

Short Communication

Online Monitoring of Volatile Fatty Acids in Biogas Plants via Data-Driven Software Sensors

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Abstract - The Volatile Fatty Acids concentration (VFAs) is a critical component for operating and controlling biogas plants for biomethane production. However, the online monitoring sensors for VFAs are too expensive and require high maintenance costs. This paper proposes data-driven software sensors that can estimate VFAs online from the available online sensor data in biogas plants. From online sensor signals for the temperature, pH, flow rates and biogas composition as inputs and VFAs concentration as the target variable, two approaches are developed: Principal Component Analysis with Nonlinear Support Vector Regression (PCA-NSVR) and a Long Short-Term Memory (LSTM) recurrent neural network. The data set was obtained from numerical simulation in the International Water Association (IWA) Benchmark Simulation Model No. 2 (BSM2) that includes the IWA Anaerobic Digestion Model No. 1 (ADM1) with dynamic influent data and noisy sensor signals. The performance of both software sensors was evaluated via mean-root square error for the testing data set. The results show that the ability of the LSTM recurrent neural network to capture the sequential dynamics in the input data makes this approach more efficient for the online estimation of VFAs.

Keywords - Biogas plants, Biomethane, Anaerobic Digestion, VFAs estimation, Recurrent neural networks, Support vector regression, Software sensors.

1. Introduction

The current challenges related to the energy transition and global warming policies promote the development of environmentally friendly and sustainable energy technologies worldwide. The production of biomethane via anaerobic digestion from organic waste has gained more attention due to its high potential as sustainable energy technology [1,2]. Anaerobic digestion (AD) has been used in wastewater treatment plants (WWTP) to break down organic matter into digestate and biogas, consisting firstly of methane (CH₄) and carbon dioxide (CO₂). It provides a versatile renewable energy source since biomethane can be used to replace fossil fuels in both heat and power generation and vehicle fuel [1].

On the other hand, to implement advanced feedback control loops for optimal operation of biogas plants, it is necessary to deploy online measurement systems for adequately monitoring critical process parameters (CPP) [7-9]. However, the current monitoring equipment for CPP in anaerobic digestion processes and biogas plants, for example, the VFAs concentration, alkalinity or bacterial populations, are too expensive and require extensive maintenance costs [10]. Only a few variables like pH, temperature, flow rates, and gaseous outflow composition are available and cost-

effective for online measurement and automation purposes [8,10,11]. One alternative is to use mathematical models of the AD process with a limited set of available online sensor data to provide an estimation of the time evolution for the key process variables by means of the so-called software sensors (or virtual sensors) [12]. The main idea behind a software sensor is to use the easily accessible online data with a mathematical model of the system to get an estimate of the critical variables of the process that are difficult, so expensive, or not available for online measure [13]. From its design principle, it can be distinguished into two categories of software sensors: model-driven and data-driven. Model-driven based or first principle models-based software sensors require in-depth knowledge of the process mechanism. For the case of biochemical processes, the first-principle models are generally based on mass balance equations with different kinetic expressions for substrate consumption and the bacterial population's growth rates [14]. Specifically for the AD process, we can find different model-based virtual sensor approaches reported in the literature, from classical Kalman filters and adaptive observers schemes to nonlinear asymptotic, interval observers, and high-order sliding mode ones [15-24]. However, model-based software sensors have drawbacks and costs associated with model derivation,



particularly in selecting a convenient kinetic structure that correctly describes the complex interactions that occur in the bioprocess. Also, the model-based soft sensors have weaknesses associated with the poor predictability of the first principle models of bioprocesses.

On the other hand, the main advantage of data-based techniques is their simplicity of implementation based on inexpensive, basic online available measurable signals [25]. Data-driven models rely only on historical data sets obtained from the process (online and offline). They can be developed quickly without requiring knowledge of the complex phenomenology involved in the biochemical process [26]. Popular machine learning algorithms like Principal Component Regression (PCR), Support Vector Regression (SVR), and Artificial Neural Networks have been used as data-driven software sensor approaches for bioprocesses [25-27]. A good review of them can be found in [13,26]. Specifically for the AD process, we can find ANN-based models for estimating and forecasting some components [28-30]. Wang et al. 2018 [28], the authors developed an ANN

software sensor for online monitoring of alkalinity in an anaerobic co-digestion system. A back propagation-feedforward NN was designed using the available online measured parameters such as pH, oxidation and reduction potential, and electrical conductivity. In Dewasme 2019 [29], a radial basis function neural network-based software sensor is designed for the estimation of VFAs, alkalinity and the biogas composition from available measurements in an AD of brewery wastewater such as electrical conductivity, temperature, pH, redox potential, suspended solids and the in- and outflows. On the other hand, in Clercq et al. 2020 [30], different machine learning regression methods such as random forest and extreme gradient boosting have been used for modelling and forecasting the bio-methane output as a function of various organic waste input in an industrial-scale anaerobic co-digestion plant. However, until the knowledge of the author, the use of typical online measured data such as temperature, pH, flow rates, and biogas composition to design machine learning-based software sensors for estimating the key components of the biogas plants is an open issue to improve the operation, monitoring, and automation of biogas plants.

