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MODELLING AND OPTIMIZATION OF BIOGAS PRODUCTION FROM FOOD WASTES (FW) USING ARTIFICIAL NEURAL NETWORK (ANN)

João Gonçalves Neto

Brunno Ferreira dos Santos

Department of Chemical and Material Engineering, Pontifícia Universidade Católica do Rio de Janeiro (PUC-Rio), Rua Marquês de São Vicente, 225, Gávea, Rio de Janeiro, RJ, CEP:22453-900, Brazil

jgnetoeng@gmail.com; bsantos@puc-rio.br

Florian Pradelle

Department of Mechanical Engineering, Pontifícia Universidade Católica do Rio de Janeiro (PUC-Rio), Rua Marquês de São Vicente, 225, Gávea, Rio de Janeiro, RJ, CEP:22453-900, Brazil

pradelle@puc-rio.br

Abstract. Biogas can be produced by anaerobic digestion from many types of organic residues, in particular from food wastes (FW). The variability of biomasses' composition and biodigesters' characteristics makes standardization difficult. Thus, the use of artificial neural networks (ANN) to investigate the effects and their interactions allows exploring several scenarios of biogas production. In the present work, a database was built with available values in 42 references in the literature in order to obtain mathematical models using reactor/feeding type, volatile solid (VS), OLR, temperature and reactor volume as input variables, and the cumulated biogas production as output. Multiple ANN configurations are considered and a statistical analysis of the model robustness is used to define the best topology. A fairly accurate prediction capability is expected. The modeling results can be compared to a more generic model already implemented by the authors for food wastes, fruits and vegetables wastes and codigestion in a former work. As a result of this modelling work, response surfaces of the ANN model are useful tools to assess if the model is predicting coherent behaviors and define optimal combination of conditions in order to maximize biogas production.

Keywords: Biogas; Food wastes (FW); Artificial neural networks (ANN).

1. INTRODUCTION

Considering the whole distribution chain from agricultural production up to consumption, a report published in 2011 estimated that around one-third of the food production (about 1.3 billion tons of food) was lost or wasted each year (Food and Agriculture Organization of the United Nations, 2019). Among them, food wastes (FW), which are the processed biomass from domestic and commercial kitchens, eateries and restaurants, represent a significant amount of them. Nowadays, this FW are disposed mainly in landfills or treated through incineration. Both alternatives negatively impact the environment and human health and did not systematically use the energy content within them (Zhang, 2014; Palaniswamy, 2017; Kuzzman, 2018).

Thus, waste-to-energy approaches are investigated and anaerobic digestion (AD) is a well-known process that can be appropriate. AD converts solid or liquid organic materials through a multi-stage biochemical degradation process in the absence of oxygen into a gaseous mixture named biogas containing mostly methane (CH₄), carbon dioxide (CO₂) and nitrogen (N₂) (Scano, 2014). Applications are cooking for raw biogas and electricity, heat and steam generation in household and industry, injection into the natural gas grid or use as vehicular fuel for upgraded biogas (Khan, 2017). According to the International Renewable Energy Agency (IRENA, 2019), the global installed capacity for electricity generation from biogas increased 105% between 2010 and 2019.

Four phases used to be considered during the anaerobic digestion process: hydrolysis, acidogenesis, acetogenesis and methanogenesis. Firstly, long chain lipids, carbohydrates and protein are hydrolysed into smaller soluble organic compounds, in a reaction considered as the kinetics-limiting step. Secondly, volatile fatty acids (VFA), such as acetate, propionate and butyrate, and by-products, such as NH₃, CO₂ and H₂S, are observed after acidogenesis. Thirdly, acetate, H₂ and CO₂ are produced from VFA in acetogenesis and then methane and CO₂ are obtained after the methanogenesis (Zhang, 2014; Mao, 2015).

