

Prediction of Temperature Conditions of Autothermal Thermophilic Aerobic Digestion Bioreactors at Wastewater Treatment Plants

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Abstract: *Energy integration plays a significant role in increasing energy efficiency and sustainability of production systems. In order to model real energy integrated systems, sometimes we don't need rigorous models for involved units, but easily implemented and fast ones instead. This study presents an approach based on Artificial Neural Networks (ANNs) for predicting the main parameters of industrial Autothermal Thermophilic Aerobic Digestion (ATAD) bioreactors that are crucial for their energy integration.*

To create such predictive ANN model, four architectures with different number of hidden layers and artificial neurons in each one of them have been investigated. The developed ANN architectures have been trained and validated with data samplings obtained through long-term measurements of the operational conditions of real ATAD bioreactors. To train the models, BASIC genetic algorithm has been implemented. Using three independent measures for validation of the models, the best ANN architectures were selected.

It is shown that selected ANN models predict with sufficient accuracy these ATAD parameters and are suitable for the implementation in an energy integration framework.

Keywords: *Wastewater treatment plant, Autothermal thermophilic aerobic digestion bioreactor, Parameters prediction, Artificial neural network, Genetic algorithm.*

Introduction

Continuously growing requirements related to the treatment and disposal of sewage sludge result in either the development of sustainable technologies of wastewater treatment or the improvement of existing ones in terms of their environmental and economic performance. Autothermal Thermophilic Aerobic Digestion (ATAD) is an example of advanced wastewater treatment technology that produces Class A Biosolids used as fertilizer in agriculture. It is realized with the help of aerobic thermophilic bacteria, where a high degree of stabilization of treated sludge is achieved. The process is self-heating as generated metabolic heat from the microorganisms leads to increase of the operating temperatures in the system and to killing of pathogens. The ATAD process is conducted in either a separate bioreactor or in a series of consecutive connected bioreactors operating in batch mode, where the sludge is treated at different operational temperatures.

ATAD facilities have a lot of advantages such as simple and flexible operation, low investment costs, class A Biosolids production etc. However the ATAD process is influenced substantially by the change in the amounts, composition and temperatures of the incoming raw sludge which leads to decrease of operational temperatures in the first bioreactors stages

and deterioration of the operational conditions of the ATAD system [9]. The latter prolongs the degradation process, hence increasing the cost of the energy needed for aeration and mixing for restoration of the normal operational conditions of the ATAD system.

Due to the fact that the heat generation and retention in the ATAD bioreactors play a key role for their performance, many researchers have analyzed opportunities to improve them in terms of their sustainability. Earlier studies on ATAD processes from an energy viewpoint have been focused mainly on the stoichiometry calculations of the kinetics of biological heat generation and identification of the parameters related to sludge stabilization [12, 13, 25]. One way to examine all aspects of the ATAD process in order to enhance its energy efficiency is the application of a mathematical modeling approach. Many of the developed mathematical models are based on Activated Sludge Models allowing simulation of the behavior of biological nitrifying and denitrifying sludge systems [5, 6]. These models comprise mass balance equations and can be applied either in thermophilic [7, 8], or both mesophilic and thermophilic conditions [8]. They can involve equations for description of physico-chemical transformations associated with the chemical equilibria and the mass transfer between the liquid and the gaseous phases in the ATAD bioreactors, as well as energy balance equations for prediction of the ATAD system temperature [3]. Recently, a mathematical model for predicting the main heat flows in ATAD biochemical reactors based on Hess's law, comprising simultaneously both conventional mass balances and energy balances formatting multi-phase matrix structure, has been proposed [2]. The model is implemented in a plant-wide modeling framework, extended with models of biochemical, physico-chemical and chemical transformations as well as mass transfer of co-existing liquid, gaseous and solid phases for description of ATAD wastewater treatment process [11].

In order to improve energy efficiency and plant capacity of ATAD system, the ATAD model has been involved in dynamic optimization framework [19, 20]. Based on an analysis of the results obtained under optimization, the parameters which have the biggest impact on the energy efficiency of the process have been identified.

