 doi:10.20944/preprints202211.0006.v1

Article

Using AI and BES/MFC to Decrease BOD_5 Measurements Prediction Time

Ivan Medvedev[1], Ksenia Polusmackova[1], Christoforos Galazis[2], Bálint Lóránt[3], Gábor Márk Tardy[3], Alexander Losev[1], Igor Goryanin[4,5,*]

1. Volgograd State University, Russia
2. Imperial College London, UK
3. Budapest University of Technology and Economics, Hungary
4. University of Edinburgh, UK
5. Okinawa Institute Science and Technology, Japan

* Correspondence: **goryanin@oist.jp**

Abstracts: Biochemical oxygen demand (BOD) is one of the most important factors to consider when evaluating water contamination. BOD_5 is the amount of oxygen consumed in five days by microorganisms that oxidize biodegradable organic materials in an aerobic biochemical manner. The primary objective of this effort is to use microbial fuel cells (MFCs) to shorten the time required for BOD_5 measurements. We created a regression artificial neural network (AI), and the predictions we obtained for BOD5 measurements were taken over 6 – 24 hours with an average error of just 7%. The outcomes demonstrated by our AI MFC/BES BOD_5 sensor's viability for use in real-world scenarios.

Keywords: Neural network; Biochemical Oxygen demand; Biosensor; Microbial Fuel Cell

1. Introduction

An MFC is a device that converts the energy of chemical bonds of organic substances into an electric current with the direct participation of bacteria. Microbial fuel cells (MFCs) have grown in popularity as a way to evaluate the quality of wastewater in recent years. A dual-chamber MFC is made up of an ion-selective membrane that can only allow protons to flow through, as well as anode and cathode chambers, while a single-chamber MFC consists of an anode chamber and an air-cathode. Electroactive bacteria form a biofilm over the anode electrode, generating electrons during the oxidation of organic materials which they move to the electrode surface. As a result, biodegradable organics in the water's composition can be inferred from the electric output. Yang et al. (2015) and Lóránt et al. (2019) claim that this technology can detect and even quantify dangerous toxic or organic substances. Thanks to electrogenic bacteria that can transform the chemical energy stored in organic material into electrical energy, MFCs may be used as an alternative technology to determine the extent of water contamination as well as a substitute energy source. The MFC is an energy-efficient device that can clean water, provide power sufficient to run low-energy devices, monitor water quality, and find dangerous compounds all at on(Rabaey and Verstraete, 2005). ce (Rabaey and Verstraete, 2005)..

A study (Tardy et al. 2021) proposed a method for using MFCs as biosensors to measure five-day biochemical oxygen demand (BOD_5). BOD_5 is one of the most important parameters to assess water pollution levels by biodegradable organic substances. Environmental agencies use it to monitor wastewater treatment plants and natural water resources. Ongoing experiments with microbial fuel cells (MFCs) as biosensors have reduced the time required to obtain the initial data needed to predict BOD_5 in wastewater (Tardy et al. 2021). The method is based on the correlation between the total amount of

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 1 November 2022 doi:10.20944/preprints202211.0006.v1

generated electricity and the BOD_5 of the sample. Compared to the conventional respirometric method with a fix 5 days long measurement, the prediction time was reduced to 1-4 days dependent on the composition of the investigated sample (Tardy et al. 2021).

An artificial neural network (ANN) is one of the well-known predictive methods used to find a solution when other statistical methods are not applicable. The advantages of using ANNs are the ability to learn from training data and to predict non-linear data, making ANNs a widely used statistical tool. In this work, we will use fully connected multilayer neural networks – multilayer perceptron (MLP). MLPs are classical feed-forward neural networks that are used in both regression and classification problems (Pal and Mitra 1992). MLPs are widely used in various fields such as remote sensing (Zhang et al. 2018) and engineering (Yilmaz and Kaynar 2011) or plant sciences (Yoosefzadeh-Najafabadi et. al. 2021) and environmental sciences (Wang and Gao 2018).

Two approaches were considered, in the first the ANN directly predicted one BOD_5 value from the raw electrical parameters. In the second, the ANN was using electrical data obtained during a measurement time, and the total charge was calculated. Further, based on the linear dependence of BOD_5 and the charge, the predicted values of BOD_5 were obtained and compared with real ones.

