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Comparison of a Model Fixed-Bed Bioreactor, Plating a Model of N-Reactors in Series Perfectly Blended and a Tubular Reactor Model, and Simulation Models

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The objective is this study is to simulate a fixed-bed bioreactor using two different arrangements, the first is the modeling of N-reactors in series perfectly blended and then developing a model of a tubular reactor, and comparing the results of both and choose which one is the most appropriate model for optimization, in addition to corroborate the hypothesis that a tubular reactor can be represented as the sum of several reactors in series perfectly mix, the general idea is to have a generic model for the bioreactor that allows changes only to the generic parameters of the kinetic and physical properties of food to make a simulation for a bioreactor that fits within the designed parameters. The main model presented uses the Michaelis-Menten kinetics, with a packed bed bioreactor, which is used to produce ethanol from glucose, based on what the two models were made. After verifying the convergence of both models was performed to compare them, in the final concentration of N-reactor model mix as compared to real data bioreactor get an error of 2.9 % compared to the concentration of ethanol at the outlet of the reactor and for the same values the error of the tubular reactor model was an error of 7.1 % compared with the ethanol concentration at the outlet of the reactor. Consequently, it was decided to perform the model of perfect mixing N-reactors and validate the model with a scale bioreactor pilot plant wich is used for the purification of contaminated water with volatile organic compounds (VOCs), the simulation result of this model proved to be a difference of 1.7 % compared to the concentration of COD from the pilot plant.

1. Model Approach (AL-Muftah and Abu-Reesh 2005)

To develop the mathematical model must be defined as the boundary conditions and assumptions that must be taken into account. To perform the simulation then the assumptions are taken into account in the model are as follows:
We work with an isothermal reactor with immobilized enzymes packed bed. Neglect the resistance of the membrane to any transport process. The enzyme activity is uniform throughout the exterior of the particle. The enzymes are immobilized in porous spherical particles, which are considered uniform throughout the reactor. The convective velocity on the surface of the particles is uniform. The pressure drop through the reactor and the radial concentration gradient is supposed to be so small that it is negligible. It is assumed that the flow of air circulating through the bioreactor is constant, so that there is sufficient oxygen supply throughout the bioreactor so that it can produce the biochemical reaction, It is assumed that no enzyme deactivation. The enzyme can be catalyzed and specified by the Michaelis-

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Menten kinetics. The enzymatic reaction is single substrate type, which only obtained a single product. Frick's law is used to model the diffusion of both substrate and product. The efficiency of the diffusivity is constant for all particles and is independent of the concentration.

1.1 Mathematical Model

To make the approach of the mathematical model to be simulated, there were two different models. The idea is to get and to choose the best model that can be used for the simulation, then perform its validation with experimental data. The model itself is a mathematical representation of the phenomenon under study, in this particular case you want to study the operation of a fixed-bed bioreactor with immobilized enzymes (Atkinsos, 1986; Bailey and Ollas, 1986; Dunn et. al 2003).

For both models we used the enzyme kinetics of Michaelis-Menten, which is most appropriate for the study of immobilized enzymes, that in case where both are considered to study biofilm.

The models will be raised are the following: the first examines the fixed-bed bioreactor as a succession of several reactors CSRT in series, this according to Fogler (2001), is a most common ways to represent a reactor plug flow, and as discussed in the assumptions, one of them is the assumption that the reactor is studied as if it were a plug flow reactor. In the second model proposes a model of tubular bioreactor with immobilized biocatalyst.

1.2 Apparent Kinetic (Lema and Roca 1998), (Znad et. al 2004)

Taking a differential flow over the length and making the transformation from hour to seconds and clearing the flow differential kinetic equation is apparent in the following way:

The apparent kinetic equation and the transformation of the saturation constant and the speed of fermentation units are suitable according to

$$N_i = \frac{r_{pm} C_i}{K_{SAT} + C_i} \tag{1}$$

Taking a differential flow over the length and making the transformation from hour to seconds and clearing the flow differential kinetic equation is apparent in the following way:

$$dN_i = r_{pm} * \frac{C_i}{K_{SAT} + C_i} \frac{\overline{\rho}}{3600} dl \tag{2}$$