The FW present highly variable characteristics, because of different sources, processing and handling methods and local eating habits, climate and seasons (Meng, 2015; Sun, 2015; Khan, 2017). The biogas yield and composition are influenced by the used microorganisms in the inoculum, the biomass (particle size, structure, composition) and the reactor geometry and characteristics. Two kind of reactors are widespread for anaerobic digestion of food wastes:

anaerobic sequencing batch reactor (ASBR) with some type of agitation and continuous stirred tank reactor (CSTR), with an intermittent (or semi-continuous) or continuous feeding. Temperature, hydraulic retention time (HRT), volatile solids (VS), organic load rate (OLR), carbon to nitrogen (C/N) ratio, pH levels, ammonia and nutrients contents are key parameters that can be optimized to appropriate levels (Grimberg, 2015; Palaniswamy, 2017; Kuzzman, 2018). Then, quantifying the interacting effects of these parameters provides valuable information for prediction and optimization of the anaerobic digestion process.

2. METHODS

2.1 Database

A database of 126 experimental conditions of anaerobic digestion of FW was built using the experimental results from 42 formerly published works found in the literature (Ariunbaatar, 2015; Banks, 2011; Browne, 2013; Chen, 2014; Chu, 2008; De Gianninis, 2017; Deepanraj, 2017; El-Mashad, 2010; Gottardo, 2018; Grimberg, 2015; Hobbs, 2018; Jabeen, 2015; Kawai, 2014; Kim, 2006; Kobayashi, 2012; Kuzzman, 2018; Lee, 2010; Li, 2015; Li, 2018a; Li, 2018b; Micolucci, 2014; Micolucci, 2018; Nagao, 2012; Paudel, 2017; Rico, 2020; Shamurad, 2020; Shen, 2013; Tampio, 2014; Ventura, 2014; Wang, 2009; Wang, 2014; Wu, 2015; Wu, 2016; Xiao, 2018a; Xiao, 2018b; Yong, 2015; Zhang, 2013a; Zhang, 2013b; Zhang, 2019). These data are used in order to determine relations between cumulative biogas production, (in l/g VS) and five characteristics (one discrete and four continuous) of the experiment listed below.

A discrete parameter provides a description of the type of reactor and feeding (ASBR, CSTR with semi-continuous feeding and CSTR with continuous feeding) and the number of stages in the digesters (one, two or three). Then, the six continuous factors are inlet biomass VS (in weight %), OLR (in g VS/(l.d), calculated for the mesophilic reactor if there is more than one phase), temperature (in °C, for more than one phase, only the mesophilic temperature is considered) and the volume of the AD reactor (in m³, for more than one phase, the volume is defined as the whole volume). It is important to notice that, for ASBR, the OLR was defined alternatively as the ratio of the initial VS and the duration of the considered AD processed (that means that ASBR is equivalent to a CSTR with constant OLR continuous feeding). As the range of variation of pH was narrow, such parameter was not investigated here. All data was taken at the end of the digestion process, when cumulated biogas volume is constant.

Among the 126 cases, a preliminary work was necessary to avoid discrepant values that will reduce the robustness of the future models (9 cases, 7.1%) and remove cases for which all parameters are not clearly defined (79 cases, 62.7%). Then, 50 of them (39.7%) are used in the next step.

2.2 ANN design and training

The ANN model was a multilayered perceptron (MLP) with three layers (input, hidden and output). The input layer represents the independent variables (Biodigester, VS, OLR, Temperature, Reactor volume) and the output layer is the produced cumulated biogas volume. In the hidden layer, the quantity of neurons required was determined by the minimum error criterion value and number of effective parameters. The model was developed using MATLAB R2018a.

The assessed activation functions in the hidden layer were logistic sigmoid (*logsig*) and hyperbolic tangent (*tansig*) and in the output layer, it was used a linear transfer function (*purelin*). Besides, the number of neurons considered for the hidden layer (HD) were limited from three to five, so that the quantity of parameters does not be higher than the amount of data registers in the training dataset.

In order to optimize parameters (weights and bias), some algorithms backpropagation method were used, such as *traingdx* based on gradient descent approach, which uses the negative gradient to minimize the error. The parameters are adjusted with changes in the momentum coefficient and the adaptive learning rate. The *trainlm* and *trainbr* algorithms are the Quasi-Newton method to minimize the error and both use Levenberg-Marquardt method in their calculation.