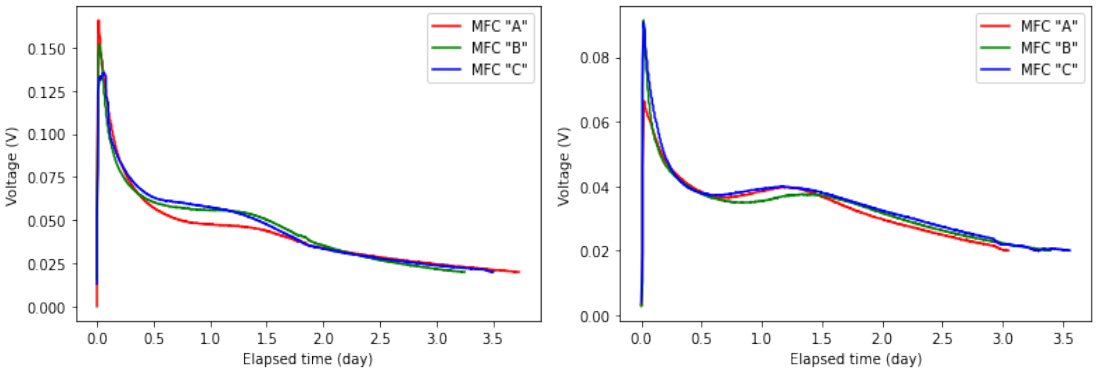
2. Material and methods

2.1. Data set

The dataset was obtained using MFCs described by Tardy et al (2021). The main purpose of a microbial fuel cell biosensor is to convert the chemical energy of biodegradable organic substances to electrical energy by the metabolic processes of exoelectrogenic bacteria that are capable of transporting the generated electrons outside the cell. The amount of generated electricity (voltage, current) is recorded. The study is based on the conclusion about the linear dependence of the biochemical oxygen demand (BOD_5) and the charge accumulated during the biodegradation in the MFC (Tardy et al. 2021).

Two types of wastewaters were used as samples for MFC: domestic and brewery wastewater. Three identical air cathode MFCs were operated in parallel, with 230 ml internal volume each. The volume of the injected substrate was 60 ml. Some cases the wastewater samples were diluted to cover a wider range of BOD_5. The external resistance was set equal to 100 ohms (Tardy et al. 2021).

During the measurements, the voltage was recorded by the data acquisition device (Graphtec midi logger GL840) every 5 minutes. It should be noted that in the initial period of each experiment, the voltage increased rapidly and reached its maximum value as a result of the rapid biodegradation of a readily biodegradable organic fraction of the wastewater. Having the readily biodegradable substrates consumed, the voltage value began to drop. When the voltage dropped below 0.02 V, the substrates were considered to be depleted and the measurements were terminated. Fig. 1 shows several examples of voltage measurement plots when domestic wastewater was used. Examples of voltage graphs for water samples from breweries are shown in Fig.2.



Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 1 November 2022 doi:10.20944/preprints202211.0006.v1

Fig. 1. Several typical examples of voltage variation over time, when domestic wastewater was used as a sample for MFC.

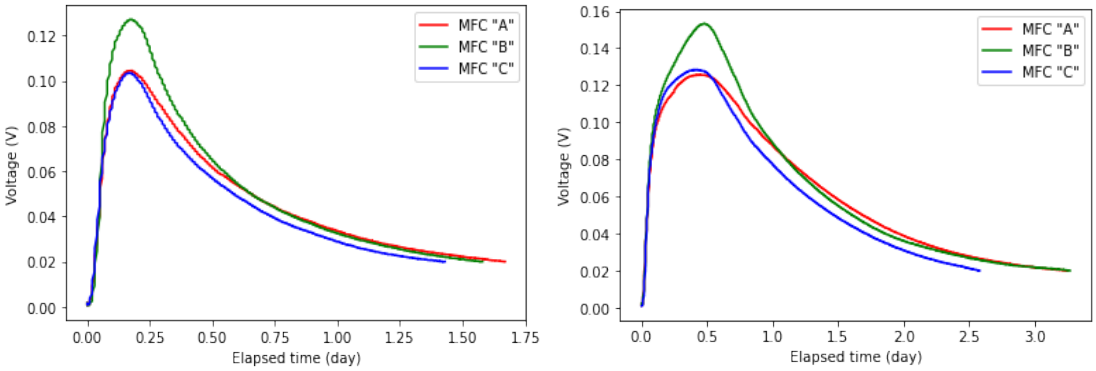


Fig. 2. Several typical examples of voltage variation over time, when brewery wastewater was used as samples for MFC.

