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Computer-Aided Evaluation of Ethanol Production from a Continuous Operating Mode using Simulink

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Computer-Aided Evaluation of Ethanol Production from a Continuous Operating Mode using Simulink

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Abstract. Fossil fuels have become a great energy source worldwide. However, its prolonged use has caused severe environmental pollution problems. Biofuels generated from biomass as a product of microbial biotechnology emerge as an alternative to the use of compounds derived from oil. Therefore, their production results in complex experiments and source investment. That is why engineering studies implementation using mathematical models and simulation techniques should be specified in bioprocesses. The latter focused on optimizing the process parameters, maximizing productivity, generating greater profitability, and reducing cost. This research aimed at the computer-assisted evaluation of obtaining bioethanol from *Saccharomyces cerevisiae* to determine the most critical factors in the production process using a continuous mode. It was determined that the feed rate significantly influences the bioethanol volumetric productivity.

1. Introduction

For many years, fossil fuels have become vital alternative energy worldwide. However, its use has negatively impacted the environment causing pollution problems [1,2]. The concern of scientists and researchers about climate change has brought with it the proposal of new researches focused on the use of renewable fuels [1], also known as biofuels, which are generated from biomass as a product of microbial biotechnology [3,4], avoiding the implementation of some stone process [5,6].

Among the most studied and implemented alternative fuels is bioethanol, made from the alcoholic fermentation of various sugars later into alcohols (-OH). Therefore, it is considered less toxic and highly biodegradable [1,6]. It occupies about 80% of the alternative fuels world production [2], is widely used in various industries and, its manufacture depends mainly on the substrate to be implemented, the flow fed into the process, and the bioreactor's operating mode, resulting in the total cost and profitability of the process in the global market [7]. However, its production is complex. For this reason, the implementation of engineering studies should be specified in bioprocesses through the development of mathematical models that describe the process with greater precision [8], as well as simulation techniques that allow optimizing the process parameters to maximize productivity, generate higher profitability, and reduce production cost [9-11]. Hence, its most studied way of ethanol production has been the batch mode using bioreactors. However, its main disadvantage is that ethanol accumulation can reach toxic levels that inhibit yeast growth, leading to reductions in productivity.

As an alternative to the above, the continuous mode offers significant advantages since it can maximize the ethanolic fermentation by adding the limiting substrate and extracting the exhausting substrate. Therefore, product concentration can remain diluted to values that allow the yeast growth.

However, the implementation of large-scale improvements cannot be directly evaluated in industrial plants due to the high risk of errors during operation, which could translate into damages and economic losses for the industry. Process simulators like Simulink software are computational tools to solve problems and develop skills and experience for an ethanol production plant's operational training.

A process simulator represents the operation of a natural plant, in which a professional can experience the operation of equipment, emergency cases, and abnormal situations during the development of a bioprocess. That is why the purpose of this study was to carry out a series of fermentation simulations to know the parameter behavior to evaluate the substrate and flow factors for bioethanol production from *Saccharomyces cerevisiae*. The latter, to determine the most fundamental factor in the production process using a simulated bioreactor operated in continuous mode.

2. Methodology

A transient mathematical framework is used to simulate biomass yeast X, substrate gradients S and ethanol concentration P based on a CSTR (continuous stirred tank reactor). The dynamic model consists of three equations as shown:

$$\frac{dX}{dt} = -DX + \mu X \quad (1)$$

$$\frac{dS}{dt} = D\left(S_{feed} - S\right) - q_s X \quad (2)$$

$$\frac{dP}{dt} = -DP + q_P X \quad (3)$$

Where D is the dilution rate and S_{feed} is the substrate concentration fed at the bioreactor. Both are mentioned in Table 1. The expressions μ, q_s and q_P are kinetic rates for biomass production, substrate uptake, and product formation and are calculated according to:

$$\mu = \frac{\mu_{max} S}{k_s + S} \quad (4)$$

$$q_s = \frac{\mu}{y_{XS}} \quad (5)$$

$$q_P = y_{PS} q_s \quad (6)$$

Here, μ_{max} is the maximal specific biomass growth rate with a value close to 1.2 d^{-1} and k_s is a substrate saturation constant with a level of 0.1 g/L. The biomass y_{XS} and ethanol y_{PS} yields were previously calculated using and Operating Training Simulator Software [12]. This research implemented a 3^2 factorial design and a response surface design to evaluate the substrate (S_{0feed}) and flow (F_0) factors in bioethanol production by *Saccharomyces cerevisiae*. Nine simulations were estimated (see Table I) and were carried out using the Simulink software. The educational and research software allows real-scale culture simulations in a stirred tank reactor that implements various operating modes.