Another opportunity for reducing the energy requirements of the ATAD system is application of heat integration of the processes [9]. An integration framework to enhance the energy efficiency of ATAD system has been developed, based on the hypothesis that the ATAD system has a sufficient energy potential that can be utilized for preheating of incoming flows [21, 24, 26].

Usage of already created ATAD models in this framework is accompanied by a lot of difficulties arising from their complexity due to inclusion of large number of parameters and variables. Moreover, existing models are developed mainly for laboratory scale case studies operating in specific temperature ranges, while in real scale case studies the presence of uncertainties in respect to the parameters of incoming flows, which varies in different seasons and days, introduces additional computational efforts.

Taking into account the above, the aim of this study is to propose an approach for modeling the industrial ATAD bioreactors based on Artificial Neural Networks (ANN) that are suitable for incorporation in an energy integration framework. Using long time industrial data and Genetic algorithm for ANN training the created models must predict the main parameters in respect of the energy integration such as the maximal operational temperatures reached at the end of batches and respective reduction of volatile solids, as well as the expected thermal shock.

The article has the following structure: Section 2 describes the developed ANN models of the ATAD bioreactor including short description of the used genetic algorithm. Results of the models' validation are shown in Section 3. Finally, short conclusions are made.

Artificial neural network modeling of ATAD bioreactors

General description of artificial neural networks

ANN are inspired by the way biological neurons transmit and process information, comprising a large number of highly interconnected artificial neurons which receive input data and process them so as to obtain output. ANN are applicable to modeling wide range phenomena in physics, computer science, biochemistry, mathematics, ecology, sociology, economics, telecommunications, color image recognition and many other areas, through consideration of only the available values of the process variables, developing conditional nonlinear functions based on the extraction of the data [1, 4, 10, 14, 15, 16, 17, 18, 23].

Artificial Neural Networks (ANNs) simulate the behavior of biological neural systems. They consist of *inputs* (like synapses through which natural neurons receive signals), *outputs* and one or more *hidden layers* with multiple neurons in them. Connections between them are modified by *weights* (strength of the respective signals). In addition, each neuron has an extra input that is assumed to have a constant value of one. The weight that modifies this extra input is called *bias*.

An illustration of *feed-forward* ANN, comprising several hidden layers with different number of neurons in each of them is shown in Fig.1.

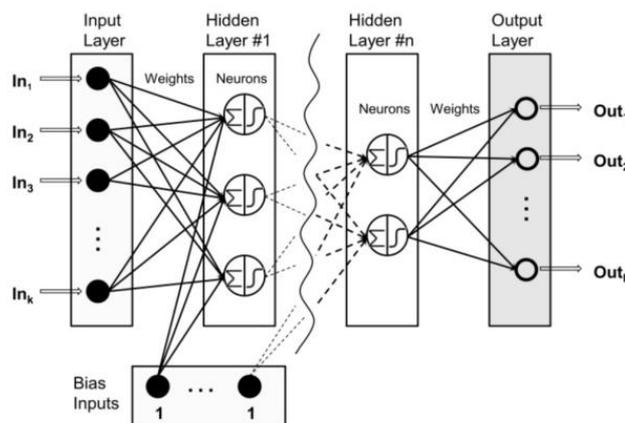


Fig. 1 *Feed-forward* ANN

In a *feed-forward* ANN the data transfer direction is from inputs to outputs. The neurons of the hidden layers aggregate these weighted values to a single value, as follows:

$$net_i = \sum_j w_{i,j} \cdot x_j + b \quad \forall i, i \in k, \forall j, j \in l, \quad (1)$$

where

i are neurons;

j – inputs;

$w_{i,j}$ – weighted coefficients of input-to-hidden connections and hidden-to-output connections;

x_j – inputs of the neural network;

b – bias inputs for each one of the neurons in the hidden layers.