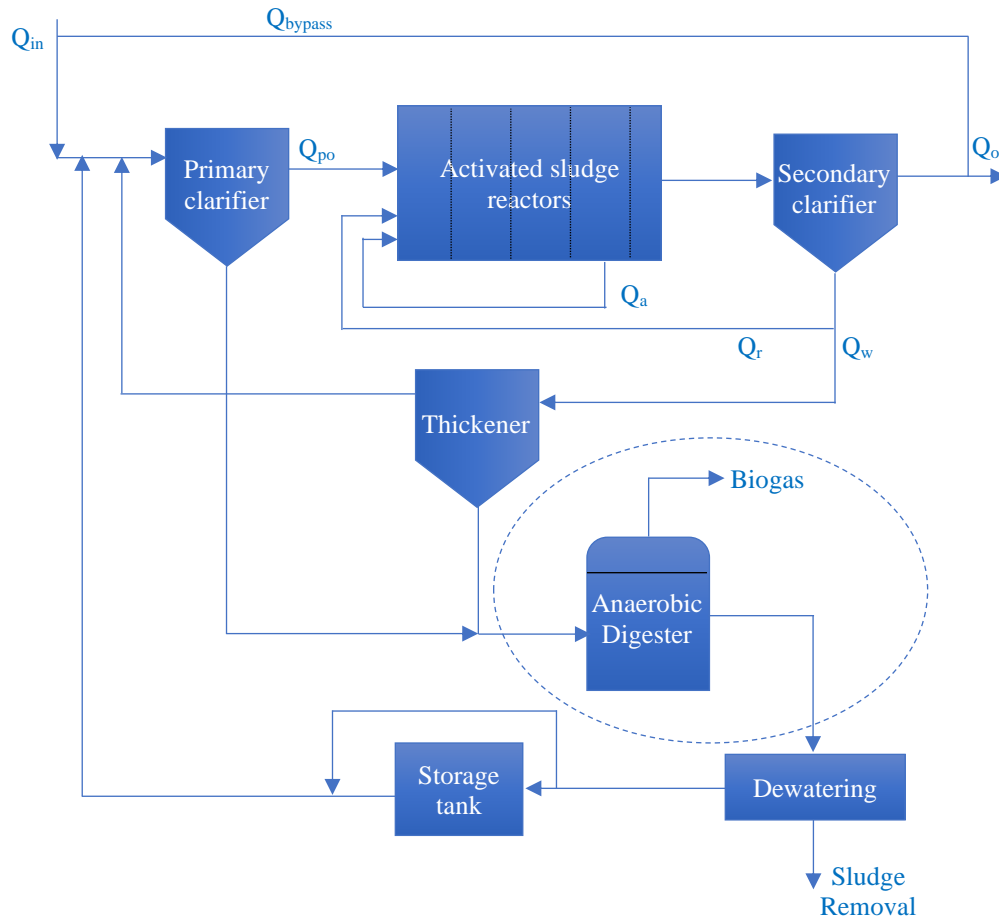


Fig. 1 Diagram of the BSM2 platform for a municipal wastewater treatment plant: The biogas plant is highlighted with a dashed line.

In this study, two machine learning techniques are implemented as software sensors for online estimation of VFA concentration in biogas plants: the first one is based on a combination of Principal Component Analysis with Nonlinear Support Vector Regression (PCA-NSVR) and, in the last one a long short-term memory deep recurrent neural network approach is developed. It is important to emphasize that in this contribution, the input features include typical online measured parameters in anaerobic digestion plants, such as temperature, pH, flow rates, and biogas composition. The data set was obtained from numerical simulation in the Benchmark Simulation Model 2 (BSM2) that represents a wastewater line of a municipal WWTP, including the implementation of the IWA Anaerobic Digestion Model Number 1 (ADM1) with dynamic influent data and noisy sensor signals [31]. The software sensors models' performance is measured using the mean-root square error technique with the testing data set. The rest of the paper is organized in the following way: in Section 2, the way to obtain the data set for the AD process is explained. After that, the PCA-NSVR algorithm is presented in section 3. Next, the architecture and characteristics of the long short-term memory deep neural network approach are shown in Section 4. Finally, some conclusions are summarized.