Table 1. Operating parameters set up. Glucose Concentration (S_{0feed}), Feed (F_0), and Dilution rate (D)

Simulation	S_{0feed} (g/L)		F_0 (mL/min)		D (h^{-1})
1	(-1)	10	(-1)	1	0.006
2	(+1)	20	(+1)	5	0.030
3	(-1)	10	(+1)	5	0.030
4	(+1)	20	(-1)	1	0.006
5	0	15	0	2	0.012
6	(-1)	10	0	2	0.012
7	(+1)	20	0	2	0.012
8	0	15	(-1)	1	0.006
9	0	15	(+1)	5	0.030

Nine simulations were started, each in Continuous Mode using the same parameters. However, different concentrations of substrate and flow rate were implemented, as expressed in Table I.

The Simulink software is used for processes control and works with codes for visualization, data monitoring, control, and simulation of industrial bioprocessing. Combining interface and programming routines uses graphical user interphases (GUI), algorithms developed using Matlab codes, block diagrams.

Figure 1 shows the diagram process for continuous ethanol production using the Simulink software

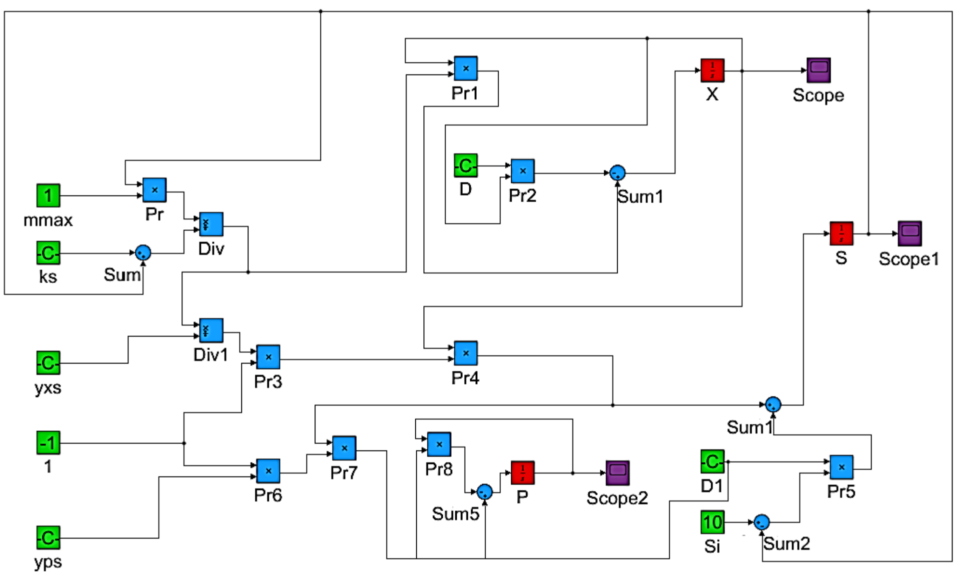

Figure 1. Bioprocess set up for ethanol production using a continuous mode (Simulink model).

3. Results and Discussions

The ethanol production in a stirred tank bioreactor operating in continuous mode can be restricted by the amount of substrate used, contamination, and operating conditions. At an industrial level, the modeling of the process allows evaluating the feed flow behavior and the biomass concentration, generating more significant process optimization, therefore, high profitability [3].

Figure 2 shows the global results of the maximum biomass and ethanol values obtained under the effect of the feed flow and substrate fed concentration. It is observed that the maximum biomass values are obtained by operating the bioreactor at a flow of 1.0 mL/min and a substrate concentration at the equipment inlet with a level of 20 g/L. Interestingly, at the same previous operating conditions, the best levels of biofuel are obtained.

