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INFLUENCE EVALUATION OF INPUT VARIABLES ON A MATHEMATICAL MODEL OF BIOGAS PRODUCTION

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Abstract. *The use of mathematical models in the biofuel industries is becoming essential to predict and optimize the final result and production efficiency of processes. Thus, mathematical models of biogas production help choosing the input values of the reactional parameters of the industrial reactors in order to evaluate the response of the variables. This work has the objective of analyzing the influences of input factors in a mathematical model, using previously evaluated methodology and factorial planning with analysis of variance (ANOVA). The results showed that two variables influenced the result of biogas production, the flow rate (positively), and the coefficient of solid production (negatively). It was also possible to observe a maximum value of biogas production of 48,484.95* $m^3\ d^{-1}$*. Also, the temperature did not have a great influence on the model and the final value of biogas production, since it presented a low normalized factor of influence. Moreover, other results also show that the predictive model resulting from factorial planning has a good predictive capacity since the sum of the average squares of the errors were null and the confidence level for all the factors was high (*$p<0.05$*).*

Keywords: *biogas, renewable energy, uasb reactor, mathematical modeling.*

1. INTRODUCTION

The use and insertion of renewable energies in the world energy matrix has been increasing gradually in some countries in the last decade. This trend happens because the energy coming from renewable sources do not have polluting characteristics is the responsible mechanism for an effective transition to a globally sustainable scenario (Lyytimäki, 2018). About Brazil's contribution to this world change, the country is among the world's leading renewable energy producers, with approximately 10% of the world's renewable energy fraction, and it is in third in the global production ranking. Brazil’s new researches show that it intends to follow the tendency to change its traditional energy matrix to clean energy because its policies keep the country committed to continuing to use and produce this type of energy (Dranka and Ferreira, 2018; Freitas et al., 2019; Lyytimäki, 2018).

One of the options for clean energy generation is based on the production of methane gas (CH_4), a fraction of the biogas, which can be used for various purposes such as electricity generation, domestic heating, vehicle fuel, and energy cogeneration. Its main production process is called anaerobic digestion, where microorganisms are responsible for synthesizing organic material during several phases until it reaches the final product, mainly composed of methane and carbon dioxide (CO_2). Its renewable characteristic is established in its neutral generation of carbon since all the production of this compound is synthesized of organic matter that already contains carbon in its composition (Scarlat et al., 2018; Silva dos Santos et al., 2018). In Brazil, the production of biogas is progressing gradually according to which policies of incentive to the production of renewable energies are applied in the country. According to Freitas et al. (2019), there were 127 biogas plants in Brazil in 2015, representing around 3835 TWh of electricity generation capacity. This number, when compared to European countries, is still small, as by 2015, there were already more than 17400 biogas plants installed in that continent (Scarlat et al., 2018). However, this scenario may change in the coming years with the creation of new companies in the renewable and sustainable sector. The projections of the Energy Research Company of Brazil indicate that production in the country can reach 9.1 TWh of electricity produced from biogas in 2030 using only municipal solid waste, which is one of the substrates used for anaerobic digestion and methane production (Flauzino et al., 2017).