In this work, a set of 56 voltage measurements was used. The longest experiment was 7550 minutes, so to equalize the dimension of all experiments, the missing values of other experiments were filled with zeros up to 7550 minutes. Since the voltage values in each experiment were recorded every 5 minutes, then 1511 discrete voltage values corresponded to 7550 minutes. Thus, the voltage dataset was presented as a matrix of 56 columns and 1511 rows. It is worth noting that 289 discrete voltage values corresponded to 24 hours of measurement, we also note that 16, 12, 8, 6 and 2 hours of measurement corresponded to 193, 145, 97, 73, and 25 discrete voltage values. In addition, the BOD_5 concentrations in mg corresponding to each experiment were reported in the data set. The BOD_5 data is represented as a vector of 56 values (y_1, y_2, …, y_{56}), where each y_j value corresponds to the BOD_5 value in the j-th experiment. The minimum BOD_5 content of the 60 ml samples was 4.13 mg and the maximum concentration was 46.84 mg, corresponding to a wide BOD_5 concentration range from ~69 to 781 mg/L.

2.2. Neural networks

The purpose of this study was to develop artificial neural network models for predicting BOD_5. We used fully connected multilayer neural networks (multilayer perceptron (MLP)) – a classical feedforward neural network, which consists of an input layer, an output layer, and intermediate layers (hidden layers), each of which consists of several neurons. The value in each of the neurons is the value of the weighted sum of all neuron values from the previous layer, converted through the activation function, plus the bias coefficient. MLP is effective in regression problems, for example, (Wang and Gao, 2018) MLP gave good results in predicting the water content of biodiesel and diesel blends in terms of temperature and composition, and for predicting gas density (Sedaghat and Kiomarsiyan 2019).

As described in the introduction, two approaches were considered. The BOD_5 direct prediction approach was that the ANNs predict one value – BOD_5 in each experiment. The approach of indirect prediction of BOD_5 consisted of the ANNs output voltage values, from which BOD_5 values were subsequently obtained. When implementing both approaches, the voltage values obtained for 24, 16, 12, 8, 6, and 2 hours of measurements were used as input data for the ANN, i.e. it was required to develop twelve ANN models in total, six ANNs for each approach.

The input data set was represented by 56 vectors (x_{1j}, x_{2j}, …, $x_{n_1 j}$), where x_{ij} is the voltage value at the i-th moment in time and j-th experiment; n_1 = 289, 193, 145, 97, 73, 25, which corresponds to the length of the voltage vectors for the first 24, 16, 12, 8, 6, and 2 hours of measurements, respectively; j = 1, …, 56. That is, the number of neurons in the

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 1 November 2022 doi:10.20944/preprints202211.0006.v1

input layers in the implementation of both approaches was 289, 193, 145, 97, 73, and 25. In each experiment, the final voltage value was reached at different times, for example, one experiment ran for two days and another for five days, but the output of the neural network requires these values to be of the same time. Therefore, the voltage measurement was complimented with zero values to generate five-day time sequences.

Three hidden layers were used for the neural networks, for each of which the Rectified Linear Unit (ReLU) activation function was used. In addition, after each hidden layer, a thinning (dropout) method was used to reduce overfitting. This method consists of eliminating a certain percentage of random neurons at different iterations during neural network training (Srivastava et. al. 2014). Then the output layer was followed, in which the dimensions differed depending on which of the two approaches was used. So, when implementing the BOD_5 direct prediction, the number of neurons in the output layer was one for all six ANNs, since only the BOD_5 value was predicted. The set of output data for direct prediction can be represented as a vector of 56 values (y_1, y_2, …, y_{56}), where each value of y_j corresponds to the BOD_5 value in the j-th experiment.

