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Application of Artificial Neural Network in the Modeling and Optimization of Volatile Acid from Anaerobic Digestion of Biomass

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ABSTRACT

Artificial neural networks (ANNs) and Brute Force algorithms (BF) are two of the most common and simplest techniques for modeling non-linear problems and linear search for an element. Very large data sets are actually compiled and fed into the ANN. An algorithm is run that iteratively makes billions of small adjustments to the weights and biases of millions of nodes. In this paper pilot-scale fermentation tests are carried out with mixtures of sewage sludge and food residues to investigate different process parameters that influence fermentation yields. A machine learning approach is used for data management and the development of a model capable of correlating process performance based on different inputs (operating parameters). To simulate the digester operation and estimate the Volatile Fatty Acid (VFA) outputs, a multi-layer ANN model with two hidden layers is developed. The ANN and BF are used to simulate and optimize the VFA from anaerobic digestion.

1. Introduction

Anthropogenic climate change, caused in various ways by the emission of greenhouse gasses, is the main reason for this catastrophe. This has obligated the government agencies and scientific communities to legislate and develop alternative solutions to overcome the aforementioned breakdown. Moreover, amidst existing options, biomass and biofuels as its main products seem to be a viable path to a sustainable development (Atadashi et al., 2012). As a result, researchers are investigating the use of renewable biomass to produce materials, fuels, and chemicals. In recent years, biomass has become a popular renewable source for energy production (Tilman et al., 2009). The use of biomass for energy production has increased in the United States by more than 60 % between 2003 and 2013 (U.S. Energy Information Administration, 2014).

Amongst different methods to produce biofuels (e.g., biogas, bioalcohols, biodiesel, etc.) from biomass, anaerobic digestion (AD) of biomass for methane production has received a lot of attention (Pilli et al., 2015). AD is a biological process in which a vast amount of biodegradable organic materials can be reduced to produce biogas (containing methane, carbon dioxide as well as traces of other gases, including nitrogen, hydrogen and hydrogen sulfide) with the help of microorganisms under anaerobic conditions. Biomass conversion into biogas takes place in four successive biological stages, that is to say hydrolysis, acidogenesis, acetogenesis and methanogenesis.

However, recent studies suggest terminating the AD

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process before the fourth stage to produce volatile fatty acids (VFAs), hydrogen (which is a clean fuel of high value) and carbon dioxide (Chang et al., 2010). In addition, unlike biogas, the storage and transfer of VFAs are much safer and easier, and they have a higher economic value than biogas.

In science and engineering, artificial neural networks (ANN) are used to solve a variety of problems, especially in areas where traditional modeling methods fail. A well-trained ANN, a data processing system inspired by biological neural systems, can be used as a predictive model for a specific application. An ANN's prediction capacity is determined by experimental data training and subsequent independent data validation. As new data becomes available, an ANN can relearn to improve its performance (Ghobadian et al., 2009).

A neural network is made up of three layers: an input layer, a few hidden layers, and an output layer. Each layer has a set number of neurons or nodes that are connected to each other. Each neuron is connected to the others via communication links and connection weights. On the linking weights, the signals flow through neurons. Each neuron receives various inputs from other neurons based on their connection weights and generates an output signal that can be generated by other neurons as well (Kalogirou, 2001; Kurt et al., 2007).

The network was subjected to two procedures to create an ANN model: Training and Testing. The network is trained to estimate the output values based on the input data during training. The network is used to estimate an output and is tested to estimate or store training data.

2. The role of ANN in anaerobic digestion systems

Neural networks have been utilized in anaerobic digestion systems for the analysis of trace gases (Strik et al., 2005), regulation of $NaHCO_3$ buffer addition, management of digester start-up and recovery, as well as for advanced control and forecasting of biogas production (Guwy et al., 1997; Holubar et al., 2002; Holubar et al., 2003).