In addition to this type of substrate, biogas can also be produced from the anaerobic digestion of cattle or pigmeat, food remains, fractions of agricultural tailings such as rice hulls, wheat, as well as animal manures, woody biomass and tree leaves (Khan and Martin, 2016; Sahota et al., 2018). Another substrate of high interest is vinasse, which is subproduct of the ethanol production. Given the number of sugar/ethanol plants in operation in Brazil, the use of vinasse could significantly contribute to increase biogas production in the country. Vinasse is the main residue generated in the production of ethanol through the fermentation process of sugarcane and its distillation, and has characteristic odor, dark color, low pH and has a high concentration of organic material in its fraction (Bettani et al., 2019; Parsaee et al., 2019; Rodrigues Reis et al., 2019). In addition to these characteristics, vinasse also has a high content of chemical oxygen demand (COD) and biological oxygen demand (BOD), which indicates the amount of oxygen required to oxidize the organic matter available in the vinasse, and this parameter indicates that the use of this residue must be controlled after distillation (Bettani et al., 2019). One of the applications of vinasse is soil fertilization, since its composition can be found nutrients such as potassium, nitrogen, and phosphorus, essential for fertilizing soils (Longati et al., 2017), but this application can cause environmental problems such as salinization, contamination of soil and greenhouse gas emissions (Bettani et al., 2019). Because of these consequences, vinasse calls attention to its high content of organic material, which is capable of being transformed into biogas, causing researchers to turn their attention to this application. The choice to produce biogas brings great benefits to a plant such as high energy recovery, reduced environmental impact, and low budget for reactor construction. Furthermore, the biogas production from vinasse would eventually convert methane, which would go to atmosphere otherwise, in carbon dioxide, which has about 25 times less green-house potential, with energy generation on the process. Thus, the process would have a double benefit. In addition, the fraction of vinasse produced in a plant can reach 8 to 10 L per liter of ethanol produced, and this ethanol-vinasse ratio offers a large amount of input to be used, for example, in Brazil it is estimated that there will be a production of 588 billion liters of vinasse in 2019 which can be used to produce biogas (Parsaee et al., 2019; Rodrigues Reis et al., 2019).

The use of vinasse to produce biogas can also bring other advantages as a contribution to the energy sector by reducing the pollutant gases, burning of the gas to produce water vapor, necessary for operations of plants. Also, there are advantages as the operation of gas turbines to generate electricity, applications in combined heat and power systems, and replacement of diesel used in agricultural machinery (Parsaee et al., 2019). Some studies have already reported the use of vinasse for the production of biogas. Cruz-Salomón et al. (2017) used vinasse to produce biogas and obtained a COD removal efficiency of 93%, indicating that the microorganisms were able to transform the organic matter into other components, mainly methane, in an anaerobic environment, and the rate of methane production per gram of COD removed was 307.5 mL CH_4 $gCOD^{-1}$. The biogas obtained in this work contained 80% of methane in its composition. Thus, biogas could be used as a fuel because it has more than 45% of the flammable fraction. Del Nery et al. (2018) also worked with UASB reactor and methane production from vinasse biodigestion and obtained a COD removal efficiency of 90.5% with a production of 200 mL CH_4 $gCOD^{-1}$, demonstrating similarity in the results obtained from the previous work.

One of the most common biogas production systems uses reactors to remove COD from the applied load, and one of these reactors is called UASB reactor (upflow anaerobic sludge blanket). This reactor is tubular with a conical part and consists of several zones, one of them is called mud blanket, where the gases are formed through the degradation of organic compounds in a continuous batch. In this type of configuration, the load enters from below and goes towards the top to exit, passing through the mud blanket that has bacteria capable of degrading the organic fractions of the load. Besides, it was found that a low hydraulic retention time (HRT) is an important parameter for the biogas process (Dutta et al., 2018; Utami et al., 2016).

Thus, this work aims to study the theoretical production of methane from a mathematical model of a UASB reactor and to analyze the influence of the input factors (HRT, Temperature, Flow Rate and Coefficient of solids production - Y_{abs}) in the model used. The power plant that provided the data for analysis is called Usina Jalles Machado S/A, located the state of Goiás, where it produces ethanol, sugar, electricity, and organic products. The plant produces about 1,112,430,590 m^3 of vinasse per year in its ethanol production plants, and this study aims to analyze the use of this vinasse for biogas production, using data provided by the plant as input data for the model. For the calculations of the theoretical biogas production, the methodology proposed by Chernicharo (1997) will be used.

2. MATERIALS AND METHODS

2.1 Model of the UASB reactor

The model used for estimation of biogas production from vinasse was modeled by Chernicharo (1997) and showed equations and models for several types of reactors, one of them the UASB reactor. In this model, some parameters are required for its implementation and are listed below.

- Average flow rate of the affluent (Q_{med}) in m^3 d^{-1};
- Maximum flow rate of the affluent (Q_{max}) in m^3 d^{-1};
- COD of the affluent (S_{0C}) in mg L^{-1};
- BOD of the affluent (S_{0B}) em mg L^{-1};
- Temperature of the affluent (T) in °C;
- Hydraulic retention time (HRT) in hours;
- Coefficient of solids production in terms of COD (Y_{abs}) in kgCOD $kgCOD_{apl}^{-1}$.