2. Data Set Collection

The data collection for the biogas plant was obtained from numerical simulations in the International Water Association (IWA) Benchmark Simulation Model No. 2 (BSM2) [31]. BSM2 is a powerful dynamic simulation model representing the physicochemical and biological phenomena in a Wastewater Treatment Plant (WWTP). The simulation platform represents a WWTP that considers dynamic influences, from short-term diurnal variations and weekend effects to long-term variations for temperature and holiday periods [31]. The WWTP comprises primary clarification followed by activated sludge process units in the water line and anaerobic digester (biogas plant), thickening and dewatering operations in the sludge line (see Fig. 1). The simulation platform used in this work includes the implementation of the IWA Anaerobic Digestion Model Number 1 (ADM1) that is a result of international collaboration among experts from multiple anaerobic process disciplines to get the most generic mathematical model for AD process reported in the literature [32]. The ADM1 includes the main biochemical and physic-chemical processes that occur in AD, and the math model contains 26 dynamic state concentration variables, 19 biochemical kinetic processes, 3 gas-liquid transfer kinetic processes and 8 implicit algebraic variables that globally represent 32 dynamic state concentrations and 6 additional acid-base kinetic processes [32]. The data set was obtained via numerical simulations outcomes for 180 days in the BSM2 platform considering the online monitoring variables recorded every 30 minutes for temperature, pH, flow rates, and biogas composition, and offline daily samples (24 hours) for VFAs concentration (see

Fig. 3 and Fig. 4). In Fig. 2 we can see the dynamic influent of the wastewater line for Suspended Solids (SS), influent flow rate and temperature.

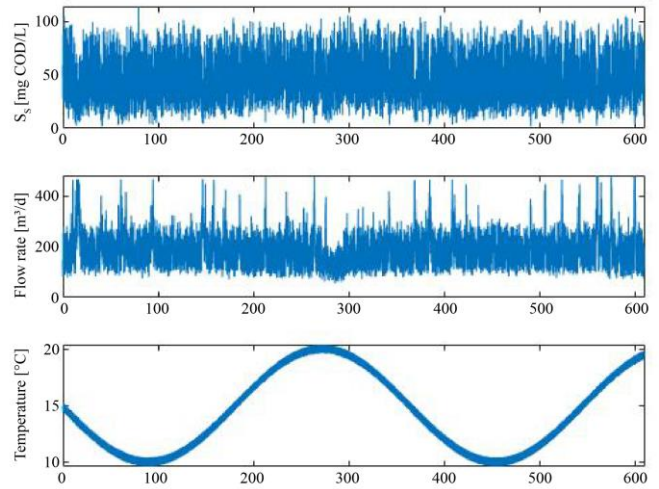


Fig. 2 Dynamic influent of the wastewater line in the BSM2 platform for suspended solids SS, influent flow rate and temperature.

In order to replicate a real operating scenario for the biogas plant, it is considered that there is noise in sensor measurement with Gaussian noise of strength 5–10 % added to all online measured process variables (see Fig. 4). Finally, the total Volatile Fatty Acids concentration was calculated as the sum of the short-chain fatty acids as $VFAs = Sva + Sbu + Spro + Sac$ where Sva , Sbu , $Spro$ and Sac represent the valerate acid, butyrate acid, propionate acid and acetate acids in the ADM1 model, respectively [32]. It is important to emphasize that in this work, the VFA concentration values are considered as offline samples taken every 24 hours (See Fig. 3). In order to match the output values with the input ones, a cubic spline interpolation tool (with the function, "interp" from MatLab) was used as is shown in Fig. 3.

3. Nonlinear Support Vector Regression

Support Vector Machine (SVM) is a supervised learning technique initially developed for classification problems. The main idea behind SVM is to find an optimal hyperplane that can maximize the distance between data points of different classes and the nearest data point of each class on the data space, which is called the margin-maximizing hyperplane [33]. Applications of SVM in nonlinear classification are made by means of mapping into a high-dimensional feature space using proper kernel functions $\phi(x, \sigma)$. Like classification, a non-linear model is usually required to model the data adequately. In the same way as the non-linear support vector classification, a proper nonlinear mapping can be used to map the data into a high dimensional feature space where linear regression is performed [33] (see Fig. 5). The nonlinear mapping can be chosen between polynomial functions, radial basis function, Gaussian functions, or others.