1.3 Balance for the bioreactor CSRT

The flux of glucose at any point of the bioreactor is given by equation 2

$$N_g = Kl_g \left(Cg_0 - Cg \right) \tag{3}$$

Differentiating with respect flow (N) with respect to length, and knowing that the hollow portion of the bioreactor is 40.8 %

$$dN_g = Kl_g \left(Cg_0 - Cg \right) \frac{0{,}408}{h} dl \tag{4}$$

Carrying a balance for glucose to any point in the bioreactor taking equation (3) and equating (4), the apparent kinetics equation yields the following equation for any point in the bioreactor

$$Kl_g \left(Cg_0 - Cg \right) \frac{0{,}408}{h} dl = r_{Mf} \frac{Cg}{K_{SAT} + Cg} \frac{\overline{\rho}}{3600} dl \tag{5}$$

A balance sheet for the bioreactor is given by the following equation where the flow of ethanol in the birth of microorganisms is equal to the flow of glucose plus cell death

$$N_e + K_{Nc} = N_g + K_{Mc} \tag{6}$$

1.4 Mass balance approach in the tubular reactor

Taking into account the assumptions made for the bioreactor, the differential material balance between the substrate and the product can be described as follows. For the substrate:

$$\frac{\partial C_{Sv}}{\partial t} = D_{Sz}\varepsilon\frac{\partial^2 C_{Sb}}{\partial z^2} - u\frac{\partial C_{Sb}}{\partial z} - (1-\varepsilon)K_L a(C_{Sb} - C_S) \tag{7}$$

For the product:

$$\frac{\partial C_{Pv}}{\partial t} = D_{Pz}\varepsilon\frac{\partial^2 C_{Pb}}{\partial z^2} - u\frac{\partial C_{Pb}}{\partial z} - (1-\varepsilon)K_L a(C_{Pb} - C_P) \tag{8}$$

In these equations take into account both the hollow space left in the reactor and, as the diffusivities of each of the elements present in the biochemical reaction, and the mass transfer constant average for the whole reactor.

The initial conditions for starting the reactor containing immobilized enzymes suspended in a solution without substrate or product. At the beginning of the operation is pumped to a constant flow substrate, generating product that comes at the same flow that goes into the product. Equations 8 and 9 are subject to the following boundary conditions. At z = 0 +

$$C_{Sb}\big|_{z=0^+} = C_{Sb}\big|_{z=0^-} + \frac{D_{Sz}}{u}\frac{\partial C_{Sb}}{\partial z} \tag{9}$$

At z = L

$$\left.\frac{\partial C_{Sb}}{\partial z}\right|_{Z=L} = \left.\frac{\partial C_{Pb}}{\partial z}\right|_{z=L} = 0 \tag{10}$$

The mass balance equations of the substrate and product particles of immobilized enzymes in spherical porous particles are given by:

$$\frac{\partial C_S}{\partial t} = D_{Sp}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_S}{\partial r}\right) - R_S \tag{11}$$

$$\frac{\partial C_P}{\partial t} = D_{Pp}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_P}{\partial r}\right) + R_P \tag{12}$$

2. Results and Discussion of Results for the Simulation Model Bioreactor

2.1 Results of model N-reactors CSRT in series

First, a simulation with values obtained from a model proposed by Lema and Roca(1998), which shows a model to simulate a fixed-bed bioreactor using glucose as substrate at a concentration of 96.2 g/L at the input, and flow of 3 L/h, to produce ethanol. By introducing the values given by Lema and Roca for the bioreactor inflow, and taking into account all the assumptions made for the model, simulation was carried out. The solution obtained for a flow of 3 L/h. These results are then compared with those obtained by Lema and Roca (see Table 1) showing the numerical values obtained at the outputs of each of the reactors CSRT.

As for this mathematical model is considered series of reactors CSRT in series is separated into the bioreactor volumes is as close as possible in order to satisfy the hypothesis which says that a tubular reactor can be represented as N-reactors CSRT in series. When making a comparison of these results with those obtained by Lema and rock, as shown in Figure 1 and Table 1, the difference between them is almost minimal, where you can see a major difference is the result of the first stage where there is an error of 14.1 %, while the fourth stage in an error of 3 % to the value resulting (Lema and Roca 1998). One of the interesting things to discuss, is that value which gives the error of 14.1 %, because it can be interpreted as a high value, which even can be despised, not knowing that the simulation program was Lemma and model can not rock planet an exact reproduction of the model proposed by them, and this causes a difference in the results also unaware that the

numerical method was used. In the case of the proposed model was used the EcosimPro simulation and modeling tool, because the mathematical approximation methods that were used are different from each other, consequently resulting in error that difference. But when making a comparison to the output value generated in the bioreactor, we can say that the model has converged efficiently, since it got error of 3 %, where in order to assume that the model was correct was expected error of less than 5 % at the outlet of the bioreactor.