The following equations are used to implement the model, considering the parameters listed above.
First, the average load of the tributary is calculated (L_0) (Eq. 1).

$$L_0 = S_{0C} \cdot Q_{med} \ \text{(kgCOD d}^{-1}\text{)} \quad (1)$$

After this step, the HRT should be defined, and for this data was used Tab. 1 available in Chernicharo (1997).

Table 1. Hydraulic retention times in UASB reactors.

Temperature of the affluent (°C)	Hydraulic retention time (h)	
	Daily average (h)	Minimum (for 4 to 6 hours)
16 - 19	> 10 - 14	> 7 - 9
20 - 26	> 6 - 9	> 4 - 6
> 26	> 6	> 4

The model proposes Eq. (2) to calculate the volume of the reactor afterward. However, this calculation can result in values that are not compatible with the volume of organic load that will be applied. Thus, there is a reconsideration step if the volume is not correct.

$$V = Q_{med} \cdot TDH \ \text{(m}^3\text{)} \quad (2)$$

With the volume calculation, the volumetric organic load (VOC), which is the amount of organic matter applied to the reactor, and hydraulic volumetric (CHV), which indicates the volume of organic matter applied daily per unit of volume of the reactor, are estimated by Eqs. (3) and (4), respectively.

$$VOC = \frac{Q_{med} \cdot S_{0C}}{V} \ \text{(kgCOD m}^{3^{-1}}\text{d}^{-1}\text{)} \quad (3)$$

$$CHV = \frac{Q_{med}}{V} \ \text{(m}^3 \text{ m}^{3^{-1}}\text{d}^{-1}\text{)} \quad (4)$$

The following equations are used to calculate and evaluate the biogas production in the reactor. The calculation is performed by estimating the COD charge of the affluent that is converted to CH_4. The model begins this step by calculating the COD removed from the organic charge affluent inserted in the reactor (Eq. 5).

$$COD_{rem} = Q_{med} \cdot (S_{0C} - S_C) \ \text{(kgCOD d}^{-1}\text{)} \quad (5)$$

Following this, the model estimates the efficiency of COD removal from the system, using an empirical model, which constants are obtained from experimental data of reactors in operation. In this step, the model offers equations obtained from adjustments of operation curves, where it was possible to observe the significant influence of HRT on the efficiency of COD removal, in this way Eq. (6) is proposed.

$$E_{COD} = 100 \cdot (1 - 0.68 \cdot TDH^{-0.35}) \ (\%) \quad (6)$$

With the efficiency calculated, it is possible to obtain the final concentration estimate of COD (S) in the effluent for the subsequent calculation of methane production with Eq. (7).

$$S = S_{0C} - \frac{E_{COD} \cdot S_{0C}}{100} \ \text{(mg L}^{-1}\text{)} \quad (7)$$

After estimating the final COD efficiency and concentration, the model goes to the final step where the biogas production is calculated with the application of Eq. (8), where the COD portion converted to methane is calculated. In this equation, the second parcel is related to methane losses caused by the accumulation of biodegradable solids inside the reactor and methane used by bacterial growth. The withdrawal of this parcel occurs with the application of the overall coefficient of solids production of the system.

$$COD_{CH_4} = COD_{rem} - (Y_{abs} \cdot Q_{med} \cdot S_{0C}) \quad (\text{kgCOD}_{\text{CH}_4}\ \text{d}^{-1}) \tag{8}$$

In order to transform the converted COD into methane in equivalent volume production of CH_4, the model indicates Eq. (9), which uses a conversion factor for the operating temperature of the reactor, calculated by Eq. (10).

$$Q_{CH_4} = \frac{COD_{CH_4}}{k(t)} \quad (\text{m}^3\ \text{d}^{-1}) \tag{9}$$

$$k(t) = \frac{P \cdot K}{R \cdot (273 + t)} \quad (\text{kgCOD m}^{3^{-1}}) \tag{10}$$

Where, P is the atmospheric pressure (1 atm), K is the COD referring to one mole of CH_4 (64 gCOD mol^{-1}), R is the gas constant (0.08206 atm L mol^{-1} K^{-1}) e is the reactor temperature (°C).