An *activation function* is applied to the aggregated weighted value to produce an individual *output* for the specific neuron (like an activated natural neuron which emits a signal through the axon which might be sent to another synapse, and might activate other neurons). For ATAD bioreactor modeling the following sigmoid function is applied:

$$F(x)_i = \frac{1}{1 + e^{-a \cdot net_i}}, \quad (2)$$

where a is the coefficient defining the slope of sigmoid function. We have chosen $a = 2$ as a most frequently used value.

The ANN model is involved in an optimization framework as an optimization criterion *least-square function* (LSF) is applied. The process is called *training with teacher* and represents adaptation of the weights of artificial neurons so as the required outputs for specific inputs are to be obtained at minimal value of LSF.

The performance of ANN is influenced substantially by the number of inputs and outputs for the model, as well as its architecture, i.e. the number of hidden layers and neurons in each hidden layer.

Determination of ANN inputs and outputs

In order to determine the parameters which have the most significant impact on energy integration of the ATAD system a detailed description of the operations of charging and discharging of the bioreactors is provided.

ATAD bioreactors operate in a batch operational mode within a cycle of 20-24 hours. Keeping a constant volume of treated wastewater in the bioreactor, each new batch N starts every day by replacing part of QS_N , % of treated wastewater with raw sludge. For the purpose, the same amount of wastewater already treated in the bioreactor is discharged producing an outgoing hot flow. The latter has a temperature equal to the maximal operational temperature (T_{max} , °C) reached inside the bioreactor before its opening and a concentration of volatile solids (VS, %) equal to those at the end of the batch. Both the maximal temperature and concentration of volatile solids reached in the bioreactor at its opening are results of the implementation of the previous batch N-1 ($T_{max_{N-1}}$, °C and VS_{N-1} , %).

Finally, the same amount QS_N , % of the raw sludge is fed from the feed tank to the bioreactor having inlet temperature TAD_N , °C, and concentrations of both the total solids and volatile solids, respectively TSS_N , % and VSS_N , %. Destroying the reactor's insulation in the beginning of the new batch for unloading and uploading respective flows and mixing the inflow with the wastewater there leads to a sharp temperature drop inside the bioreactor to the minimal one, T_{min_N} , °C, causing thermal shock on the microorganisms and taking time to restore the required temperature conditions. Then the bioreactor is insulated, the ATAD process is started reaching the maximal temperature, T_{max_N} , °C and reduction of the volatile solids, VS_N , % at the end of batch N after approximately 24 hours.

The purpose of ANN modeling is to determine the expected temperature drop, maximal operational temperature reached at the end of batch and respective reduction of volatile solids, so following the above description we have selected required inputs and outputs for modeling of the bioreactors as listed in Table 1.

Table 1. Selected inputs and outputs for modelling

	Bioreactor	
	Inputs	Outputs
Feed amount of raw sludge, [%]	QS _N	
Composition of total solids in raw sludge, [%]	TSS _N	
Composition of volatile solids in raw sludge, [%]	VSS _N	
Temperature of the feed, [°C]	TAD _N	
Temperature inside the bioreactor before opening in a current day, [°C]	Tmax _{N-1}	
Volatile solids in bioreactor on the next day, [%]		VS _N
Temperature drop in bioreactor, [°C]		Tmin _N
Temperature inside the bioreactor before opening on the next day, [°C]		Tmax _N

To create the required ANN models we have used long time daily industrial records of the temperatures inside ATAD bioreactors, reduction of volatile solids at the end of each batch, amount of charged raw sludge with its composition in terms of total solids and volatile solids and the temperature. All the data are measured, and aiming to exclude large deviations in measured values we have subjected them to the analysis determining respective intervals of confidence.

Thus, the upper and lower confidence limits for each set of measured data have been determined accepting a confidence interval of 95%:

$$\bar{X} \pm 1.96 \frac{S}{\sqrt{n}}, \quad (3)$$

where \bar{X} , S and n are mean, standard deviation and size of the data set.

In this way only the data sets contained within determined limits are used for modeling.