In order to evaluate the quality of the model, the coefficient of determination (R²) and the sum of squared errors (SSE) were used to compare experimental and calculated data, as shown in Equation 2 and 3.

$$SSE = \sum_{i=1}^n (Y_{observed} - Y_{predicted})^2 \quad (1)$$

$$R^2 = 1 - \frac{\sum_{i=1}^n (Y_{observed} - Y_{predicted})^2}{\sum_{i=1}^n (Y_{observed} - Y_{mean})^2} \quad (2)$$

A statistical analysis of the database was performed, in order to determine which variables have more influence over the cumulative biogas volume produced and, consequently, to indicate which combination of variables should be investigated in the form of response surfaces charts using the predicted results of the ANN best model.

3. RESULTS

3.1 Data statistical analysis

The database screening resulted in a set of 50 different experimental conditions that were separated into three datasets for the ANN: training, testing and validation. The full data distribution can be observed in the following histograms.

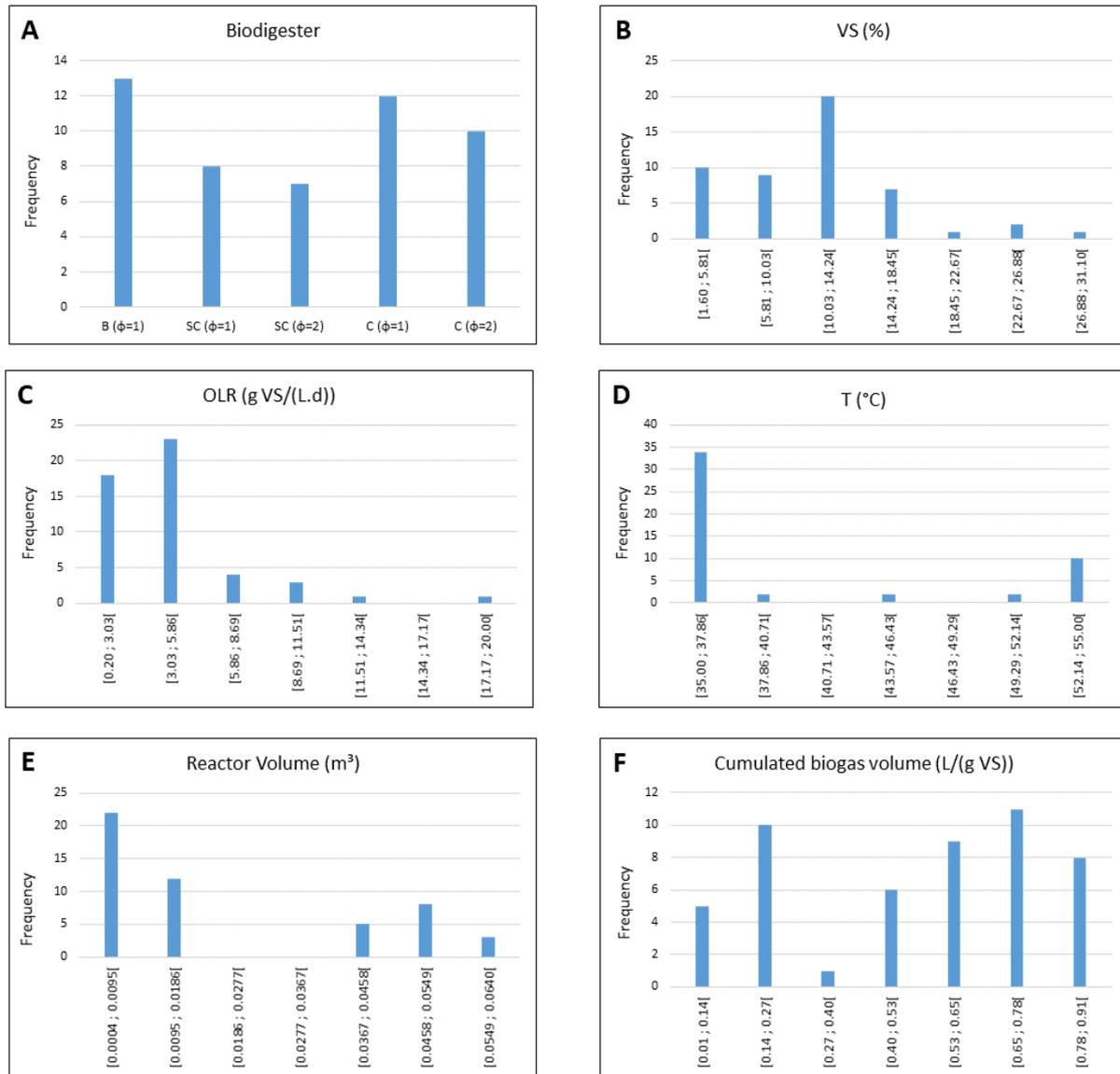


Figure 1. Data distribution for each of the system's variable. For the biodigester, B means Batch, SC means Semi-continuous, C means continuous and ϕ is the amount of phases.