Therefore, to finish the model application, it is necessary to estimate the methane content of the biogas produced, and for this data, the model indicates the range of 70-80% for the calculation.

The mathematical model used in this work was previously validated by Lobato et al. (2012), through tests with three types of scenarios (worst, typical and best) to validated the model by comparing with these same three scenarios of real-scale UASB reactors. The results showed significant agreement between the model and the results of the real-scale reactor.

2.2 Methodology

In this work, a model simulation plan was used to verify the predictive capacity of the model, as well as the relevance of the input factors to the final biogas yield. Thus, it was used the planning based on Central Composite Design (CCD) in STATISTICA software, with 24 simulations with normal levels plus two simulations in the central points and 8 with points below or above the endpoints (rotatability = α = 2), and without repetitions in the center point. This planning is defined by levels −2, −1, 0, 1 and 2, and this analysis are used mainly for experiment planning or optimal point analysis for response variables (Alshehria et al., 2016). For this process, three steps were applied: estimating the coefficients in a mathematical model, predicting the response and checking the adequacy of the model. Also, the planning was used to analyze the influences of the input parameters of the model in the final production of biogas, being analyzed the flow, coefficient of production of solids, temperature, and HRT. The levels used for the simulations as well as the planning matrix, are listed in Tables 2 and 3, respectively.

In addition to experimental planning, analysis of variance (ANOVA) was used to evaluate the factors with significant effects on the final biogas production result, as well as their confidence levels with the confidence interval value $p<0.05$.

Table 2. Levels and input data for experimental planning and simulations.

Level	Flow rate (m^3 d^{-1}) (1)	Y_{abs} (kgCOD $kgCOD_{apl}^{-1}$)(2)	Temperature (°C)(1)	HRT (h)(2)	COD (mg L^{-1})(3)
Low (−1)	3072.0	0.11	45	6	20644.7
Center (0)	5209.0	0.17	52.5	7	20644.7
High (1)	7346.0	0.23	60	8	20644.7

(1)data from Usina Jalles Machado S/A
(2)data taken from the methodology described in Chernicharo (1997)
(3) average value taken from Del Nery et al. (2018), Reis et al. (2019) and Santa Cruz (2011)

3. RESULTS AND DISCUSSIONS

3.1 ANOVA results

Table 4 summarizes the main results obtained in the ANOVA test, where the R^2 value found for the model was 0.9998. This value demonstrates the good predictive capacity of the model since this parameter explains that the variation of 99.98% of the result can be attributed to the factors used as input parameters for the model. This result was expected because the model had previously been verified and validated. Also, the parameter p, which considers the 95% confidence level to be accepted as a predictive model presented a value lower than 0.05 for all parameters, and this result demonstrates that the model is predictive for all input factors and that all variations of the model can be considered validated. In Tab. 4, SS means the sum of squares and MS means of the sum of squares. About these values, it is possible to conclude that the predictive model is good because the SS and MS present higher values when the parameters are considered and compared to the values of SS and MS of the errors.

Table 3. Matrix of experimental planning with CCD and result of simulations of biogas production.

Flow rate	Y_{abs}	T	HRT	Biogas(1)
−1	−1	−1	−1	18162.93
−1	−1	−1	1	19362.44
−1	−1	1	−1	19019.67
−1	−1	1	1	20275.77
−1	1	−1	−1	14025.52
−1	1	−1	1	15225.03
−1	1	1	−1	14687.11
−1	1	1	1	15943.19
1	−1	−1	−1	43432.58
1	−1	−1	1	46300.94
1	−1	1	−1	45481.29
1	−1	1	1	48484.95
1	1	−1	−1	33538.90
1	1	−1	1	36407.26
1	1	1	−1	35120.92
1	1	1	1	38124.58
−2	0	0	0	5218.91
2	0	0	0	52931.51
0	−2	0	0	36256.22
0	2	0	0	21894.20
0	0	−2	0	27735.34
0	0	2	0	30415.08
0	0	0	−2	26501.44
0	0	0	2	30809.23
0	0	0	0	29075.21
0	0	0	0	29075.21