In the realm of estimating, predicting and modeling statistical and analytical data, Artificial Neural Networks (ANN) stand out as a potent modeling tool that offers a swift and cost-efficient alternative to conventional analytical techniques (Betiku et al., 2015; Nguyen et al., 2020).

It is worth noting that Artificial Neural Networks demonstrate superior accuracy compared to the Response Surface Method (RSM) in forecasting higher biogas yields (Dahunsi et al., 2016).

Some studies have used neural networks to forecast how much biogas can be made from different substances in order to understand their characteristics and makeup (Gueguim et al., 2012; Beltramo et al., 2016; Verdaguer et al., 2016). Holubar and his team of researchers (Holubar et al., 2002) used different types of neural network models to understand and control how methane gas was made in tanks that did not have oxygen and were constantly stirred. They were studying how the amount of waste being put into the tanks affected the production of methane.

It was found that the new models could accurately predict the amount and type of gas produced by the reactors. Strik and colleagues (Strik et al., 2005) made a model to predict certain gases like hydrogen sulfide and ammonia using ANN. The model could accurately predict the trace gases even when conditions were changing.

Ghatak and other researchers in 2018 (Ghatak et al., 2018) used a neural network model to guess how biogas production changes at different temperatures. Scientists also use neural network to guess how much methane will be produced in anaerobic digestion which helps them avoid sudden increases in production and increasing efficiency, using information from the process as it happens (Holubar et al., 2002; Abu et al., 2010).

Temperature, acidity, waste chemicals, organic compounds, alkaline substances, solid particles and gas production are the main factors used as input data in ANN models (Holubar et al., 2002; Abu et al., 2010; Yetilmezsoy et al., 2013). Ozkaya and colleagues (Ozkaya et al., 2007) presented ANN models for foreseeing the methane division in landfill gas from anaerobic absorption from field-scale landfill bioreactors at the Odayeri Clean Landfill, Turkey.

The neural network models' performance evaluation indicated that the network output closely matched the corresponding target, yielding correlation coefficient of 0.951 and 0.957 as well as mean squared errors (MSE) of 0.00263 and 0.00250 for the predicted CH_4 fraction in the operation with leachate recirculation and the operation without leachate recirculation, respectively.

Umar Alfa and colleagues (Umar et al., 2024) demonstrated the efficacy of various machine learning algorithms in predicting volatile fatty acid (VFA) levels in the manufacturing process involving primary and secondary sludge. The models achieved a precise fit, boasting an ideal coefficient of determination of 1.0 during training and a respectable correlation coefficient of 0.902 during testing, indicating robust generalization capabilities.

Abu Qdais and colleagues (Abu et al., 2010) gathered operational data from a plant over a 177-day period to investigate the impact of digester operational parameters, including temperature (T), total solids (TS), total volatile solids (TVS), and pH, on biogas production. The study utilized an artificial neural network (ANN) model in conjunction with a genetic algorithm to optimize methane production, resulting in an optimal methane yield of 77 %, surpassing the maximum value of 70.1 % recorded in the plant's records. The model demonstrated a correlation coefficient of 0.87 and a performance mean squared error (MSE) of $6 \cdot 10^{-5}$.

3. Methods

3.1. Data preparation

The provided dataset consists of nine independent experiments, five of which are without pH control and thermal treatment, two with thermal treatment, one with pH control and one with both pH control and thermal treatment. Each experiment includes rows of seven input variables (Organic Loading Rate, Hydraulic Retention Time, temperature, sludge, food waste, day and pH) and the corresponding output values of nine Volatile Fatty Acids (acetic, propionic, isobutyric, butyric, isovaleric, valeric, isocaproic, caproic and heptanoic) as well as soluble chemical oxygen demand (CODsol) and the ratio of the total VFA to CODsol. Table 1 summarizes the operating conditions of all nine Continuous stirred-tank reactor (CSTR) runs; the data reported in this table represents the minimum and maximum values (for OLR and pH), the exact data (usually fixed in a single CSTR run, for waste activated sludge (WAS) and Organic Fraction of Municipal Solid Waste (OFMSW) content, HRT and T), and the application (true) or not (false) for the thermal pretreatment or pH-control strategy.