As expected, Figure 1 shows how there is a lack of literature related to the biodigestion of FW for temperatures between the mesophilic and thermophilic regions, as it is known that this type of systems tend to be optimized for either. Besides, no research was found for reactor volumes between 0.0186 and 0.0367 m³. On the other hand, OLR data seems to be more abundant for values around 5 (g.VS/(L.d)). For the other variables, data is reasonably distributed.

After the analysis of the histograms, a statistical study was conducted to evaluate the effect of each variable through a polynomial approximation, resulting in the following Pareto chart.

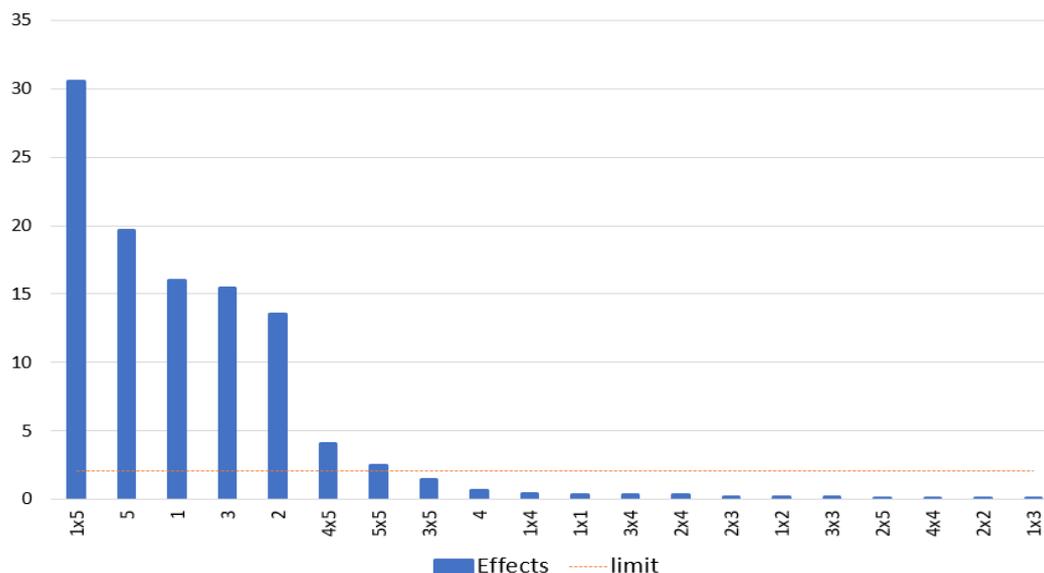


Figure 2. Pareto chart to evaluate the effect of each input variable. (1) Biodigester; (2) VS; (3) OLR; (4) Temperature; (5) Reactor volume.

From Figure 2, it is possible to observe that the only variable that does not present a considerable linear influence over the biogas production is the temperature. This result could be justified by the lack of information already commented. In contrast, the reactor volume was the only parameter to have a significant quadratic impact on the output. Regarding the combined effects, biodigester/reactor volume (1x5), temperature/reactor volume (4x5) and OLR/reactor volume (3x5) were the pairs that have shown considerable impact over the product synthesis, although OLR/reactor volume is close to the relevance limit and, therefore, was also considered.

3.2 ANN development

The database division was performed randomly and resulted in training, testing and validation sets with 39, 8 and 3 entries, respectively. Training and testing results can be found in Table 1, for all training algorithms, activation functions and number of neurons on the hidden layer (HD) considered, including the amount of parameters present in each network (NP).