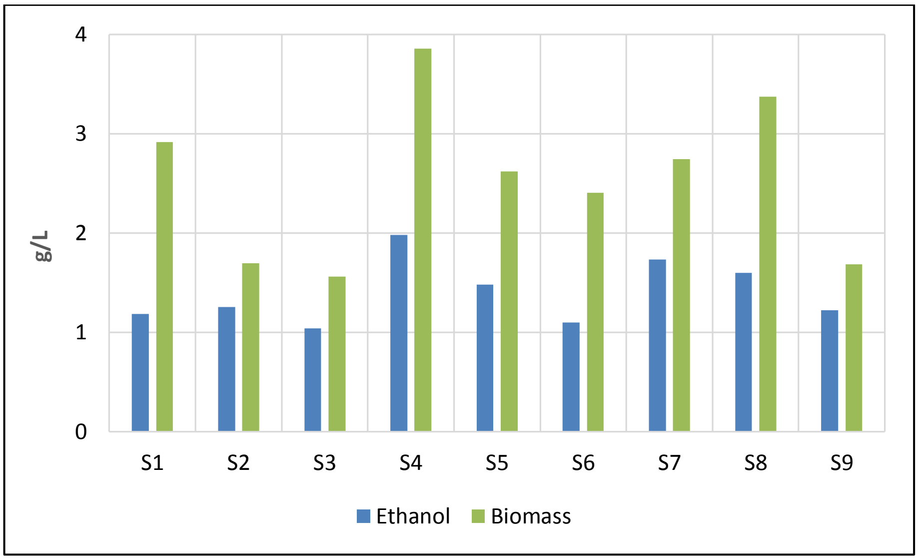

Figure 2. Maximum concentrations of ethanol and biomass obtained in the simulations carried out

The results obtained in the simulations carried out the Simulink software allowed observing different scenarios by relating the flow factor, where a substrate feeding of 10, 15, and 20 g/L, respectively, reached the stable ethanol state at day 5 using a F_0 = 5 ml/min (see Figures 3C, 4C, and 5C). However, when using an F_0 = 2 ml/min, at least 15 days are required to produce ethanol at a stable state (see Figures 3B, 4B, and 5B). Lastly, when using a flow rate equal to 1 ml/min, a considerable increase in time required to stabilize the ethanol concentration is shown in Figures 3A, 4A, and 5A. Therefore, more than 20 days are needed to reach a stable state.

However, simulation four on day 20 produced close to 2 g/L of ethanol (Figure 5A). The maximum biomass concentration occurred on the sixteenth day in simulation 4, being 3.85 g/L when implementing an F_0 = 1 ml/min and S_{0feed} = 20 g/L, followed by simulation 8 with 3.37 g/L using F_0 = 1 ml/min and S_{0feed} = 15 g/L.

On the other hand, the lowest biomass concentrations occurred 6 days after starting the process in simulation 3 (Figure 3C), being 1.56 g/L with S_{0feed} = 10 g/L and F_0 = 5 ml/min and, the simulation 9 (Figure 4B) with 1.69 g/L using S_{0feed} = 15 g/L and F_0 = 5 ml/min. When using a S0feed = 10 g / L in simulations 1, 3, and 6, the highest ethanol production was obtained in simulation 1 (Figure 3A) when using an F0 = 1 ml/min, 1.18 g/L. Simulations 5, 8, and 9 were implemented a S0feed = 15 g/L where simulation 8 produced 1.59 g/L of ethanol (Figure 4A) with an F0 = 1 ml/min, while the lowest production is shown in simulation 9 being 1.22 g/L (Figure 4). Finally, simulations 2, 4, and 7 produced more than 1.2 g/L of ethanol when using S0feed = 20 g/L (Figure 5).