Then, we have chosen samplings for ANN learning and validation of designed model. We have set apart approximately 1/3 of the data for validation. The remaining data sets are used for determining the number of samplings for training the ANN model. According to the well-known empiric rule the number of samplings for training is determined so as to be at least twice the number of weighting coefficients.

Artificial neural network architecture

Based on the available data we have investigated two architectural types for the model with one (H1) and two (H2) hidden layers, which differ in the number of neurons in each layer. An original software code has also been designed.

For the selection of ANN architecture the number of neurons is determined according to the following empiric rule:

$$NN \approx 2 \cdot \sqrt{In \cdot Out} , \quad (4)$$

where In is the number of inputs;
 Out – number of outputs.

In this order the acceptable number of neurons for the ATAD bioreactor is 6-9 and the investigated architectures ((I,H1,O) and (I,H1,H2,O)) for its modeling are (5,6,3); (5,7,3); (5,5,3,3) and (5,6,3,3), respectively.

Training of ANN models using BASIC genetic algorithm

For training of the proposed four ANN architectures, BASIC genetic algorithm (GA) has been implemented [22]. The purpose is to determine the main model parameters (weighting coefficients) at which the LSF has a minimal value. Obtained minimal values of the LSF are the following: 128.25-(5,6,3); 125.12-(5,7,3); 130.14-(5,5,3,3) and 132.08-(5,6,3,3) respectively.

The used BASIC GA follows all common steps of genetic algorithms. The continuous search space [0, 1] and real representation schemes are exploited for both real and integer variables. At the first generation, BASIC GA initializes a population of randomly created individuals. It works with a predefined constant size of the population. Applying morphogenesis functions their phenotypes are determined. Afterwards they are used to calculate the values of the objective function and to determine respective fitness functions. At the next steps the evolutionary operators take place to create the offspring. Firstly, a biased selection for reproduction is carried out. The algorithm operates with the fitness function values to provide the most prospective samplings for crossover. They gather in a sampling pool. Then, the samplings go to recombination. Randomly chosen individuals form couples, whose number is equal to the number of samplings. If, for a given couple, a predefined crossover probability has happened, their chromosomes recombine providing two children, otherwise parents pass directly in the offspring. Finally, the mutation takes place. Each gene of each offspring's chromosome goes to mutation if a predefined mutation probability has happened. In the last stage, selection for replacement is carried out to produce a new population for the next generation. The offspring decodes to obtain the respective solutions. Both the parents' and children's chromosomes collect in a replacement pool. The elite individual corresponding to the best solution in the pool passes to the new population. Further selection goes unbiased randomly drawing chromosomes from the pool until the next population is completed. At the end of this phase, the number of generation increases.

BASIC GA uses the generation number as a stop criterion. It checks for the stop criterion fulfillment. If it is met, the obtained best solution is proposed as a problem solution. In the opposite case, the loop is closed through the fitness functions calculation for the new population. BASIC GA involves a different number of schemes in the genetic operators, which makes it adaptive to various optimization problems.

Validation of ANN

Finally, models' validation takes place using samplings selected for this purpose.

For efficiency estimation of developed ANNs and their ability for precise predictions, three measures – *root mean square error (RMSE)*, *mean absolute percentage error (MAPE)*, and *linear correlation coefficient (R)*, have been used.

Root mean square error represents the square root of the average of the summing square predicting errors and is defined as follows:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (P_i - Q_i)^2}, \quad (5)$$

where P_i and Q_i are calculated and measured values for Tmax, Tmin and VS, respectively, and n is the number of data samplings.

The second measure is the mean absolute percentage error. It represents the percentage of the mean ratio of the error related to the measured data. *MAPE* is defined as:

$$MAPE = \frac{1}{n} \sum_{i=1}^n \left| \frac{P_i - Q_i}{Q_i} \right| \cdot 100. \quad (6)$$

The lower the values for *RMSE* and the *MAPE* are, the more accurate the prediction is.