Table 1. ANN training and testing results for all considered topologies (In bold: identification of the best ANN configuration)

ANN ID	Training Algorithm	Activation Function HD	Number of Neurons HD	Training Dataset SSE	R ² Training Dataset	R ² Testing Dataset	NP
net1	trainidx	tansig	3	10.004	0.328	0.907	22
net2			4	2.771	0.814	0.537	29
net3			5	3.061	0.795	0.718	36
net4		logsig	3	7.984	0.463	0.464	22
net5			4	7.840	0.474	0.692	29
net6			5	5.304	0.644	0.729	36
net7	trainbr	tansig	3	14.625	0.061	0.894	22
net8			4	14.794	0.062	0.886	29
net9			5	14.644	0.059	0.887	36
net10		logsig	3	14.579	0.059	0.799	22
net11			4	14.887	0.052	0.865	29
net12			5	14.042	0.074	0.000834	36
net13	trainlm	tansig	3	0.536	0.964	0.931	22
net14			4	0.440	0.970	0.070	29
net15			5	0.217	0.985	0.290	36
net16		logsig	3	1.629	0.891	0.754	22
net17			4	3.511	0.764	0.761	29
net18			5	0.137	0.991	0.279	36

As it can be seen in Table 1, trainbr algorithm presented the higher SSE during training, while trainlm presented the best performances in relation to this parameter. On the other hand, no major tendencies could be observed when comparing the different activation functions and the different number of neurons in the hidden layer. The trainbr algorithm also presented more occurrences of the coefficient of determination (R^2) of the training being greater than the one from the testing dataset. This indicates a strong possibility of underfitting, where the performance of the ANN in the test is better than in the training. In some instances, it was also possible to observe overfitting, as the model had high performance in the training dataset, followed by a considerable decrease in the testing.

From all analyzed topologies, net13 presented the best results, as it had better performance when R^2 from both training (0.964) and testing (0.931) datasets are considered. With this in mind, net13 was evaluated through the validation dataset, in which it also presented a considerably good R^2 (0.902). The application of net13 in each dataset can be better observed in Figure 3, where the model and experiment are compared in relation to the cumulative biogas volume through two different plots. In the first one, the output Y axis is relate to the model prediction, while the targets T axis represents the experimental data. In addition, the linear fit equation is presented, where the aim would be $Y = T$. The coefficient of correlation (R) was also included. The second plot shows the experimental and predicted cumulative biogas volume for each sample of the datasets.