(1) values of the model results in $m^3\ d^{-1}$ of biogas

It is also possible to observe with the results of Tab. 4, by the SS value, that some factors had more influence on the response value of the model (biogas) when they are varied, as the flow, which presented the highest value of SS, and it was the factor that most influenced the result. This result was expected because the relationship between flow and final biogas production is directly proportional. This result can also be explained by the amount of organic load applied to the reactor due to the flow of mass coming from the flow rate, and because they are directly proportional variables, the more flow, the more organic load can be consumed and transformed into biogas. The factor that influenced the least when it varied was the temperature since its consequences in this model were minimal. The variations of this parameter are typically used to correct other factors such as asepsis of the equipment or adequacy for the bacteria that will be used in the degradation process of the organic matter. Guo et al. (2013) studied the effects of temperature on the production of biogas from the pig manure and obtained similar results for the influence of temperature, where they varied between 28 and 38 °C and obtained only 5% more biogas production, which demonstrates that temperature does not influence the response variable.

About the regression coefficient, it is possible to observe which are the influencing parcels for the final value of biogas production. The Y_{abs} parcel had the greatest negative influence on the equation, as did all the multiplicative components that had Y_{abs} in one of the terms. This influence can also be observed in Tab. 5, which shows the normalized estimate value of the effects of each factor, calculated by the ANOVA application. The negative influence of the Y_{abs} is explained by the biogas loss factor in the equation of the model since this coefficient indicates the amount of oxygen lost in the process of growth of microorganisms and solids accumulation in the oxidative matter (Chernicharo, 1997).

Table 4. ANOVA table of the results obtained after the simulations with the mathematical model.

Factor	SS	MS	Regression coefficient
1 Flow Rate (L)[(1)]	3.3989×10^9	3.3989×10^9	5.22
Flow Rate (Q)[(2)]	9.0746	9.0746	0.00
2 Y_{abs} (L)	3.0940×10^8	3.0940×10^8	−9583.99
Y_{abs} (Q)	9.0746	9.0746	200.29
3 Temperature (L)	1.0721×10^7	1.0721×10^7	7.63
Temperature (Q)	9.0746	9.0746	0.01
4 HRT (L)	2.6608×10^8	2.6608×10^8	1303.57
HRT (Q)	9.0746	9.0746	−104.25
1 x 2	3.4716×10^7	3.4716×10^7	−11.49
1 x 3	1.2002×10^6	1.2002×10^6	0.02
1 x 4	2.9179×10^6	2.9179×10^6	0.20
2 x 3	1.0951×10^5	1.0951×10^5	−183.85
2 x 4	2.5000×10^5	2.5000×10^5	−0.02
3 x 4	9.2044×10^3	9.2044×10^3	3.20
Pure error	0.00001	0.00001	-

[(1)]L = linear relation
[(2)]Q = quadratic relation

Based on the factor that indicated the greatest effect among the parameters (Flow rate) the other values were normalized, and it can be seen that Y_{abs} has the greatest influence of the other three factors that are leftover, as already expected by previous analyzes. The HRT and the temperature had sufficiently equal performances of influence in the result, presenting values in the same order of magnitude.

Table 5. Effects of the factors on the production of normalized biogas for the value of the flow.

Factor	Flow rate	Y_{abs}	Temperature	HRT
Estimated normalized effect	1	−0.3017	0.05616	0.08848

3.2 Surface performance results

Figures 1 to 6 show the results of the influences and interactions between the factors after the planning is performed in the form of response surfaces. In these images, it is possible to observe how each component influences the final value of biogas production from the mathematical model implemented. In all figures, the predominance of ramps indicates that these factors influence the response variable linearly. In Figures 1, 2 and 3, it can be observed that for any value, the Flow Rate parameter positively influences the biogas production. Fig. 1 shows that to obtain an optimal point between Flow Rate and $Y_{abs,}$ it is necessary to apply average flows and lower solids production coefficients. This result was expected because the solids production coefficient causes biogas production to decrease if the value is high. As the coefficient of solids increases, the solid particles present in the mixture will require more oxygen to oxidize, which results in a reduction in biogas conversion efficiency. As for Figures 2 and 3, for any temperature or HRT value, the biogas production value will increase with the increase of the Flow Rate factor. This can be explained by the normalized effects that are listed in Tab. 5, where both the Temperature and HRT factors did not have significant effects on the model. However, it is important to point out that the maximum flow rate value provided by the plant is 7346 $m^3\ d^{-1}$, so the biogas production values does not reach their maximum value on the ramp peaks, but rather in the variables near the maximum flow rate value.