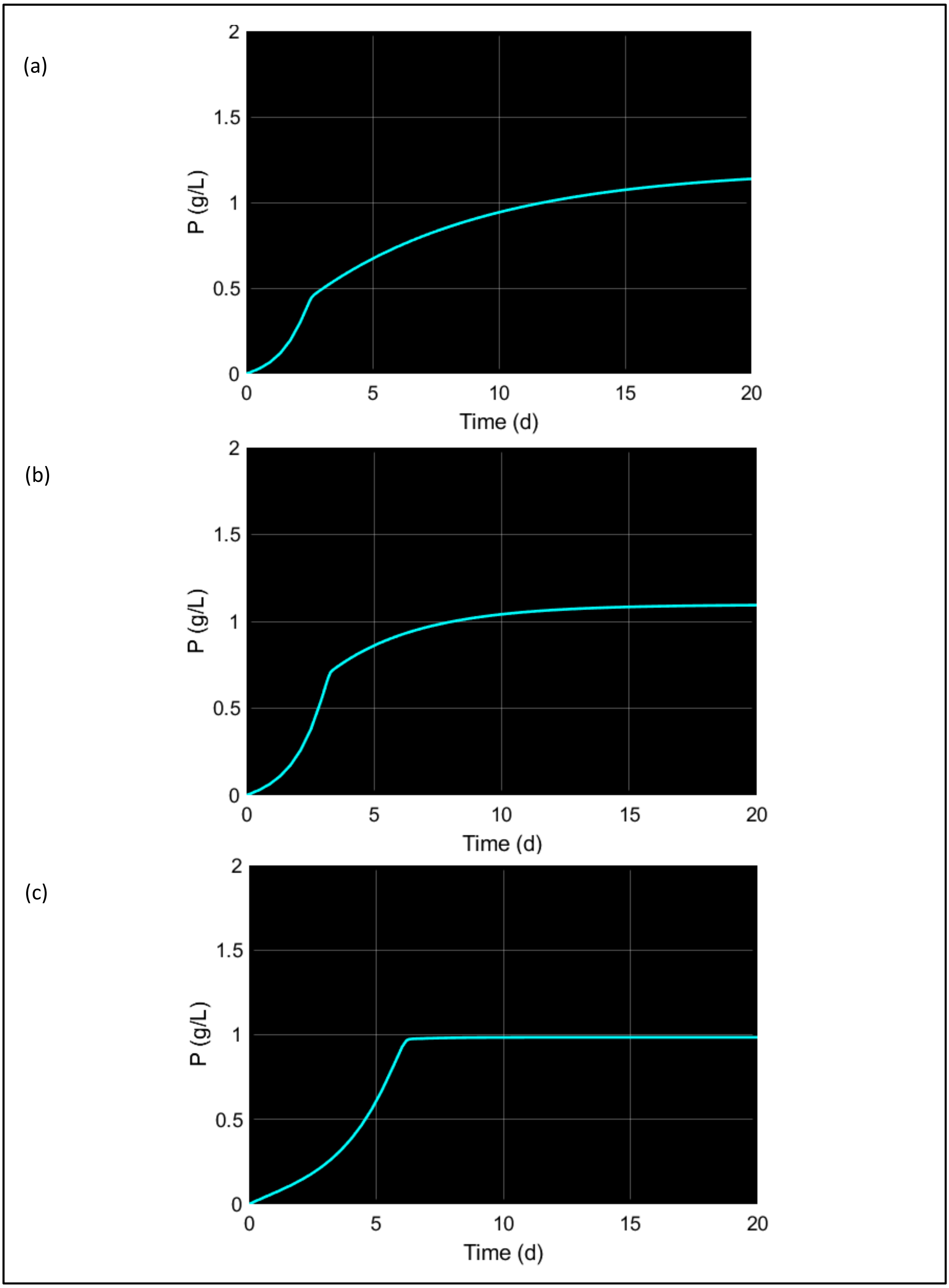

Figure 3. Flow rate effect on ethanol production using a feeding glucose concentration of 10 g/L. (a) F0 = 1 ml/min; (b) F0 = 2 ml/min; (c) F0 = 5 ml/min.