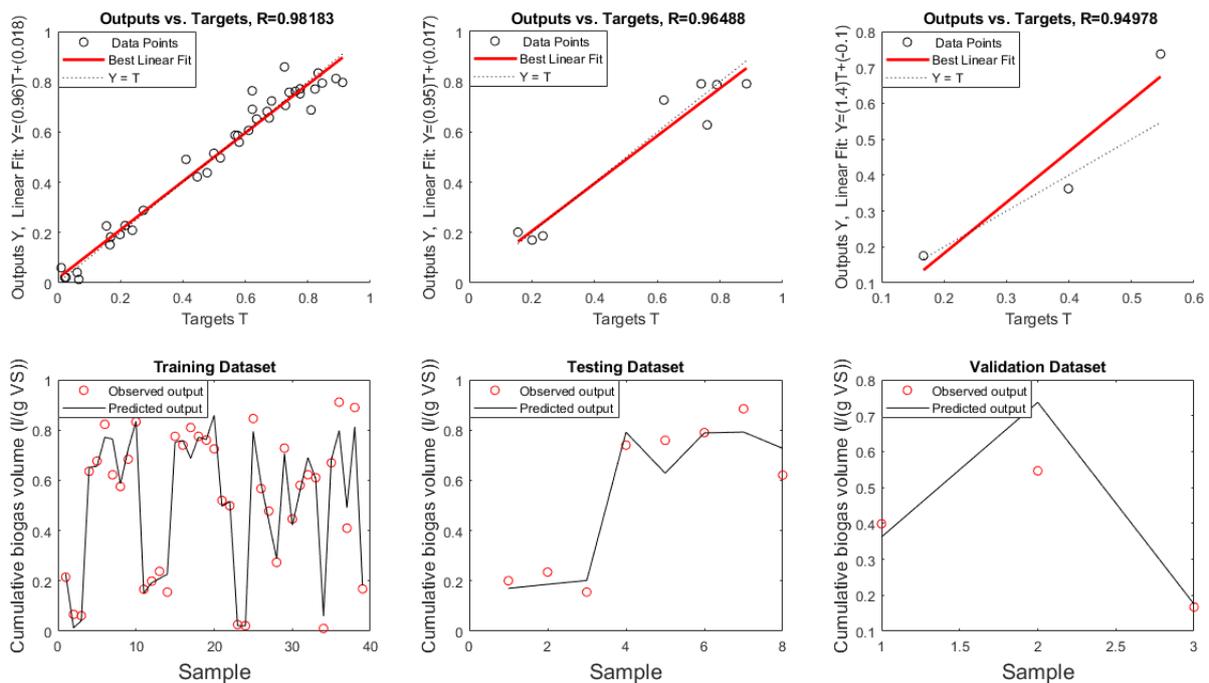


Figure 3. Performance of the best ANN (net13) for the training, testing and validation datasets.

As indicated in the Figure 3, the predicted and experimental data are not dispersed, which indicates the model has a good prediction capability for the analyzed system. In all three datasets, the best linear fit approximates the $Y=T$ line, as intended, the best case being the training, followed by the testing set, which is coherent, because these behaviors would not be expected to happen for all datasets in an overfitting or underfitting scenario.

3.3 Investigation using the best ANN

The best ANN model was applied considering the previous statistical analysis. In each case, two different parameters were evaluated through the whole database range while the remaining inputs were fixed according to Table 2. These values were calculated for the continuous variables through the average of the most populated groups observed in the histograms. Particularly for the temperature, the mesophilic region was selected for the calculation.

Table 2. Fixed values for each input not being analyzed.

Input Variable	Fixed Value
Reactor/feeding	Batch
VS (%w)	10.09
OLR (g VS/(l.d))	3.08
Temperature (°C)	36.36

The first investigation considered the variation of volume for each reactor/feeding type and can be observed in Figure 4. The model indicates the volume has an almost linear influence over the biogas productions for every case. In the considered conditions, the batch reactor presented a better performance than all other systems, being maximum for lower reactor volumes. The linear behavior was not expected, as biodigester processes are usually known for their high non-linearity.

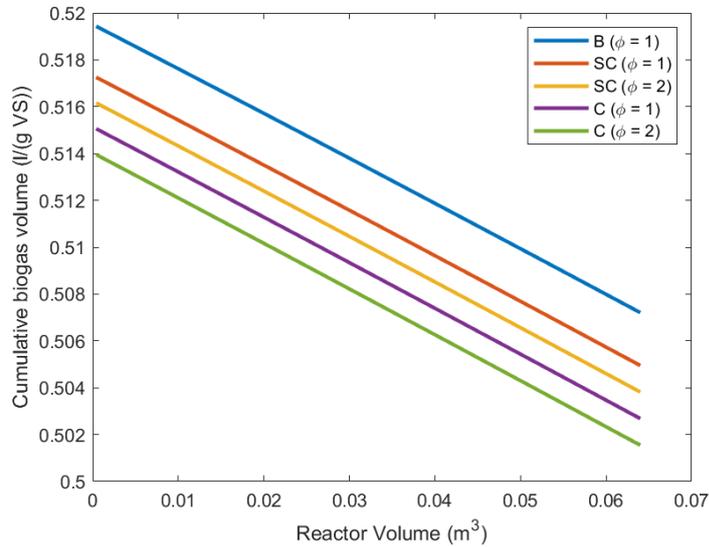


Figure 4. Performance of the best ANN (net13) for the training, testing and validation datasets.

Figure 5 expresses the variation of OLR and the reactor volume. Again, the behavior seems to be considerably linear as the prediction seems to have resulted in a flat surface. Lower OLR and reactor volumes seem to maximize production, being coherent with the previous figure.