Figure 4 shows the effect of Temperature and Y_{abs}. It is possible to observe that lower values of solid production coefficient are significant in biogas production. It is possible to note that the production reaches the maximum when the temperature is maximum and the coefficient is minimum, with few variations when the temperature changes, because the production remains in the range between 30,000 and 40,000 $m^3\ d^{-1}$ of biogas. The effect of temperature indicates that with increasing this parameter the biological activity of bacteria also increases, and thus they synthesize the organic matter present in vinasse. However, it should be noted that most reactors work in mesophilic conditions, with temperatures around 40 °C, so, observing Fig. 4, it is possible to notice that when reaching the mesophilic temperature, biogas production does not exceed value of 32,500 $m^3\ d^{-1}$. The surface behavior of Fig. 5 shows the similarity when compared to Fig. 4, with maximum yield when Y_{abs} is minimal, and HRT is maximum. The relation between HRT and Temperature is shown in Fig. 6, in which case the biogas production reaches its maximum (about 32,200 $m^3\ d^{-1}$) when the two factors are at their maximum points, due to their low levels of effect (Table 5). The biogas production values varied little (25,000 - 35,000 $m^3\ d^{-1}$) when compared to the other group of factors. The results of figures 5 and 6 showed that with increasing temperature and HRT and decreasing coefficient, high biogas production values are found, however, it is possible to observe that the maximum values for HRT and temperature are 8 and 60 °C. respectively. Therefore, the maximum biogas production values are around 30,000 $m^3\ d^{-1}$ because of these two values. And considering the mesophilic temperature, these values can decrease by up to 28,000 $m^3\ d^{-1}$.

Similar results were found in the work of Cancelier et al. (2015), where they studied the production of biogas from swine manure using response surfaces and obtained values of positive effects for COD and Temperature. These results indicate that the increase of these factors increases the value of the final response (biogas production). Also, they presented equivalent response surfaces when the Temperature parameter is varied, which shows that its increase is a positive response factor for the model, with a maximum level of 44 °C, a result similar to the one found in this study, where at 43,5 °C the maximum production level was reached.

Similar results were also found by Safari et al. (2018) who worked with biogas production optimization by integrating surface response analysis with the production process on a laboratory scale. In this paper, they also relate temperature as a factor that positively influences the final result of biogas production, and they found an optimal operating point at 40.36 °C, close to the mesophilic condition.

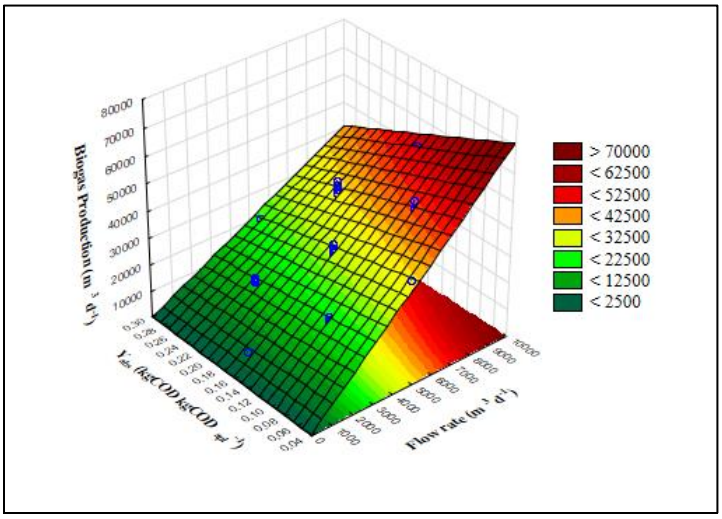

Figure 1. Response surface between factors: Y_{abs} and Flow Rate.