When BOD_5 the indirect prediction was implemented, the output set was represented by 56 vectors (y_{1j}, y_{2j}, …, $y_{n_2 j}$), where y_{ij} is the voltage value at the i-th time point in the j-th experiment; n_2 = 1486, 1438, 1414, 1366, 1318, 1222, which corresponds to the length of the voltage vectors obtained after 2, 6, 8, 12, 16 and 24 hours of measurements, respectively; j = 1, …, 56. Therefore, the number of neurons in the output layer for the indirect prediction was 1486, 1438, 1414, 1366, 1318, and 1222 respectively, which matches the voltage vectors for each time measurement.

The parameters used for neural networks in the BOD_5 direct prediction approach is shown in Table 1, and the indirect prediction approach in Table 2.

Table 1. Neural network parameters for the direct prediction approach.

Input	Dense 1	Dropout1	Dense 2	Dropout2	Dense 3	Dropout3	Output
25	128	30%	128	30%	64	50%	1
73	128	10%	128	50%	64	50%	1
97	128	10%	64	30%	64	50%	1
145	96	10%	96	10%	64	40%	1
193	128	10%	128	30%	128	30%	1
289	128	10%	128	10%	64	30%	1

Table 2. Neural network parameters for the indirect prediction approach.

Input	Dense 1	Dropout1	Dense 2	Dropout2	Dense 3	Dropout3	Output
25	128	30%	128	30%	64	50%	1486
73	128	20%	64	50%	64	50%	1438
97	128	25%	128	50%	64	50%	1414
145	128	10%	64	30%	64	50%	1366
193	128	10%	64	10%	64	50%	1318
289	128	10%	128	20%	64	50%	1222

As described earlier, a dataset of 56 experiments was used in this work. Of these, 16 experiments (8 experiments with domestic wastewater and 8 experiments with wastewater from breweries) were used as the test set for the final evaluation of the models once model tuning and training were completed. With the remaining 40 experiments, the K-fold cross-validation (K=5) method was applied to assess the quality of the ANNs during parameter selection. The data set of 40 experiments were divided into 5 blocks, with each block clustered into 8 experiments. In the first stage, the first block (20% of the data) was used as a validation block, and the remaining 4 blocks (80% of the data) were used as training. In the next stage, the second block (20% of the data) was used as validation and the remaining blocks (80% of the data) as training data. And so on, until each block of 20% has been used in the validation.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 1 November 2022 doi:10.20944/preprints202211.0006.v1

According to the obtained five estimates, the average value of the loss function was calculated. The root means square error (MSE) was defined as the loss function to be minimized during training. Moreover, when implementing the BOD_5 direct prediction approach, the MSE of the predicted BOD_5 values relative to the actual BOD_5 values were minimized. The formula for the direct MSE is (1):

$$MSE_1 = \frac{1}{n}\sum_{i=1}^{n}(y_i - \overline{y_i})^2, \quad (1)$$

where n is the number of ANN output values (in all cases equal to 1) multiplied by the number of experiments in the validation set (there were 8 experiments in each of the 5 validation blocks); y_i – real values of BOD_5; $\overline{y_i}$– predicted values (the value of the weighted sum of all neuron values from the previous layer plus the bias factor converted through the activation function) BOD_5.

And when implementing the BOD_5 indirect prediction approach, the MSE of the predicted voltage values relative to the real ones was minimized. The formula for the indirect MSE is (2):

$$MSE_2 = \frac{1}{n \cdot n_2}\sum_{j=1}^{n}\sum_{i=1}^{n_2}\left(y_{ij} - \overline{y_{ij}}\right)^2, \quad (2)$$

where n is the number of experiments in the validation set (there were 8 experiments in each of the 5 validation blocks);); n_2 = 1486, 1438, 1414, 1366, 1318, 1222, which corresponds to the length of the voltage vectors obtained after 2, 6, 8, 12, 16, and 24 hours of measurements, respectively; y_{ij} – real voltage values at the i-th moment of time in the j-th experiment; $\overline{y_{ij}}$ – predicted stress values at the i-th time point in the j-th experiment.

To minimize the loss function during training, the Adam optimizer (adaptive moment) was used in this work. For the BOD5 direct prediction approach, the learning rate was 0.001, the rest of the parameters of the Adam method were left at the default settings for the Keras library.