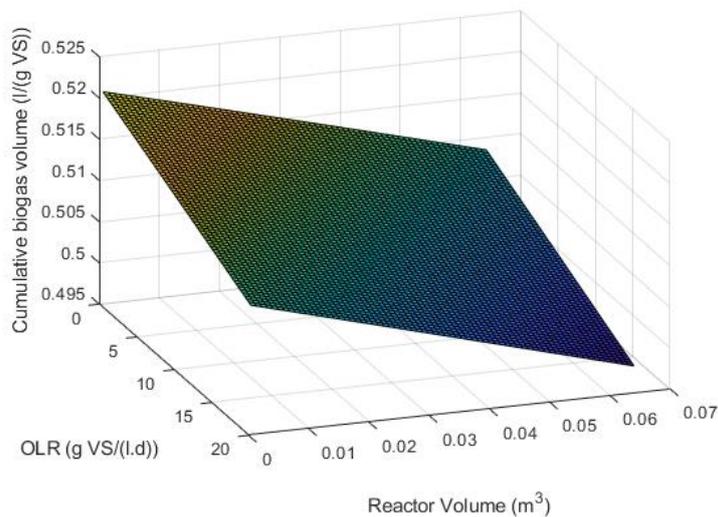


Figure 5. Response surface for OLR-Reactor volume.

The last analyzed case is related to the variation of temperature and reactor volume, which is presented in Figure 6. The response surface indicates maximum production at mesophilic temperatures, also with smaller reactor volumes. Unexpectedly, the increase in production at thermophilic temperatures is not present as the general behavior is considerably flat. This can be due to the lack of data in this region for ANN training.

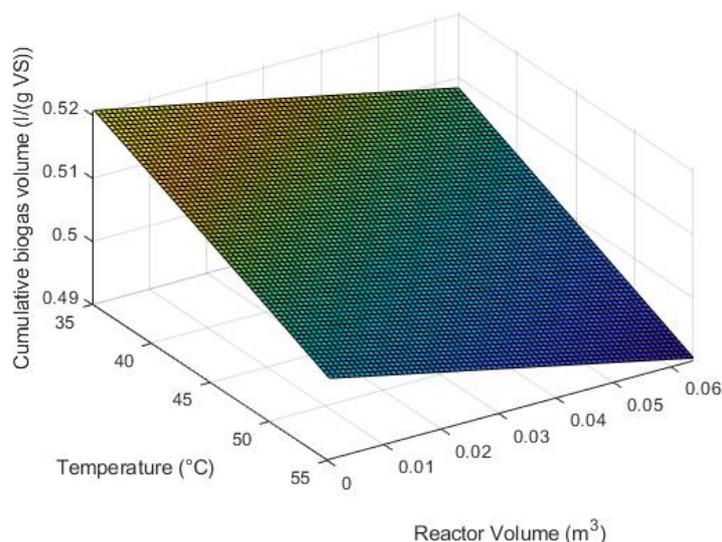


Figure 6. Response surface for OLR-Reactor volume.

It was possible to observe more linear tendency for all analyzed variables that could be related to the investigated conditions. It is also important to point out how little the cumulative biogas production changes (around 0.5 to 0.52 l/(g VS)), especially in Figures 4 and 5. This indicates the influence of the chosen variables may not be as expressive as expected from the statistical analysis. Besides, the size of the database is one of the major concerns in ANN modeling, because relation between the amount of parameters present in the network and the total of entries in the database limits the quantity of inputs that can be considered. As a result, the relatively small database used in this study constrained the model to having the considered inputs, although variables such as pH, retention time, carbon to nitrogen ratio and others are expected to also have a certain level of influence over the system. Therefore, the mostly flat behavior observed could be due to a limitation of the model, even though it presented excellent results in the training, testing and validation phases.

4. CONCLUSION

The biodigestion of food wastes has an important role in society, as it not only translates in an alternative energy source, but also gives a productive destination to an otherwise discarded material. A characteristic of these processes is the biological chemical reactions involved that are complex to model, which justifies the attempt to use artificial neural networks. In this study, 126 experimental data were found in the literature, although only 50 were presented the complete information needed for model implementation. This system was limited in terms of how many variables can be included in the model, due to the total amount of entries in the database, so the reactor/feeding type, temperature, OLR, VS and reactor volume were included. This final database was randomly separated between training, testing and validation datasets in which the best ANN (net13) had a determination coefficient of 0.964, 0.931 and 0.902, respectively. Although net13 has shown an excellent prediction capability for all datasets, the investigation performed according to the most influential variables pointed out by the previous statistical analysis resulted in a more linear behavior than expected. This could be justified by the size of the database, since other variables could not be included without the number of ANN parameters surpassing the amount of data entries. Therefore, the ANN model presented an excellent prediction capability for the given database and to better capture possible non linearity of the system, more data would be needed to allow more variables to be investigated.

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