the MATLAB and ANSYS CFX results for cell growth in the inner chamber of the reactor



Fig. 11. Cell growth with ANSYS CFX: (a), with MATLAB (b): S1 - concentration of substrate at the outlet of the reactor; S - concentration of substrate necessary for cell growth; X - concentration of cells.

The results obtained are shown in the above figures with different magnitudes in time, as in MATLAB the time is represented in hours, while in ANSYS CFX it is in seconds. The disturbances that are seen on the graph obtained with ANSYS (Fig. 11a) appear after 18 hours. In general, the two graphs are identical, which can be considered as a verification of the computer simulation model used.

CONCLUSION

The two-step procedure combining MATLAB and CFD can be successful in predicting the SMBR design at given productivity and produce visualization of bioreactor fluid dynamics in a way as to avoid pathological condition of cell death. The case study shows that a lab-scale SMBR equipped with a frame membrane could ensure substrate bioconversion of up to 90% for 25 h at zero cell death simulated as reference strain rate less than 0.8 s^{-1} introduced as moderate agitation rate of 22 rev/min. and air velocity of 0.55m/s. The ANSYS CFX software environment makes it possible to formulate a comprehensive computer model and describe the hydrodynamic situation in the bioreactor and around the membrane module in detail. Accordingly, the computer model, thus created, is verified by using the results obtained from calculations with MATLAB.

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