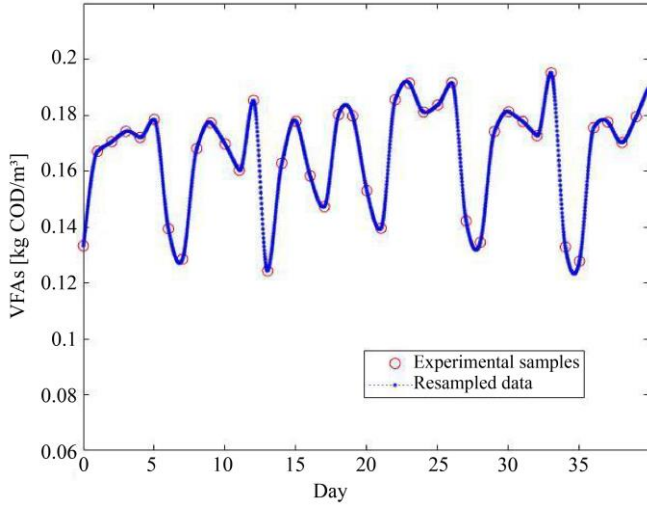


Fig. 3 Offline measured values for the VFAs concentration every 24 hours.

In order to apply Nonlinear Support Vector Regression (NSVR) to online estimation of VFAs in AD process the noisy measured signals for temperature, pH, flow rates and biogas composition were chosen as input features, while the VFAs were the output target, the schematic diagram of the NSVR-based soft sensor is shown in Fig. 5. The mapping of the normalized input signal from the data space to the feature space was done by using a Gaussian kernel function of the form:

$$\phi(x, \sigma) = -\frac{1}{(\sqrt{2\sigma})^n} e^{-\frac{\|x\|^2}{2\sigma^2}} \quad (1)$$

Where $x \in \mathcal{R}^n$ is the normalized input signal vector of dimension $n = 6$ and σ is the width of the Gaussian kernel. The data set was divided between the training and testing sets, assigning 80 % (144 days) to the training data and the rest to the testing data (36 days). All computing and algorithms were executed in the MATLAB® R2022b platform.