For the BOD5 indirect prediction approach, the learning rate was 0.0001, the rest of the parameters of the Adam method were left at the default settings for the Keras library. Adam is an efficient stochastic optimization method that combines the benefits of methods such as AdaGrad and RMSProp (Kingma and Ba 2015).

After the final selection of all parameters, such as the number of neurons in the layers and thinning percentages, the number of epochs for each of the 12 ANNs were selected, at which the average MSE over 5 validation blocks was minimal. These epochs for 12 ANNs were used to train the final ANNs on a sample of 40 experiments and tested on a leave-out sample of 16 experiments.

3. Results and discussion

3.1. Results of direct prediction of BOD_5 using ANN

Six ANN models were developed for the BOD_5 direct prediction approach. After training 40 sets in K-fold cross-validation, a set of weights were stored that resulted in a minimum loss value. These weights were applied for inference.

To compare actual and predicted BOD_5 values, the mean absolute percentage error (MAPE) was used (3):

$$MAPE = \frac{1}{m}\sum_{i=1}^{m}\frac{|y_i - \overline{y_i}|}{|y_i|}100\% \quad (3)$$

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 1 November 2022 doi:10.20944/preprints202211.0006.v1

and the maximum absolute error (MAX) (4):

$$MAX = max|y_i - \overline{y_i}|, \qquad i = 1, \dots, m, \tag{4}$$

where m = 16 when assessing BOD_5 on the test set (because there were 16 experiments in the test set) and m = 8 when assessing BOD_5 on each of the validation blocks; y_i – real values of BOD_5; $\overline{y_i}$ – predicted BOD_5 values.

In addition to the errors described above, to estimate the predicted values of BOD_5 relative to the actual values of BOD_5, the coefficient of determination was used (R^2) (5):

$$R^2 = 1 - \frac{\sum_{i=1}^{m}(\overline{y_i} - y_i)^2}{\sum_{i=1}^{m}(y_i - \hat{y}_i)^2}, \tag{5}$$

where $\hat{y}_i$ are the average overall real values of y_i. The larger the value of R^2 (close to 1), the better the accuracy of the linear relationship between the actual and predicted results.

The errors of the predicted BOD_5 compared to the actual values of BOD_5 for K-fold cross-validation are shown in Table 3.

Table 3. Mean errors over 5 validation blocks.

Input	MAPE	MAX	R^2
2 hours	39.63 %	15.79 mg	0.208
6 hours	23.39 %	9.56 mg	0.65
8 hours	20.06 %	10.43 mg	0.73
12 hours	16.63 %	9.22 mg	0.745
16 hours	12.4 %	5.41 mg	0.845
24 hours	8.14 %	3.39 mg	0.938

Next, the models were trained on 40 sets and tested on a delayed sample of 16 experiments. The results are shown in Table 4.

Table 4. Model errors on delayed set.

Input	MAPE	MAX	R^2
2 hours	36.6 %	25.36 mg	0.385
6 hours	21.02 %	18.74 mg	0.659
8 hours	15.76 %	9.46 mg	0.857
12 hours	13.59 %	10.62 mg	0.875
16 hours	11.23 %	11.33 mg	0.877
24 hours	8.72 %	9.61 mg	0.923

It can be seen that the results on the test set do not differ much from the results obtained during cross-validation for 5 blocks. The models were able to predict the correct values, corresponding to the expected ones, when the voltage values for 24, 16, and 12 hours were applied to the input (determination coefficient on the delayed sample: 0.923, 0.877, 0.875).

A high level of BOD_5 (more than 220 mg/l) can cause the growth of excess biomass, therefore, for wastewater, the indicator BOD_5 (more than 220 mg/l) indicates water pollution. In total, there were 10 different types of wastewater with pollution and six types of wastewater without pollution in the test sample, therefore, indicators of specificity, sensitivity, and accuracy were also calculated to evaluate the neural network. Sensitivity was calculated as the ratio of the number of polluted waters correctly identified by the neural network to the true number of polluted waters in the test. Specificity was calculated as the number of unpolluted waters detected by the neural network to the true number of unpolluted waters in the test. Thus, the sensitivity was 1 when the input data was 24 hours of measurements, 0.9 for the cases of 16 and 12 hours, and 0.8 for the remaining cases (8, 6, and 2 hours). The specificity was 1 for 24, 12, and 8 hours of measurements, 0.83 for 16

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 1 November 2022 doi:10.20944/preprints202211.0006.v1

hours, and 0.67 for the 6 and 2-hour cases. In addition to specificity and sensitivity, accuracy was also calculated as the ratio of the number of correctly guessed water states (contamination or not) to the amount of data in the test set (16 experiments). The accuracy was 1 for the entry at 24 hours of measurement, 0.975 for 12 hours, 0.875 for the entry at 16 and 8 hours, and 0.75 for the entry at 6 and 2 hours.