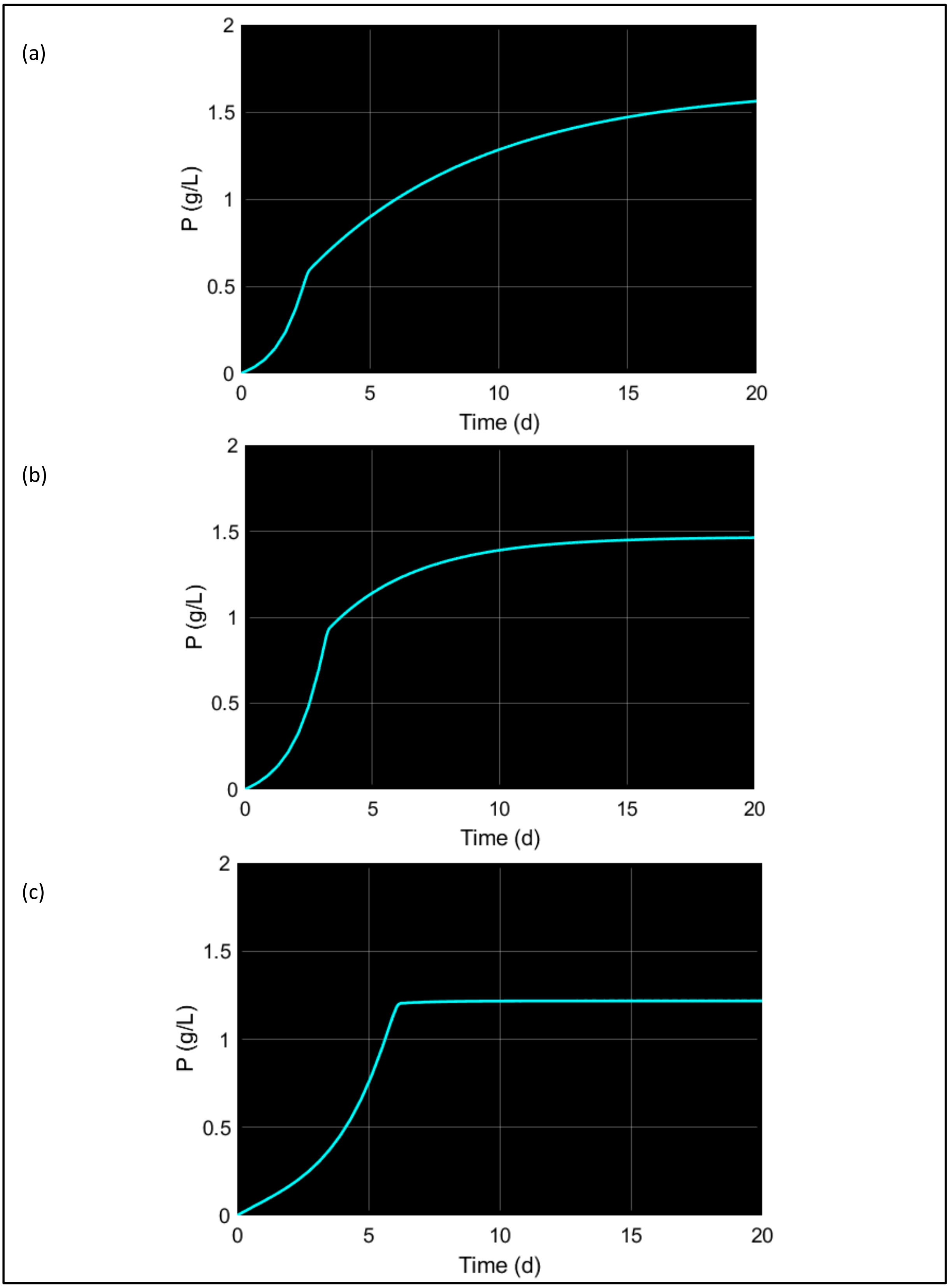

Figure 4. Flow rate effect on ethanol production using a feeding glucose concentration of 15 g/L. (a) F0 = 1 ml/min; (b) F0 = 2 ml/min; (c) F0 = 5 ml/min.