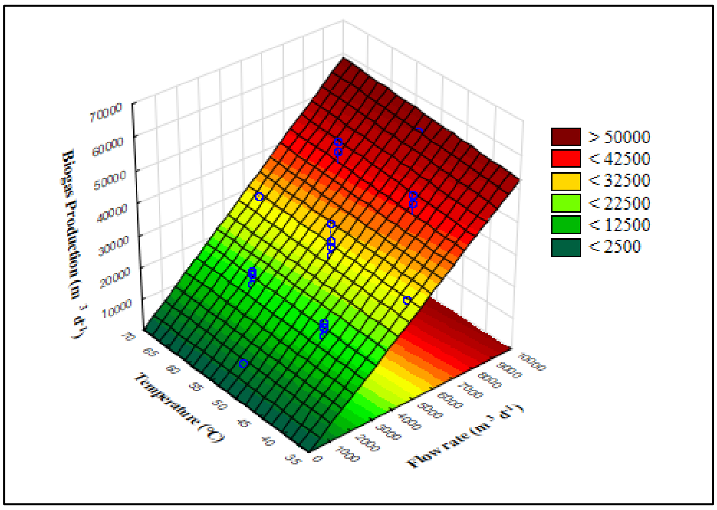

Figure 2. Response surface between factors: Temperature and Flow Rate.

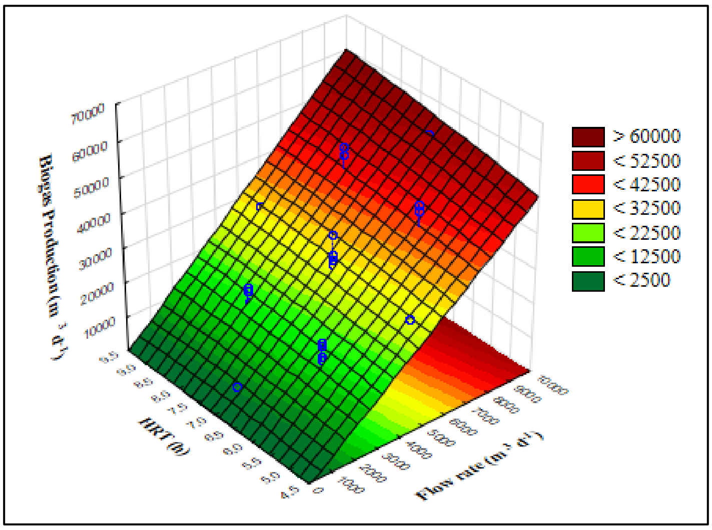

Figure 3. Response surface between factors: HRT and Flow Rate.

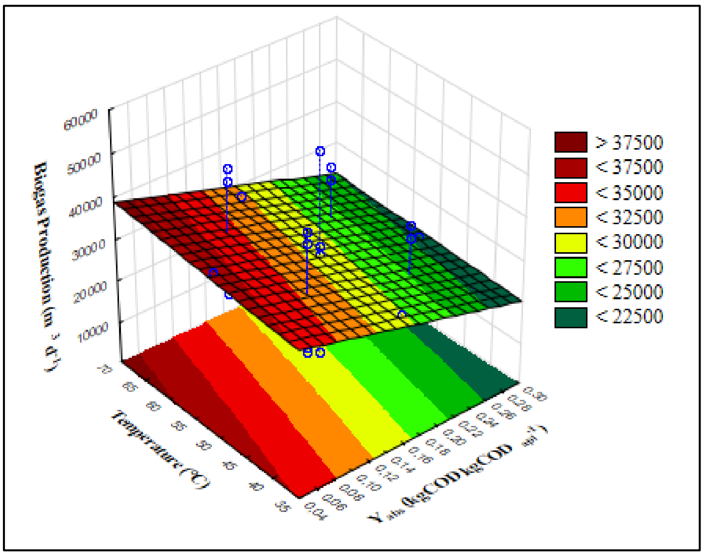

Figure 4. Response surface between factors: Temperature and Y_{abs}.