At the beginning rows with missing values are removed. Because of the scarcity of the available data and increasing the accuracy of the model that will be presented later, OLR, pH and VFA/CODsol ratio were interpolated as a function of day individually for each experiment using a cubic spline, as illustrated in Figure 1. The other inputs such as temperature, HRT, WAS and OFMSW content were kept constant during each process so there was no need to interpolate them. It should be noted that since the study was carried out using a semi-continuous fermentation reactor, it is expected that the interpolated data are fairly accurate

Table 1
Summary of operating conditions with (true) and without (false) pH control and thermal treatment for all the nine CSTR runs

Experiment number	pH control	Thermal pretreatment	OLR ([min, max])	HRT	T°C	WAS content (V/V, %)	OFMSW content (V/V, %)	pH ([min, max])
1	FALSE	FALSE	[12.5,17]	5	55	60	40	[4.6, 6.2]
2	FALSE	FALSE	[8.5, 13]	6	55	70	30	[5, 5.8]
3	FALSE	FALSE	[8, 13]	6	42	70	30	[5.3, 6]
4	FALSE	FALSE	[8, 12.5]	6	37	70	30	[4.9, 6]
5	FALSE	FALSE	[16.5,20]	5	55	50	50	[4.3, 5.1]
6	FALSE	TRUE	[7, 13.5]	6	37	70	30	[5, 6]
7	FALSE	TRUE	[7.5, 11]	6	25	70	30	[5.5,6.3]
8	TRUE	FALSE	[8, 14]	5	37	70	30	[6.8, 7.7]
9	TRUE	TRUE	[7, 14]	5	37	70	30	[8.3, 9.3]

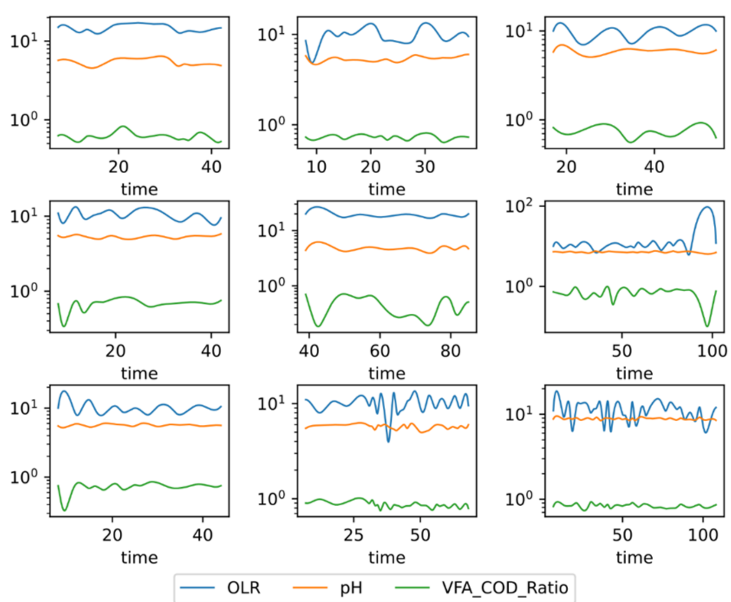

Figure 1. Interpolated data

3.2. Building a regression multilayer perceptron

A multilayer perceptron (MLP) is a feedforward neural network (FNN). An FNN is an artificial neural network (ANN) in which the signal moves only in one direction (from the inputs to the outputs). An ANN is a computational model inspired by the networks of biological neurons of the human brain. A biological neuron or nerve cell is a cell found in animal brains. It consists of a cell body containing the nucleus, dendrites and a single axon. The axon splits off into multiple branches called telodendria, and at the tip of these branches are structures called synapses, which are connected to the dendrites or cell bodies of other neurons.