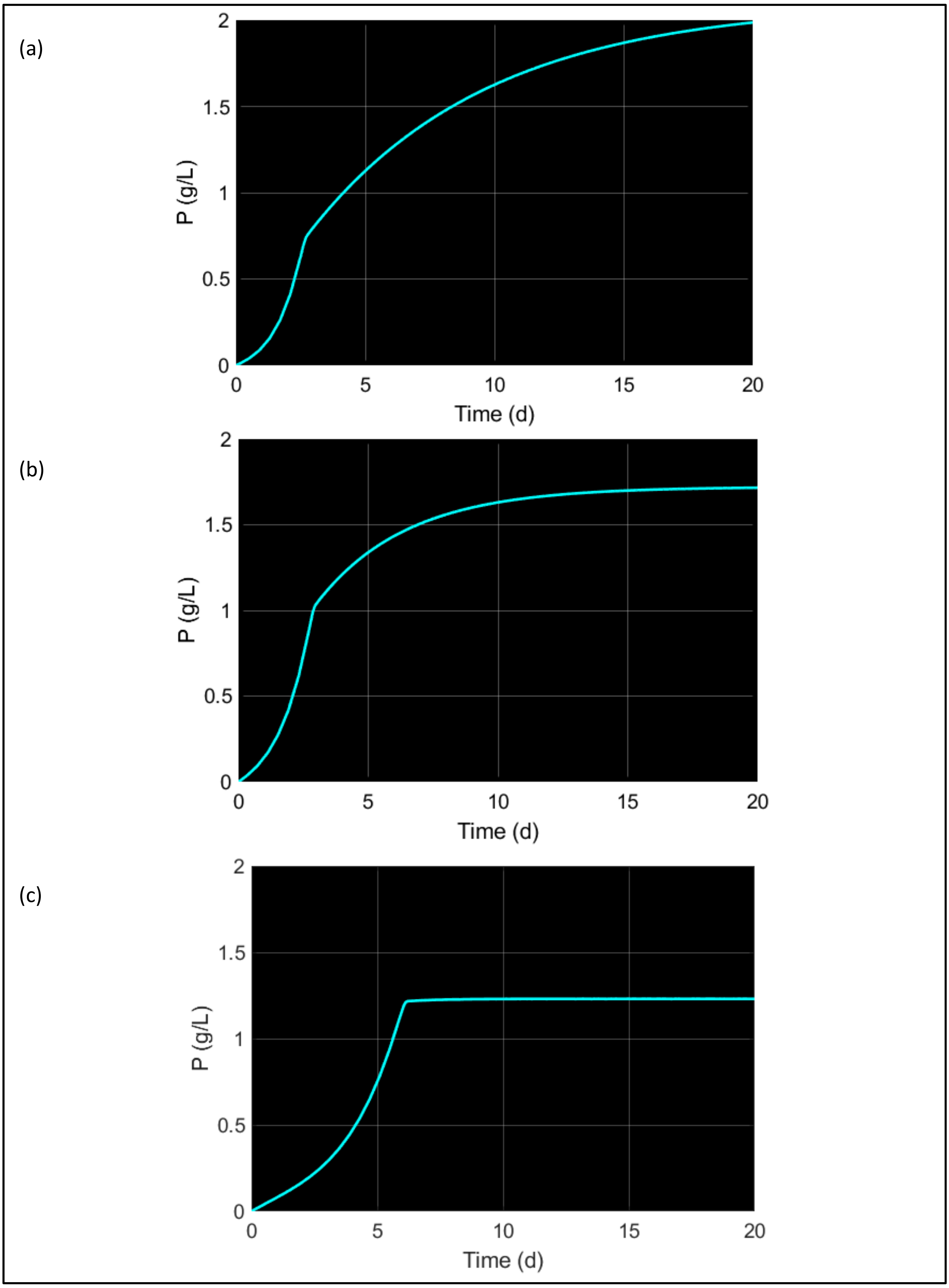

Figure 5. Flow rate effect on ethanol production using a feeding glucose concentration of 20 g/L. (a) F0 = 1 ml/min; (b) F0 = 2 ml/min; (c) F0 = 5 ml/min.

The preceding suggests that ethanol production is favored when using 5 ml/min flow rates. The latter suggests a relationship between the biomass-ethanol concentrations and the flow rate implemented. Furthermore, in a study [10], researchers evaluated the glucose concentration in the feed stream and the dilution rate by implementing a non-linear analysis of the cybernetic model. The mentioned work concluded that the dilution rate plays an essential role in the cellular metabolism of microorganisms where biomass cells are sensitive to a high dilution rate, which is directly related to the flow rate.

Likewise, glucose can enrich the cells in a continuous stirred tank reactor (CSTR), achieving a vital biomass yield in ATP when implementing other carbohydrates as a carbon source in SBR and CSTR reactors [11-13]. The latter is because most microorganisms can metabolize monosaccharides, mainly glucose, to carry out their metabolic reactions and bioproducts.

Likewise, the maximum volumetric productivities of biomass and ethanol were reached in simulations 2 and 9, respectively: 0.050 g/Lh and 0.054 g/Lh for biomass and 0.037 g/Lh and 0.036 g/Lh for ethanol (both simulations implemented an F_0 = 5 ml/min).

On the other hand, simulations 1 and 8 obtained the lowest values in the volumetric productivity of biomass with 0.017 g/Lh and 0.020 g/Lh and ethanol being 0.0071 g/Lh and 0.0095 g/Lh when implementing a flow rate of 1 ml/min. Results can be seen in Figure 6.

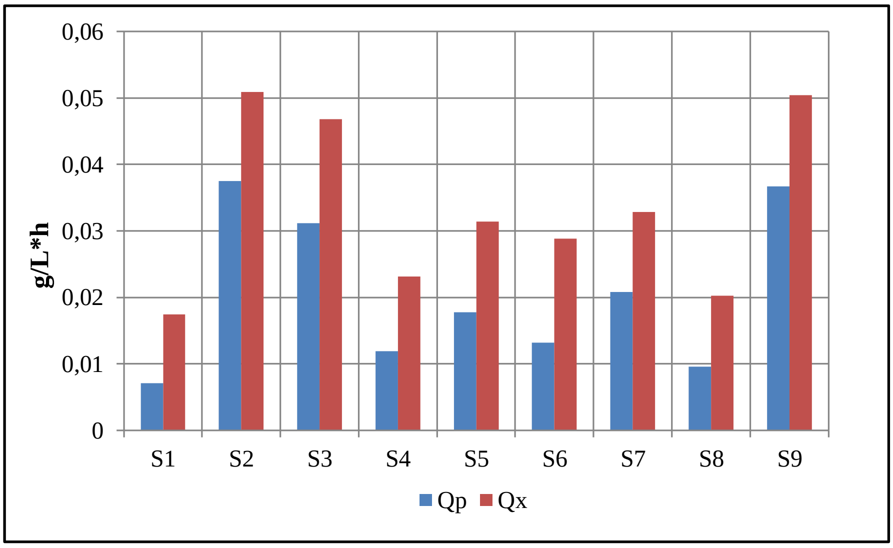

Figure 6. Volumetric productivity of ethanol and biomass obtained.