3.2. Results of indirect BOD_5 prediction using ANN

The indirect prediction approach of BOD_5 using ANN was that, knowing the voltage and external resistance, which, as already described earlier, was set to 100 Ohm to accelerate the biodegradation process, the current strength can be obtained according to Ohm's law. By numerically integrating the current over time, the total charge can be calculated as shown in the formula below (6):

$$Q = \int_{t_s}^{t_e} I\, dt, \tag{6}$$

where Q is the total charge (C), I is the current in the external circuit (A), t_s (s) is the starting time of the experiment, t_e (s) is the end time of the measurement. Due to the linear relationship between BOD_5 and charge, the resulting total charge can be used to estimate BOD_5.

When implementing this approach, six ANN models were developed that predict voltage values after a certain measurement time. After selecting epochs that give the minimum mean square error over 5 validation blocks, ANNs were trained for 40 experiments with voltage measurement and tested on 16 experiments from the test set.

The ANN was able to predict the correct values corresponding to those expected when the input voltage values were applied for 24, 16, and 12 hours and in some cases even 8 and 6 hours. For example, some graphs of the predicted and experimental voltage values, when voltage values obtained for 12 hours were applied to the ANN input, are shown in Fig. 3.

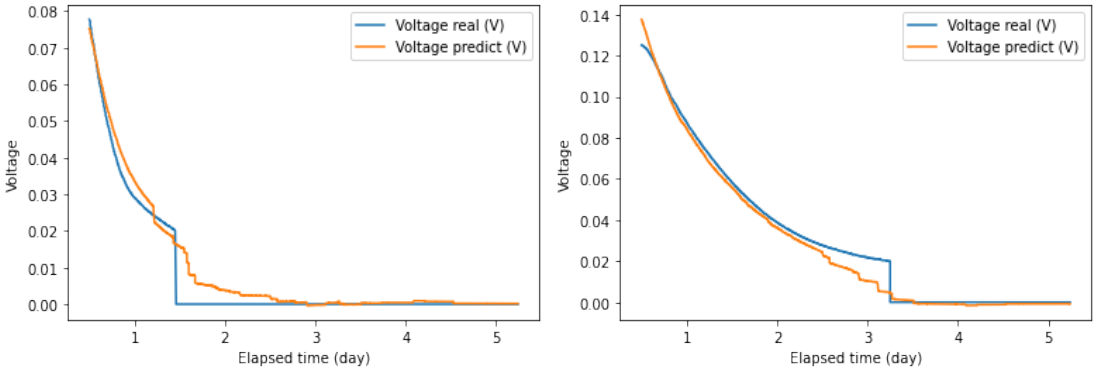


Fig. 3. A few examples of the ratio of real to predicted voltage when voltage values measured over 12 hours were used as input to the ANN. Blue graph – real voltage data, orange – obtained using a neural network.

As a rule, in experiments in which the voltage did not peak and did not begin to decrease after the input time allowed, the results were worse compared to those experiments in which the voltage peak was reached before the time of the input data measurement. Therefore, when using voltage values obtained for 6 and 2 hours as input data, the measurement results deteriorated significantly in comparison with other cases (see Fig. 4, which shows the ratio of the real and predicted voltage graphs, when voltage values were applied to the ANN input received within 2 hours). The voltage did not peak and did not begin to decrease by this time.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 1 November 2022 doi:10.20944/preprints202211.0006.v1