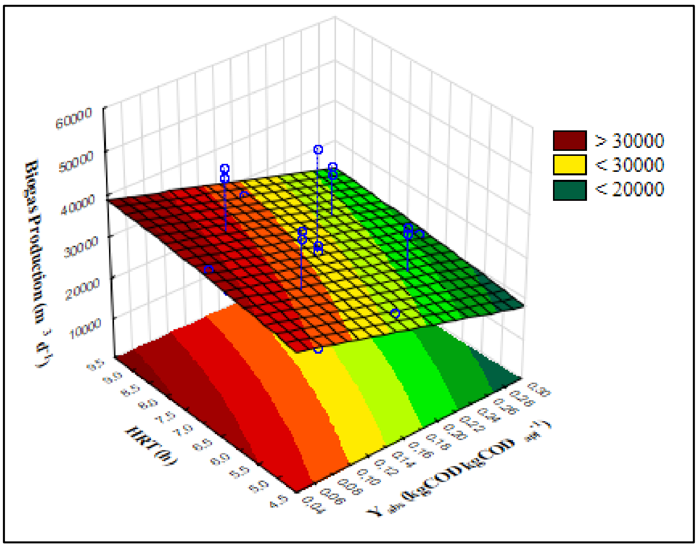

Figure 5. Response surface between factors: HRT and Y_{abs}.

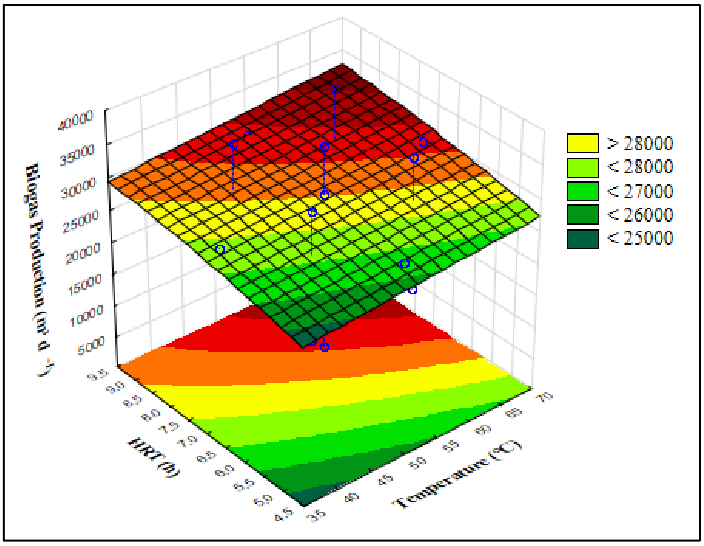

Figure 6. Response surface between factors: HRT and Temperature.

4. CONCLUSION

The experimental planning technique was used to observe and evaluate the influences of the input variables of a model for prediction of biogas production. Four variables were analyzed (Flow Rate, Y_{abs}, Temperature, and HRT) and their influences on the final biogas production result were described by the ANOVA and response surface results. The Flow Rate was the variable that most influenced the final value of biogas production because it has a direct relationship with the biomass conversion in biogas since the organic load that enters the reactor depends exclusively on the Flow Rate. The ANOVA results showed that Y_{abs} influences the model negatively while the other variables influence positively, and in addition, the results showed that the model described after the experimental planning had good predictability, since all parameters presented a confidence order above 95% and the sum of the squares of the errors was practically null (0.00001).

The results also showed that the second variable that most influenced the final production of biogas when varied was the Y_{abs} because it is directly related to the amount of oxygen lost during the oxidation process of the organic matter.

Finally, the results of the response surfaces of the model showed that three variables have a directly proportional influence on the final biogas production which are Flow Rate, Temperature, and HRT, and when placed together with Y_{abs}, they have an indirect correlation with the final production of biogas. In addition, this analysis has shown great predictive power to indicate which variables most influence the mathematical models for biogas production, as it uses highly reliable statistical analyzes. The optimum operating point was found using the values of 7346, 0.11, 60 and 8 for Flow Rate, Y_{abs}, Temperature, and HRT respectively, with a maximum yield of 48484.95 $m^3\ d^{-1}$.

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