The response surface technique establishes a relationship between the experimental and the observed parameters, analyzing the effect of the factors applied in the process, thus generating a mathematical model capable of identifying the variable of interest in the process [14-16]. According to the results obtained by evaluating flow and substrate effect on biomass and ethanol productivity (see Figure 7), it is observed that the predominant factor is the flow rate so that slight variations in substrate concentration increase the productivity of both biomass and ethanol. However, the substrate affects the productivity of the process to a lesser degree since significant changes are not reflected in a considerable increase in productivity. According to [5], the high substrate concentrations allow a high ethanol production because the raw material can more easily bind to the enzyme's active site, thus generating higher productivity.

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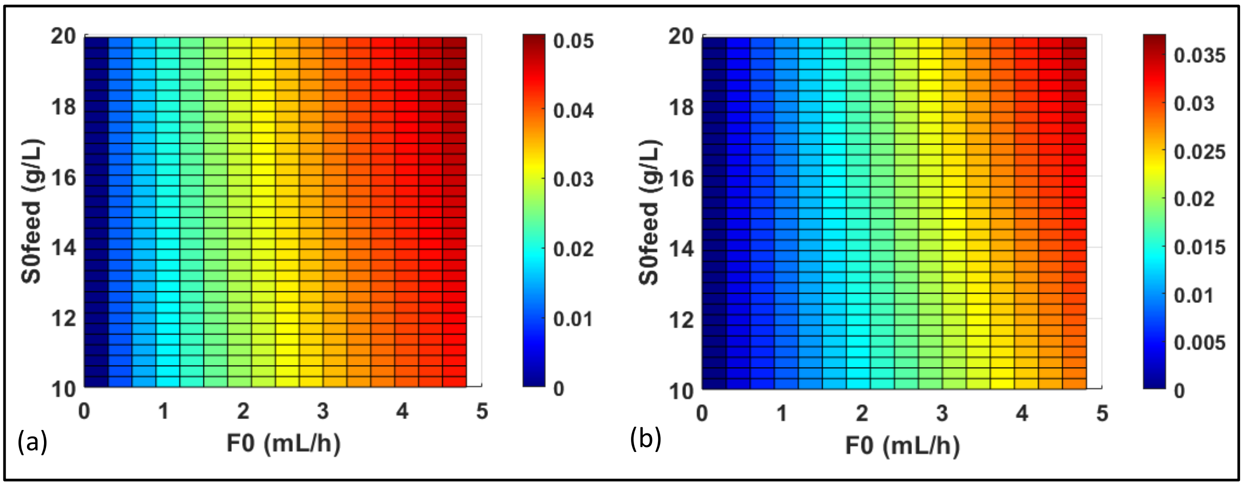

Figure 7. Contours of (a) Biomass Qx and (b) Ethanol productivities evaluated for different Volumetric productivity of ethanol and biomass obtained.

However, it should be noted that the excessive increase in substrate concentrations causes various problems in the enzymatic capacity of the microorganism, resulting in the proliferation of inhibitory compounds that end up limiting mass transfer in the bioprocess [17].

Therefore, the bioethanol industry generates greater interest every day by playing a fundamental role in forming a sustainable energy system capable of reducing greenhouse gases and increasing the production of renewable fuels [18].

The efficiency of a biological process can be improved by employing engineering studies that allow the modeling and optimization of process variables [19-21]. The mathematical modeling of the bioprocess allows controlling key factors such as the substrate concentration and the fed flow, guaranteeing the minimization of waste through the optimal use of raw materials, achieving greater profitability, stability, and productivity in the process.

4. Conclusions

Bioethanol is considered an ideal substitute for fossil fuels, playing a fundamental role in forming a sustainable energy system. Furthermore, the modeling of a bioprocess at an industrial level makes it possible to evaluate the behavior of the feed flows and the concentrations obtained from biomass and ethanol, generating more significant optimization of the process and, therefore, high profitability. The results of this study suggest that the use of flow rates with values of 1 ml/min favor biomass production, while ethanol production is favored when using flow rates of 5 ml/min; as well as, the high concentrations of substrate favor a high production of ethanol, by generating greater incorporation of the molecule with the active site of the enzyme.