A perceptron is made up of a single layer of Threshold logic unit (TLUs) (Figure 2), each connected to all of the inputs. A fully connected layer, also known as a dense layer, is one in which all of the neurons are connected to every neuron in the previous layer (i.e., its input neurons).

The perceptron's inputs are fed to input neurons, which are special passthrough neurons that output any input they are fed. The input layer is made up of all the input neurons.

The MLP presented here consists of an input layer with seven nodes, including HRT, temperature, sludge/food waste ratio, OLR, pH and two binary nodes indicating if a row of the dataset belongs to an experiment carried out with or without pH control and thermal treatment, two hidden layers with 256 and 224 nodes and one output layer with only one node representing the ratio of VFA to CODSOL (Figure 3).

The number of nodes in each hidden layer was determined using KerasTuner library. Both hidden layers use ReLU activation function. The model uses the mean squared error (MSE) as the loss function during the training. In addition, one third of the whole interpolated dataset were used for testing (two third for train set), and one third of the train set were used for validation.

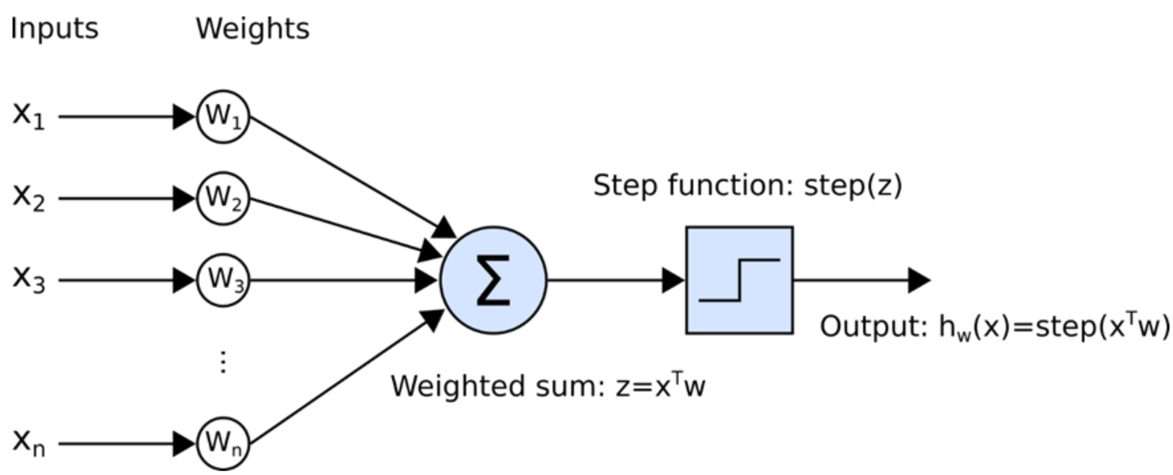

Figure 2. Threshold logic unit

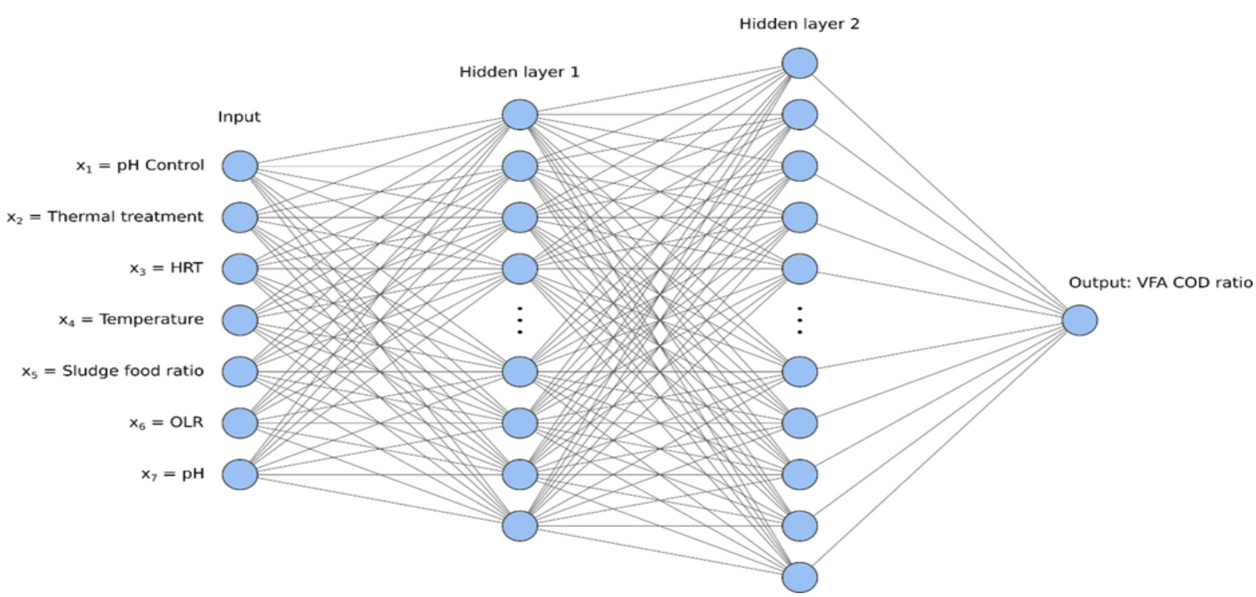

Figure 3. The regression MLP

4. Results and discussion

After compiling (training) the model using the MSE loss and fitting it on the training set for 10.000 epochs (number of complete passes of the training algorithm through the training set) and evaluating it on the validation set (to provide an unbiased evaluation of the model fit on the training set during tuning the internal parameters of the model), it has been get an MSE of about 0.0018 during training (Figure 4) and 0.0027 during evaluation using the test set. In other words, the model could predict the unseen data (test set) with the MSE of about 0.0027. Also, Figure 5 and Figure 6 illustrate that the model predicted the test set fairly accurately.

Figure 5 shows all the VFA/CODSOL ratio collected in all the nine CSTR runs, without any trend but just a sequence of data experimentally obtained (blue line). The predicted VFA/CODSOL values (pink dots; by the model) are often overlapped the real data (experimentally obtained).