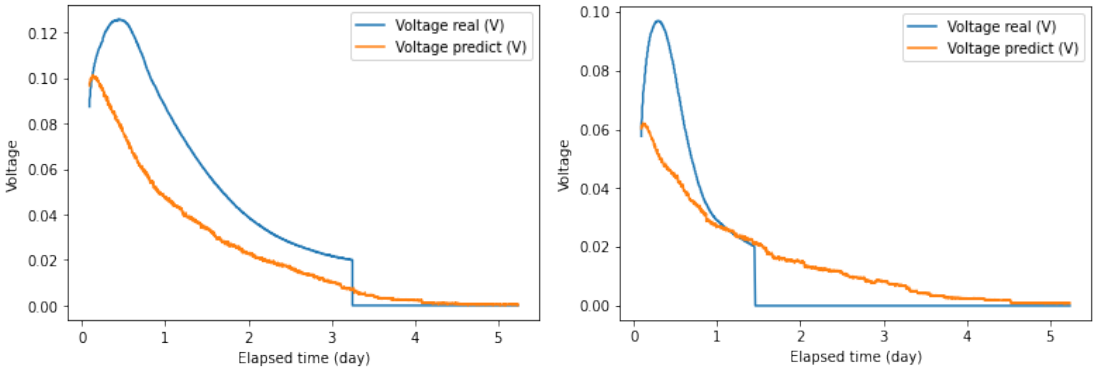


Fig. 4. A few examples of the ratio of real voltage to predicted voltage, when voltage values measured over 2 hours were used as input data for the ANN. Blue graph – real voltage data, orange – obtained using a neural network.

Knowing the voltage and external resistance, the current strength was calculated according to Ohm's law. Then the total charge was calculated by numerically integrating the current as a function of time. At the same time, taking into account that during the development of the ANN, empty voltage values were filled with zeros up to 5 days, when calculating the integral, regression voltage values were discarded, which were less than 0.01 V. To equalize the dimensionality of all experiments, we filled in the missing stress values with zeros until day 5, so the regression stress gradually tended to zero over time, but these near-zero values could introduce an additional error in obtaining BOD5. At the same time, if we cut off the regression voltage at 0.02 V, we could finish the experiment earlier than the real one would go, since the regression voltage did not always reach 0.02 V exactly at the time when 0.02 V was achieved at a real experiment. Therefore, it was decided to cut off the regression voltage when it had already passed the cutoff point but had not yet reached zero, namely, when it was less than 0.01 V. Several examples of the ratios of the charge obtained from real data and the charge obtained from predicted data are shown in Fig. 5 and Fig. 6.

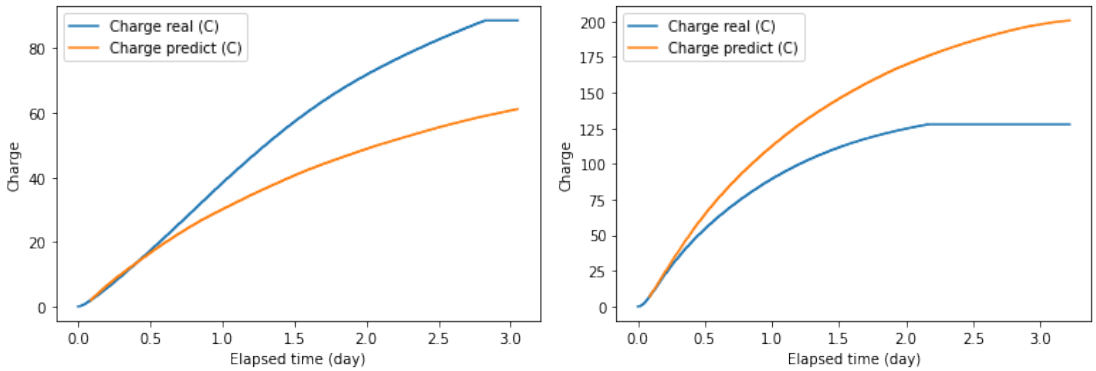


Fig. 5. The ratio of the real and predicted charge, when voltage values measured over 2 hours were applied to the ANN input. Blue graph – charge values obtained from real data, orange – charge values obtained from predicted data. .