The linear correlation coefficient R represents a measure of the strength of the straight-line or linear relationship between measured data and data calculated by the model. The best fit between measured and calculated values would have $R = \pm 1$. The linear correlation coefficient R is given by:

$$R = \frac{n \cdot \left(\sum_{i=1}^n P_i \cdot Q_i \right) - \left(\sum_{i=1}^n P_i \right) \cdot \left(\sum_{i=1}^n Q_i \right)}{\sqrt{\left[\left(n \cdot \sum_{i=1}^n Q_i^2 - \left(\sum_{i=1}^n Q_i \right)^2 \right) \cdot \left(n \cdot \sum_{i=1}^n P_i^2 - \left(\sum_{i=1}^n P_i \right)^2 \right) \right]}}. \quad (7)$$

The trained ANN with selected architectures has been validated using the above measures. The values of *RMSE*, *MAPE* and R for chosen models are listed in Table 2.

Table 2. Values of RMSE, MAPE and R for ANN model

ANN	RMSE			MAPE			R		
	Tmax	Tmin	VS	Tmax	Tmin	VS	Tmax	Tmin	VS
(5,6,3)	2.072	1.242	0.144	2.757	2.046	4.019	0.972	0.987	0.953
(5,7,3)	2.069	1.198	0.137	2.721	1.929	4.051	0.971	0.988	0.965
(5,5,3,3)	1.728	1.334	0.355	2.202	2.268	12.77	0.976	0.972	0.753
(5,6,3,3)	5.865	5.837	0.437	8.947	9.17	13.66	0.452	0.449	0.339

Note: The architecture (5,6,3,3) is excluded from further consideration

Data listed in Table 2 present very good consistency between the values of the measures for architectures (5,6,3) and (5,7,3). According to that, *RMSE* and *MAPE* have almost equal values. The values of the correlation coefficients tend to 1 that denote the presence of a very high correlation between measured and calculated data for the Tmax, Tmin and VS. However, the measures for the architectures with two hidden layers have very different values. While the values of *RMSE*, *MAPE* and R for the architecture (5,5,3,3) are closer to the same measures for the models with one hidden layer, the architecture (5,6,3,3) has

3-4 times larger values for the *RMSE* and *MAPE*, and *R* presents a weak to modest correlation for *T*_{max}, *T*_{min} and *VS*.

Hence, we have done a comparison between these correlation coefficients and the critical value for *R* of 0.3809 within the confidence level of 95%. One can see that *R* for *VS* is less than it, which means this correlation coefficient is not significant. That is the reason the ANN model with the architecture (5,6,3,3) is rejected from further consideration. Despite the fact that *R* for *T*_{max} and *T*_{min} exceeds the critical value.

On Fig. 2 a comparison is shown between measured values for *T*_{max}, *T*_{min}, *VS* and their calculated values obtained at the architectures (5,7,3) and (5,5,3,3) for the ATAD bioreactor where a very good level of prediction can be seen.