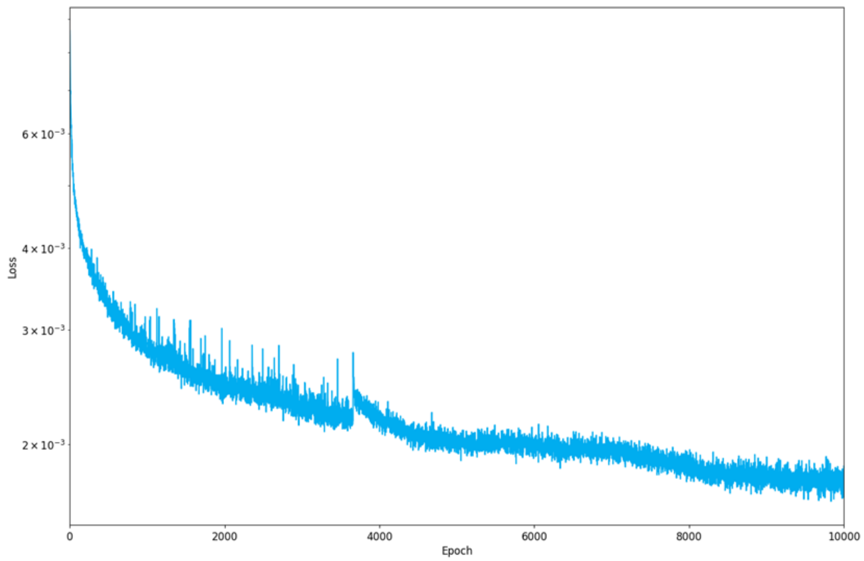

Figure 4. Learning curve: the mean training loss measured over each epoch

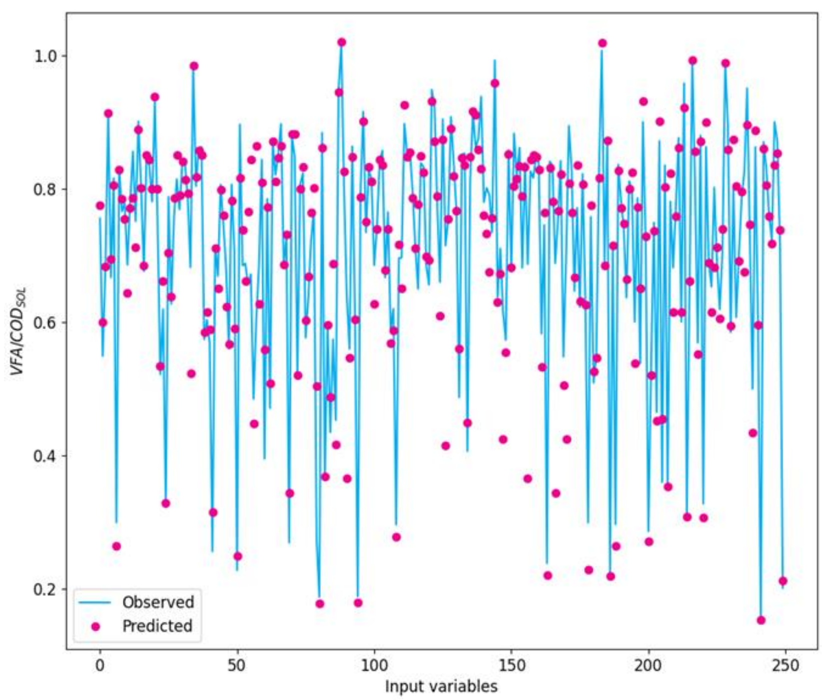

Figure 5. Actual versus predicted VFA/CODSOL values for the first 250 rows of the test set

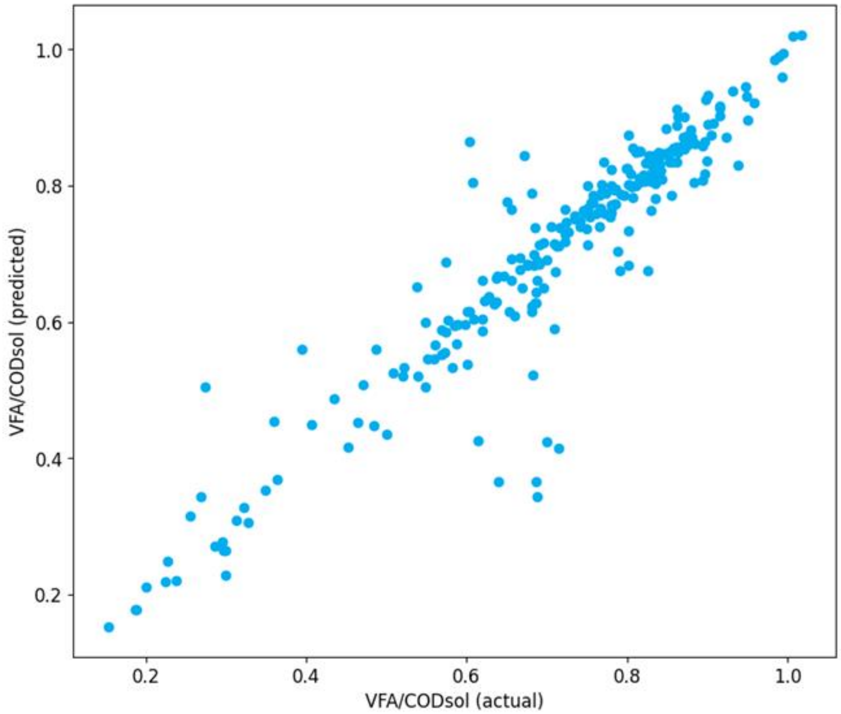

Figure 6. Actual versus predicted VFA/CODSOL values for the first 250 rows of the test set