2.2 Results of the model of the bioreactor packed

As It was described in the previous section, this model was compared with data obtained by Lema and Roca (2008), to allow for a good approximation of the model, when compared with the model of a tubular reactor, it can be evaluated only the output bioreactor until it reaches steady state, without considering the influence of weather on the operation of the bioreactor. The bioreactor simulation took into account both the dispersion of fluid in the axial direction as in the radial direction, with both are assumed to be constant both above and in the radius of the bioreactor. The simulation was conducted by varying height, as per mentioned reference. A comparison between two models is show in table 1.

Table 1: Comparison of the concentrations of the different models

Height of the Bioreactor(cm)	**Model Proposed by Lema and Roca**	**Model of N Serial CSRT Reactors**	**Model of Tubular Reactor**
	Concentration (g/L)	**Concentration (g/L)**	**Concentration(g/L)**
0	96.2	96.2	96.2
7.5	18.2	14.42	24.3
15.5	0.59	0.28	1.1
23.5	1.56×10^{-3}	1.51×10^{-3}	1.68×10^{-3}
27	2.43×10^{-3}	2.35×10^{-4}	5.56×10^{-4}

Table 2: Comparison of the results of the tanks in series model and the tubular reactor

Model of N Serial CSRT Reactors		**Model of Tubular Reactor**	
Concentration(g/L)	**Error (%)**	**Concentration(g/L)**	**Error (%)**
96.2	0	**96.2**	0
14.42	24.1	**24.3**	26.3
0.28	14.1	**1.1**	54.5
1.51×10^{-3}	3.1	**1.68×10^{-3}**	7.9
2.35×10^{-4}	2.9	**5.56×10^{-4}**	7.1

The simulation at the first height (h = 7.5 cm) shows that in an output value of 24.3 g/L glucose generating an error of 26.3 % compared with the value obtained experimentally by simulating the second height (h=15.5 cm), a value of glucose concentration of 1.1 g/L which is obtained and it represents a 54.55 % error with respect to the experimental value at this point. This part has to tell the difference between the two proposed mathematical models, one can observe that the first level of data collection are similar values, but as you progress through the height of the model can see how the values are moving away, this is seen in the differences given by the errors. When performing the simulation for the output of the bioreactor (h = 27 cm), the concentration of glucose was obtained at the output of 5.56×10^{-4} g/L, which means an error of 7.1 % compared with the experimental value of this height. The latter value corresponds to the output of the reactor, detail to comment that the output values are much improved reactor for behavior that had been observed, this means that for the tubular reactor model at the end there has been a correction and the output value greatly resembles the experimental value.

3. Model Validation

With the validation that is done is to compare the model results presented experimental data that the results of the model generates the smallest difference between the two, all the assumptions considered

in the model, so that if the difference can considered negligible. One can say that the generated model is valid for those values. In the event that the error obtained in this model is big enough to say that the model does not generate enough consistent values, you can make corrections in the mathematical model, to make these values have the least deviation possible, thus validating the model.

As it was discussed above, there are two different models for a simulation with each of them, the first making a model of the tubular reactor packed-bed reactors in N-Reactors CSRT, and the second assuming a bed tubular reactor fixed a certain height, to determine which model is most appropriate is the percentage error that occurs when comparing the concentration of substrate at each height of the bioreactor and the value generated by each model to the same height. Another consideration that was done and as with the results shown in the simulation model of N-reactors CSRT is that the results shown at each stage of the bioreactor pilot plant heights were similar therefore can be taken as similar volumes to model effects of N-reactors in series perfect mix. Due to the investigation and silver in his articles and books some authors such as (Fogler, 2001; AL-Muftah and Abu-Reesh 2005; Hasan, et al. 2007; Mitchell, et al. 2010), that for the simulation of a tubular reactor packed bed or use the approximation of N-reactors CSRT in series. The results obtained by entering the pilot plant data on both proposed models are shown in theTable 3 as well as the error obtained in each stage of the bioreactor (see Table 3).