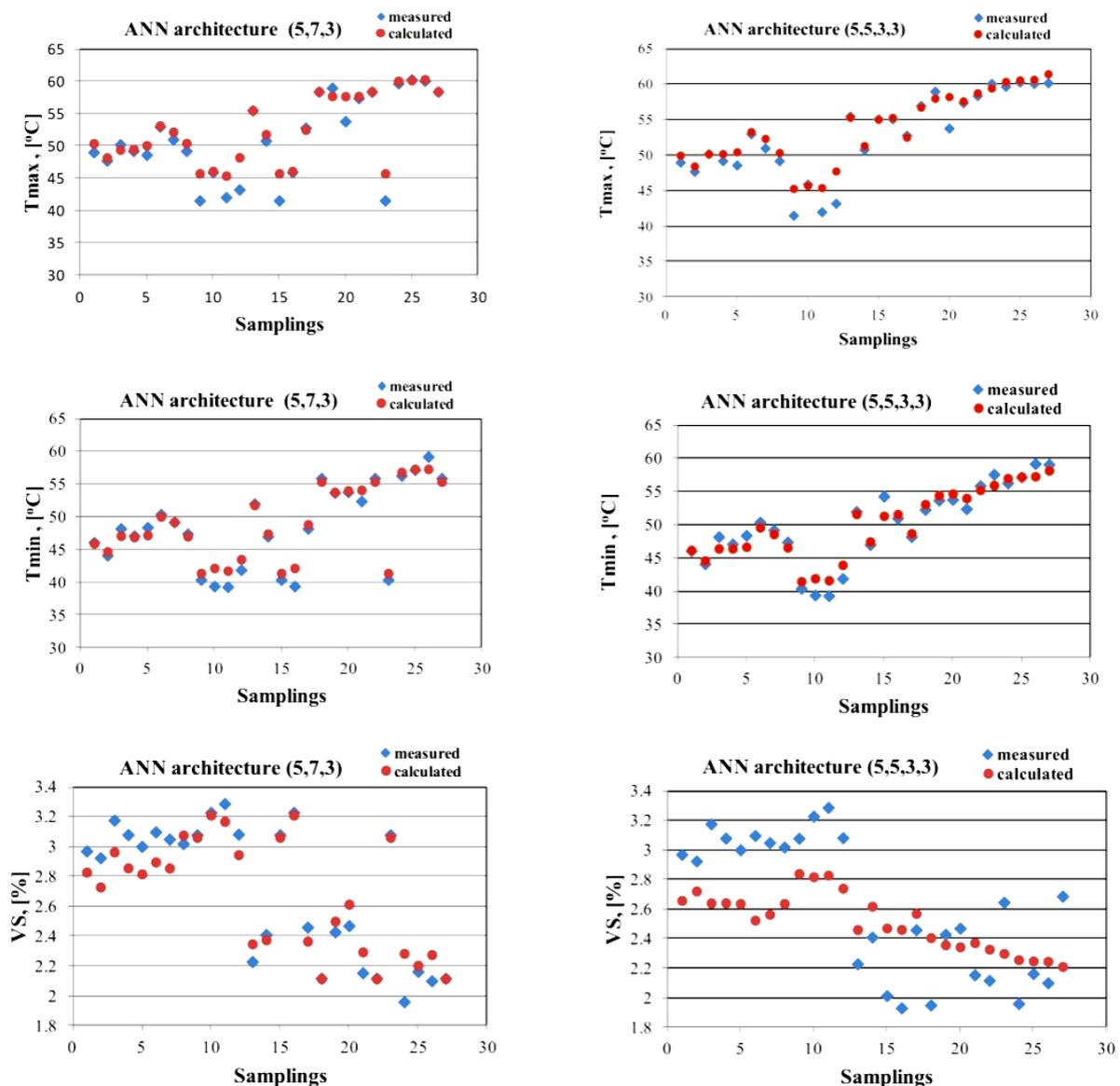


Fig. 2 Comparison between measured and calculated values for *T*_{max}, *T*_{min} and *VS* for the ANN architectures (5,7,3) and (5,5,3,3)

Therefore, we have selected three models providing very good coincidences between the measured and calculated values as the most prospective for modeling the ATAD bioreactors. They have architectures (5,6,3), (5,7,3) and (5,5,3,3), respectively.

Conclusions

This study provides an opportunity for predicting the maximal operational temperatures reached at the end of batches, the respective reduction of volatile solids and the expected thermal shock in real scale industrial ATAD bioreactors by using Artificial Neural Networks. Our proposed ANN modes are sufficiently suitable and simple to be incorporated within the energy integration framework in order to improve the energy efficiency of ATAD systems. We have investigated different ANN architectures involving one or two hidden layers with different number of artificial neural neurons in each one. For training and validation of such developed ANN models, data sets of the operational conditions of real ATAD facility have been used. For training of the developed ANNs a robust optimization tool – BASIC genetic algorithm has been implemented. The performance of created ANN models has been evaluated by using specific measures such as root mean square error, mean absolute percentage error and linear correlation coefficient. Based on a comparison between the values of the different measures, the best ANN architectures for predicting the required parameters of the ATAD bioreactors have been selected.

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