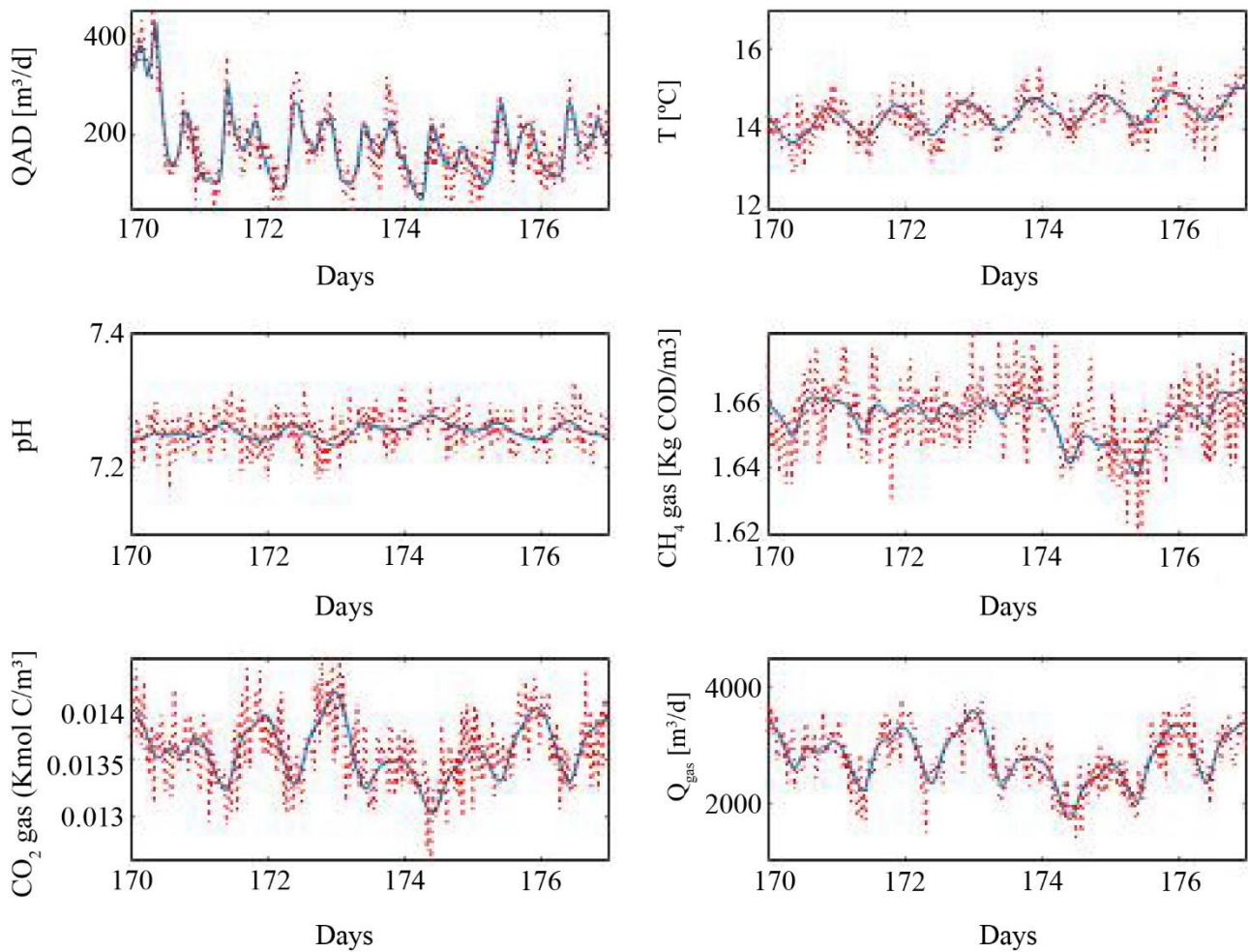


Fig. 4 Online measurement signals for temperature, inlet flow rate, pH, outflow gaseous rate and biogas compositions: the noisy corrupted signals are highlighted with dotted lines

In order to have an idea of the correlation degree between the input and output variables, the correlation coefficient matrix was computed for all data sets; it can be seen that the gaseous outflow data is more correlated with the VFA concentration (see Table 1). We consider using a statistical reduction dimension method before the NSVR to simplify the original sensor data from this result. We chose the PCA method to consider previous results regarding Principal Component Analysis (PCA) combinations with NSVR as software sensors. The essence of PCA consists of simplifying the original data space with minimum loss of overall dispersion, getting the way to a reduction of dimensionality in which the input data is represented [34].

The performance of the PCA/NSVR-based software sensor was evaluated with the root mean square error (RMSE),

that is, the standard deviation percentage of the residuals (prediction errors) calculated as:

$$RMSE = \sqrt{\frac{\sum_{k=1}^N (VFA_k - \widehat{VFA}_k)^2}{N}} \quad (2)$$

Where VFA_k is the actual value, \widehat{VFA}_k is the estimated value predicted by the software sensor, and N is the total number of data points in the testing set.

Considering that the gaseous phase inputs correlate more with the VFAs, we evaluate the software sensor performance with 3 and a total of 6 inputs similar for the PC's (Table 1).

Table 1. Correlation coefficient matrix for the input and output variables for the AD process

	Q_ad	Tem	pH	CH4	CO2	Q_gas	VFAs
Q_ad	1,000	0,025	-0,080	-0,163	0,001	-0,089	0,028
Tem		1,000	-0,250	-0,111	0,129	0,061	-0,123
pH			1,000	0,104	-0,199	-0,121	-0,078
CH4				1,000	0,155	0,327	0,344
CO2					1,000	0,525	0,341
Q gas						1,000	0,494
VFAs							1,000