When comparing the two models proposed, the model of N-reactors CSRT in series is chose; because this model gives the lowest percentage error considering the concentrations obtained at different heights in the bioreactor (see Table 3). Assuming that the model of N-reactors to assess the result to the output of each reactor, it becomes easier to compare the values obtained in the mathematical model with those obtained in pilot silver and compare results. In contrast to the tubular reactor model that was done was to simulate the reactor at different heights to produce the results of this model to the different heights of the bioreactor.

The experimental results were obtained from a fixed-bed bioreactor that uses the heart of the corn cob as packing, which allows setting there enzymes that can produce the enzyme kinetics. This bioreactor is designed to remove VOCs that gives gasoline when dissolved in water. One of the assumptions taken into account to assume that using a Michaelis-Menten kinetics of the bioreactor is that it does is make a reduction of COD (mg /L), and thus assume that all VOC is a single substrate for this enzyme kinetics to apply (Huelves and Matos 2003).

From the data shown above and a thorough review of the compounds present in gasoline as a VOC, the following assumptions were made to validate the model. VOCs present in water are as follows: toluene, benzene, xylene and acetone. Since these compounds are determined a medium viscosity and diffusivity for each one of these compounds. Lineweaver-Burk method was used to determine the parameters of the Michaelis-Menten kinetics. The values obtained were as follows: KM=15.1 g/L and Vmax=196.08 h-1 No bacterial growth or death because both are considered equal. The dimensions of the bioreactor used to validate the model were: a height of 2 m and a diameter of 15 cm. The package, is the heart of the corn cob was assumed to have an average area of 10.3 cm^2 and a diameter of 1.8 cm, and a hollow space 40 % of the volume and flow bioreactor operation was 6.25 L/h.

Table 3: Comparison between the model simulation and pilot plant.

Pilot Plant		**Model of N Serial CSRT Reactors**		**Model of Tubular Reactor**	
COD (mg/L)	**Height (cm)**	**COD (mg/L)**	**Error (%)**	**COD (mg/L)**	**Error (%)**
4000	**0**	4000	0	4000	0
1800	**40**	2212.2	22.9	2287.8	27.1
1666.7	**80**	1992.9	19.5	2496.7	49.8
1560	**120**	1708.2	9.5	1837.7	17.8
1453	**160**	1498	3.1	1544.5	6.3
1293.3	**200**	1304.9	0.9	1330.8	2.9

Having obtained all the necessary data is loaded into the model and the simulation is performed in order to generate the data, as shown in table 3. There are five stages in the bioreactor, thus for the simulation, take five reactors CSRT serial and thus able to compare each output of the reactor with the experimental values of each step and calculating the error, to take respective measures to determine if the model is made valid or whether to make an adjustment the model, so that it can adapt to the data and reduce the error in the simulation result.

4. Conclusions

1. Because of the similarity between the results obtained in the simulation model of perfect mixing reactors in series and model of packed-bed reactor, it was decided to use the model perfectly mixed reactor, because it has less numerical difficulties when making simulation and the easiness of the time of the proposed model validation.
2. The proposed mathematical model chosen fits and represents, the behavior of a packed bed bioreactor using immobilized enzymes as a catalyst, when evaluated with respect to initial data, leaving only to validate the proposed model.
3. Due to the limitation of the tool used in this study to develop the model without dimensionless variables, avoiding the need to work with different areas and avoiding the problems of convergence of values is required.
4. During the compilation of experimental values built the Lineweaver-Burk plot for determination of Km and Vmax values, these values obtained by regression analysis, with a regression coefficient of 0,9698, thus verifying that it is a reliable method for the determination of the parameters before mentioned.
5. The selected model converges properly, this can be observed that when getting the values of simulation and a comparison with experimental data, in the corresponding points you show a negligible error.
6. The proposed model is valid to simulate a packed bed bioreactor with immobilized enzymes, which are governed by the Michaelis-Menten kinetics.
7. The choice of model model N-reactors CSRT in series is that this model has the least amount of nonlinear equations which, the face of an optimization, calculation means less time and easy of resolution.

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