In order to obtain the optimal values of VFA/CODSOL ratio in the acidogenic fermentation process as a function of operating parameters, a simple brute-force search was carried out using the values' ranges provided in TABLE 2. The highest experimental value of VFA/CODSOL (as output) in the provided dataset was 0.99, as ideal value to achieve. By considering all the past experiments, the highest VFA/CODSOL ratio value (0.86) was obtained in a CSTR run performed by applying thermal treatment to the feedstock, without pH control and with the corresponding input values of OLR of 8.0 kg VS/(m^3d), HRT 6 days, temperature (T) 37 °C, WAS content 70 % (v/v), OFMSW content 30% (v/v) and average pH of 5.9.

The maximum value of VFA/CODSOL was found to be 0.9999965, suggested by the optimal value by the model.

The results are depicted in Table 3. These results show the operating parameter to be applied, for the optimal valorization of such feedstock (composed by WAS and OFMSW); in other words, for the maximization of the acidification performances, among others the VFA/CODSOL ratio.

Table 2
The range of input variables for brute-force search

	HRT (D)	T (°C)	WAS/OFMSW (%, V/V)	OLR (KG VS/m^3 D)
MIN	5	15	0	5
MAX	10	70	100	25

Table 3
Optimal values of fermenter operational parameters for maximum vfa/codsol ratio

pH control	Thermal pretreatment	HRT (d)	T (°C)	WAS (%, v/v)	OFMSW (%, v/v)	OLR (kg VS/m^3 d)	pH
0	0	5	55	30	70	21	10.5
0	1	7	23	80	20	16	9
1	0	9	19	90	10	24	8
1	1	6	36	80	20	14	10.5

5. Conclusion

In this study, a regression MLP was developed to simulate the production of VFAs in a continuous fermentation reactor. The MLP model with two hidden layers with ReLU activation functions and one output node, was found to capture most of the important patterns in VFAs production, as it provided an MSE value of 2.7×10^{-3} for the test, which measures the amount of error in the model and evaluates the mean squared difference between the observed and predicted values. Using a simple brute force search, optimal values for HRT, temperature, sludge, food waste, OLR and pH can be predicted to maximize the ratio of VFAs to CODSOL considering four different conditions (without pH control and without thermal treatment, without pH control and with thermal treatment, with pH control and without thermal treatment, and with pH control and with thermal treatment).

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Primena veštačke neuronske mreže u modelovanju i optimizaciji isparljivih kiselina tokom anaerobne digestije biomase

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Višeslojni model
Anaerobna digestija
Fermentacija

I Z V O D

Veštačke neuronske mreže (ANN) zajedno sa Brute Force algoritmima (BF) predstavljaju dve od najčešćih i najjednostavnijih tehnika za modelovanje nelinearnih problema i linearnu pretragu za pronalaženje elementa. Veoma veliki skupovi podataka se zapravo sakupljaju i unose u ANN. Algoritam se pokreće i iterativno vrši milijarde malih prilagođavanja težina i pristrasnosti miliona čvorova. U ovom radu, koristili su se pilot testovi fermentacije u manjem obimu sa mešavinama kanalizacionog mulja i ostataka hrane, kako bi se istražili različiti parametri procesa koji utiču na prinose fermentacije. Pristup mašinskog učenja je korišćen za upravljanje podacima i razvoj modela sposobnog da koreliše performanse procesa na osnovu različitih ulaznih parametara. Kako bi se simulisao rad digestora i procenili izlazi isparljivih masnih kiselina (VFA), razvijen je višeslojni ANN model sa dva skrivena sloja. ANN i BF su korišćeni za simulaciju i optimizaciju VFA iz anaerobne digestije.