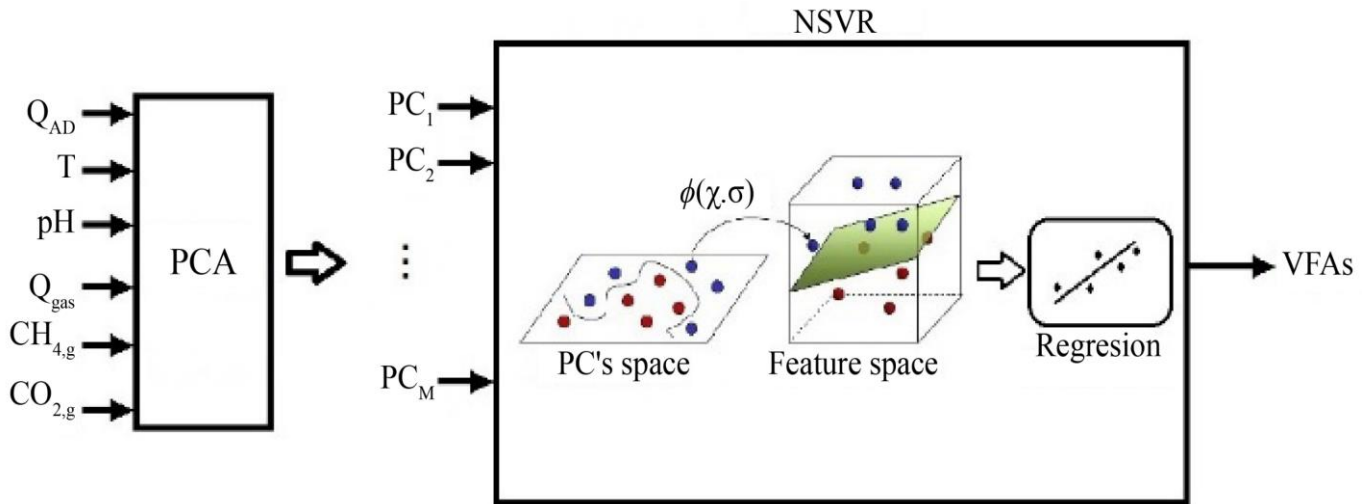


Fig. 5 Schematic diagram of the PCA/NSVR-based virtual sensor.

Table 2. RMSE for the PCA/NSVR-based soft sensor

Number of inputs	Without PCA	PCA (3)	PCA(6)
3	0,0179	0,0179	
6	0,0168	0,0211	0,0167

As we can see, the best combination was with 6 inputs and 6 PC's (Table 2), then this one was chosen as the configuration of the PCA/NSVR's soft sensor. The validation of the PCA/NSVR-based software sensor for the testing data is shown in Fig. 6. It is shown that the VFAs estimated follow with acceptable performance the fluctuation of the actual values.

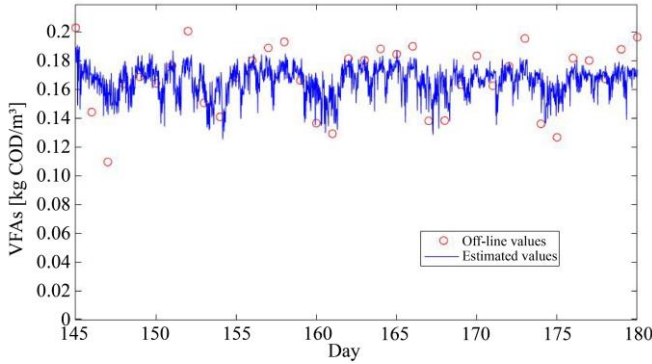


Fig. 6 Validation of the PCA/NSVR-based soft sensor for the online estimation of VFAs concentration with test dataset

4. Long short-Term Memory Deep Recurrent Network

Traditional static artificial neural networks ANN do not have the capacity to represent the inherent dynamics in sequential input data. This drawback makes them limited to model processes with complex dynamics like a biogas plant. However, in the last few years, recurrent architectures of ANN formed with activation functions and feedback connections have been considered feasible options for solving different dynamics pattern recognition problems [35].

Due to the recursive components in their architecture, Recurrent Neural Networks (RNN) have the ability to remember past information and process new events from the sequential input data [36]. The sequential input data can be collected from the plant's online sensor measurements, making the RNN more suitable to model complex dynamics in a real bioprocess. Also, since deep learning architectures are composed of multiple layers of nonlinear modules, they achieve better generalization in the case of highly varying nonlinear systems [27].

Additionally, the advantages of recurrent deep networks in dealing with big data from sensor measurements make them a promising tool for designing software sensors for complex biochemical processes [37]. Long short-term memory LSTM networks are an improved version of RNN that avoids the problem of vanishing and exploding gradient in the learning process proposed originally in Hochreiter et al., 1997 [38]. LSTM networks have specific units with the capacity to remember information for long- or short-time intervals.

The LSTM units are composed of the following elements: a central cell that controls the memory of the unit; the input and output gates that control the flow of input and output information, combining with previous states with weights; and a forget gate that determines how the cell will keep the previous states (see Fig. 7) [36]. In zoom of the RNN's diagram, $x(t)$ represents the input data at time t , and $h(t-1)$ indicates the hidden units at time $t-1$, while $C(t-1)$ and $C(t)$ represent a candidate value at time $(t-1)$ and (t) , respectively.

Each element in the LSTM block has an activation function, either a sigmoid function or tangent hyperbolic function, and a set of weights is specified in its design and training procedure, respectively.