References

[1] Fernandez C, Pantano N, Serrano E and Scaglia G 2020 Multivariable Tracking Control of a Bioethanol Process under Uncertainties *Mathematical Problems in Engineering* **2020** 1
[2] Jambo S, Abdulla R, Marbawi H and Gansau J 2019 Response surface optimization of bioethanol production from third generation feedstock - *Eucheuma cottonii Renewable Energy* **132** 1
[3] Shokrkar H, Abbasabadi M and Ebrahimi S 2018 Model-based evaluation of continuous bioethanol production plant *Biofuels, Bioproducts and Biorefining* **13** 11
[4] Yi F, Lawell C, Thome K 2018 A Dynamic Model of Subsidies: Theory and Application to the Ethanol Industry

[5] Khandaker M, Qiamuddin K, Majrashi A, Dalorima T, Sajili M and Hossain A 2018 Bio-Ethanol Production from Fruit and Vegetable Waste by Using *Saccharomyces Cerevisiae*. *Bioscience Research* **15(3)** 1703
[6] Cutzu R and Bardi L 2017 Production of Bioethanol from Agricultural Wastes Using Residual Thermal Energy of a Cogeneration Plant in the Distillation Phase *Fermentation* **3(2)** 24
[7] Chouaibi M, Daoued K, Riguane K, Rouissi T and Ferrari G 2020 Production of bioethanol from pumpkin peel wastes: Comparison between response surface methodology (RSM) and artificial neural networks (ANN) *Industrial Crops and Products* **155** 1
[8] Ortega F, Pérez O and López E 2016 Phenomenological-Based Semiphysical Model of Continuous Alcoholic Fermentation Process *Información tecnológica* **27(271)** 21
[9] Araque J, Niño L and Gelves G 2020 Industrial Scale Bioprocess Simulation for Ganoderma Lucidum Production using Superpro Designer *Journal of Physics: Conference Series* **1655** 1
[10] Ciesielski A and Grzywacz R 2019 Non-linear analysis of cybernetic model for aerobic growth of Saccharomyces cerevisiae in a continuous stirred tank bioreactor. Static bifurcations *Biochemical Engineering Journal* **146** 88
[11] Rombouts J, Mos G, Weissbrodt D, Kleerebezem R and Van Loosdrecht M 2019 Diversity and metabolism of xylose and glucose fermenting microbial communities in sequencing batch or continuous culturing *FEMS Microbiology Ecology* **95(2)** 1
[12] Alvarado K, Bayona J, Consuegra J, Parada D, Sepúlveda N and Gelves G 2020 Use of Operational Training Simulation in the Study of Ethanol Operating Conditions: A Powerful Tool for Education and Research Performance Improvement *Journal of Physics: Conference Series* **1655** 1
[13] Kihara T, Noguchi T, Tashiro Y, Sakai K and Sonomoto K 2019 Highly efficient continuous acetone–butanol–ethanol production from mixed sugars without carbon catabolite repression Bioresource Technology Reports **7** 1
[14] Caspeta L, Coronel J, Montes de Oca A, Abarca E, González L and Martínez A 2019 Engineering high- gravity fermentations for ethanol production at elevated temperature with Saccharomyces cerevisiae *Biotechnology and Bioengineering*, **116(10)** 2587
[15] Han W, Xu X, Gao Y, He H, Chen L, Lian X and Hou P 2019 Utilization of waste cake for fermentative ethanol production *Science of the Total Environment* **673** 383
[16] Triwahyuni E, Sudiyani Y and Abimanyu H 2015 The effect of substrate loading on simultaneous saccharification and fermentation process for bioethanol production from oil palm empty fruit bunches *Energy Procedia* **68** 138
[17] Betiku E and Taiwo A 2015 Modeling and optimization of bioethanol production from breadfruit starch hydrolyzate vis-à-vis response surface methodology and artificial neural network *Renewable Energy* **74** 87
[18] Bi C, Zeng J, Zhang W and Wen Y 2020 Modelling the Coevolution of the Fuel Ethanol Industry, Technology System, and Market System in China: A History-Friendly Model *Energies* **13(5)** 1
[19] Niño L, Acosta A and Gelves G 2013 Evaluación de pretratamientos químicos para la hidrólisis enzimàtica de residuos lignocelulósicos de yuca (Manihot esculenta Crantz). *Revista Facultad de Ingeniería Universidad de Antioquia* **69** 317
[20] López L, Peñuela, M and Gelves G 2016 Improving of gas-liquid mass transfer in a stirred tank bioreactor: A CFD approach. *International Journal of Applied Engineering. Research* **11(9)** 6097
[21] Niño L and Gelves G 2015 Simulating gas-liquid mass transfer in a spin filter bioreactor. *Revista Facultad de Ingeniería* **1** 163