The architecture of the LSTM network-based software sensor proposed in this work is shown in Figure 7. Firstly, the input data for the 6 measured signals (features) were normalized by centring with respect to their mean and dividing by their standard deviations according to:

$$\bar{x}_i = \frac{x_i - \mu_i}{\sigma_i} \quad (3)$$

Where x_i , \bar{x}_i are the i -th input and the normalized value, respectively, and μ_i , σ_i are the corresponding mean and standard deviations. Next, the first layer is a sequence input layer whose size is the same as the number of inputs to the network model (for this case, it is equal to six), followed by a Bidirectional Long Short-Term Memory layer with the number of hidden units in the forward and backward sequence was chosen initially at 100; next layer is a dropout layer that is useful to prevent overfitting; after that was added a fully connected layer whose output size specifies the size of the output for the layer (for this case is equal to one); and finally a regression output layer for the neural network is added.

The input data was divided in the same way that the PCA-NSVR software sensor, *i.e.*, 80 % (144 days) to the training data and the rest 20 % to the testing data (36 days). The adaptive moment estimation algorithm (Adam) was chosen for training the neural network because it is a more computationally efficient optimization algorithm and converges better within the same training epochs than the stochastic gradient descent SGD one [39]. The maximum number of epochs was fixed at 60 with an initial learning rate equal to 0.01. The loss function used in the training process was the RMSE defined in (2).

The validation of the LSTM network-based software sensor for the testing data is shown in Figure 8. Unlike the NSVR software sensor in Fig. 8, it is shown that the VFAs estimated fit closer to the actual values, avoiding noisy fluctuations. The RMSE computed for the LSTM virtual sensor is lower than for all combinations obtained with the NSVR ones (see Table 2), with a value of 0.0108.

4.1. Improving the Deep Network Architecture

In order to improve the LSTM network-based software sensor performance and avoid possible overfitting, the effect of the number of hidden units on the RMSE is considered. In Fig. 9, RMSE is shown as a function of the number of hidden units. We can see that the best software sensor performance is presented in around 100 hidden units. The performance of the LSTM network-based software sensor with 100 hidden units is shown in Figure 10.

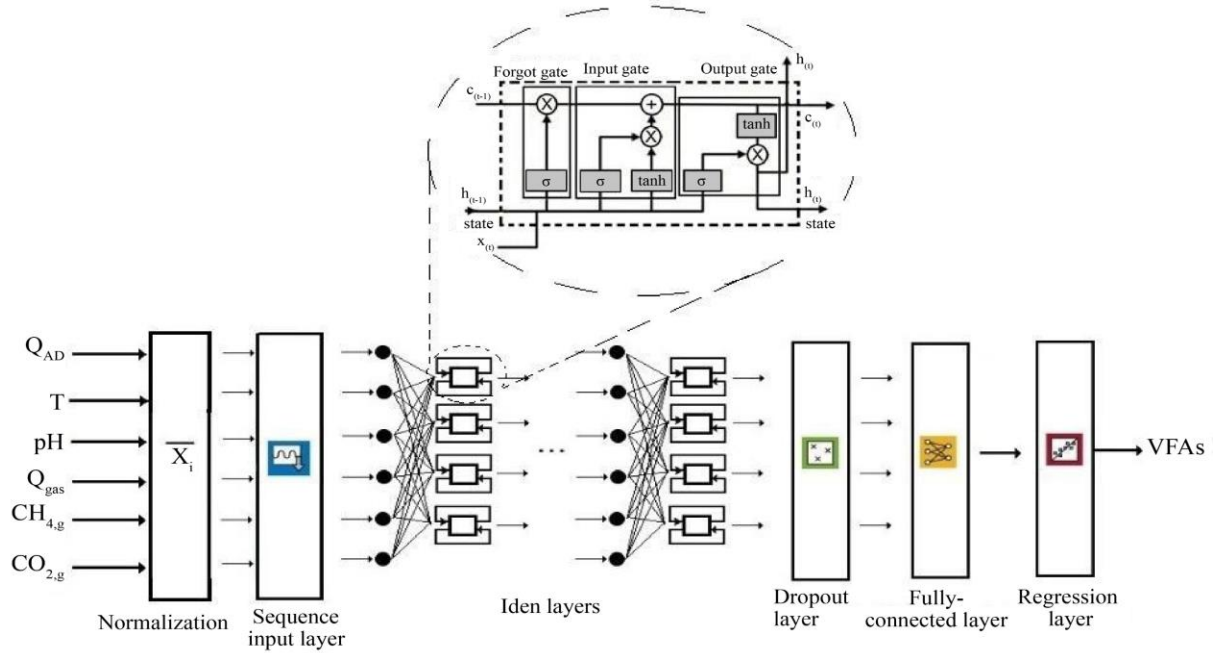


Fig. 7 Recurrent neural network structure for the LSTM-based software sensor

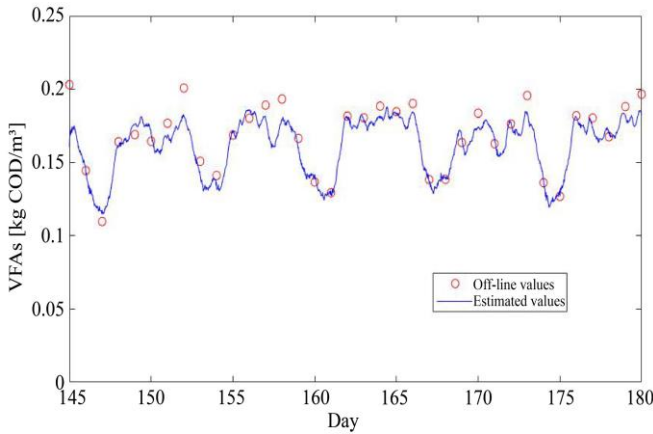


Fig. 8 Validation of the LSTM network-based software sensor for the online estimation of VFAs concentration with the test dataset.

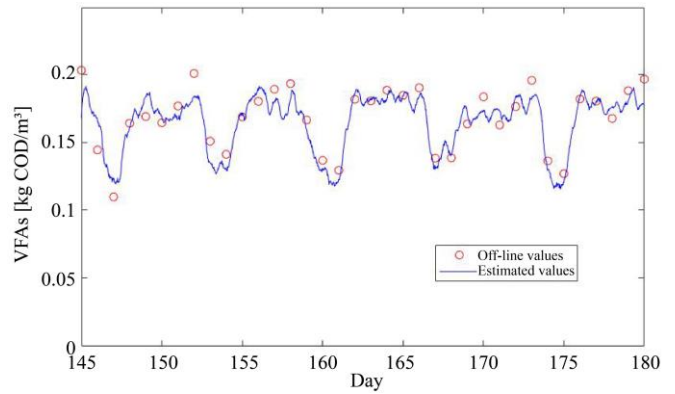


Fig. 10 Validation of the LSTM network-based software sensor with 100 hidden units

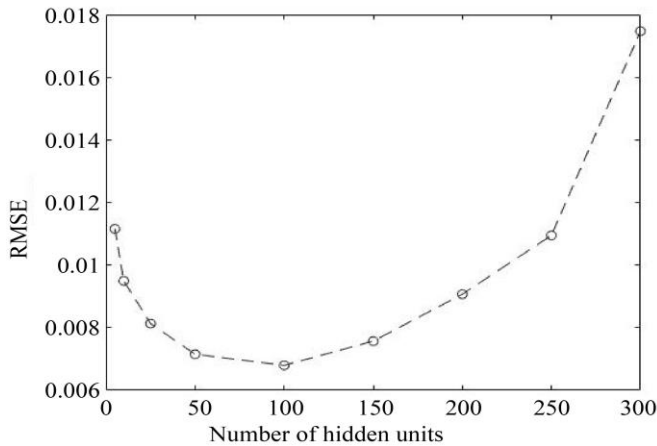


Fig. 9 Root mean square error (RMSE) as a function of the number of hidden units in the LSTM network architecture.

Finally, with respect to future implementation of these classes of software sensors with real biogas plants online measured data, it is important to consider that commonly, the offline laboratory measures of the VFAs concentration are made with a low sampling rate of the order of 1-3 days. In this case, it would be necessary to modify the LSTM network architecture to one able to process the input data as a sequence and the output as a scalar value, with a structure like "sequence to one". This issue will be addressed in future contributions.

5. Conclusion

In this article, two machine learning models, nonlinear support vector regression and Long Short-term Memory (LSTM) recurrent network, were studied as software sensor approaches for the online monitoring of total Volatile Fatty Acids concentrations (VFAs) in biogas plants from the online

sensor data for temperature, pH, flows rates and biogas composition as input features. The NSVR approach showed good performance with easy implementation and low computational cost. However, taking into account the mean-root square error as performance criteria, the LSTM recurrent network approach showed the best fitting with the actual

values. The capacity of the LSTM recurrent networks to capture the dynamics of the sequential input data makes this approach more efficient for representing the complex dynamics of the biogas plants. It provides a good estimation of their critical components.

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