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 1 November 2022 doi:10.20944/preprints202211.0006.v1

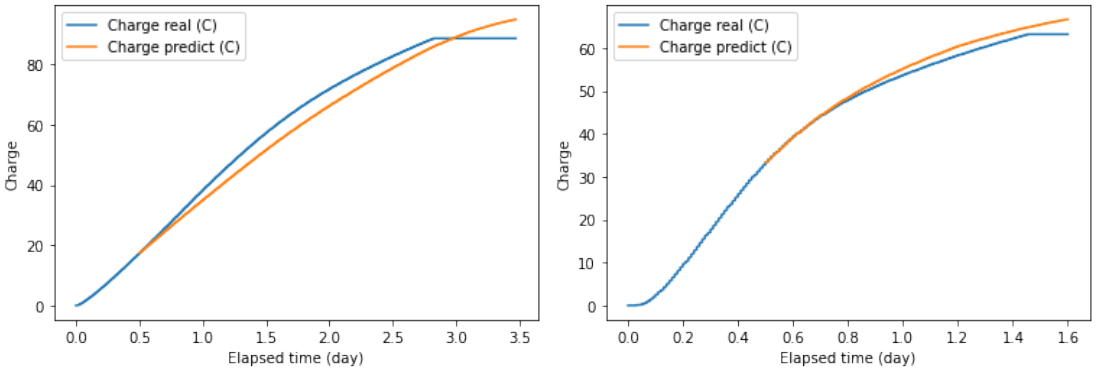


Fig. 6. The ratio of the real and predicted charge, when voltage values measured over 12 hours were applied to the ANN input. Blue graph – charge values obtained from real data, orange – charge values obtained from predicted data.

Due to the linear dependence of BOD_5 and charge, the resulting total charge was used to estimate BOD_5. Moreover, the values described in paragraph 3.1 (MAPE, MAX and R^2) were used for the assessment. The results of these values for comparison BOD_5 obtained by the formulas of linear dependence on the predicted charge with reference values BOD_5 are shown in Table 5.

Table 5. Errors of BOD_5 obtained from the predicted charge.

Input	MAPE	MAX	R^2
2 hours	48.35 %	20.06 mg	0.483
6 hours	15.62 %	10.32 mg	0.867
8 hours	11.95 %	8.72 mg	0.907
12 hours	10.66 %	5.53 mg	0.946
16 hours	8.42 %	4.69 mg	0.961
24 hours	7.5 %	4.49 mg	0.976

As in the case of direct prediction BOD_5, sensitivity, specificity and accuracy were calculated. The sensitivity was 1 when the input data were 24, 16, and 12 hours of measurements, 0.9 for 8 hours of measurements, and 0.8 for other cases (6, 2 hours). Specificity was 1 for 24, 16, 12, and 8 hours of measurements 0.5 for 2 hours. The accuracy was 1 for the inputs at 24, 16, and 12 hours of measurements, 0.9375 for 8 hours, 0.875 for the input at 6 hours, and 0.6875 for the input of 2 hours of measurements.

3.3. Discussion

Firstly, ANN models were used to predict directly the values of BOD_5, one value for each experiment. With this approach, acceptable results were obtained when compared to reference values of BOD_5 for 24, 16, and 12 hours of measurement. This approach is more reliable since only one value is predicted, but it is less informative since it does not reflect the process of voltage change.

Using the second approach, ANN models predicted the voltage values from which a charge can be calculated and, as a consequence, BOD_5. Moreover, as soon as the predicted voltage data reached small values (Tardy et al. 2021) a value of 0.02 V was determined as the end point of the measurement, and then the charge was considered until the day when the predicted voltage became less than 0.01 V. In comparison with the first approach, the results were better (see Table 4 and Table 5), but for entries at 6 and 2 hours, and in some experiments for entries at 8 and 12 hours, the results, as in the first approach, gave a high error because voltage did not reach the peak and did not begin to decrease by this time.

 doi:10.20944/preprints202211.0006.v1

4.Conclusions

ANN models were trained on voltage data obtained by MFC for 24, 16, 12, 8, 6, and 2 hours and used to predict BOD_5 values. Two approaches were considered in the prediction of BOD_5 – when the ANN directly predicts BOD5, and when the ANN predicts voltage, from which BOD_5 can be calculated. The results obtained during cross-validation and on the delayed test set did not differ much from each other. When using the voltage values obtained at 12 hours as input, the error on the delayed set was 13.59% in the first approach and 10.66% in the second. For cases when voltage values measured for more than 12 hours were input to the models, the relative error was even smaller, for an entry at 24 hours, the relative error was 8.72% and 7.5% for the first and second approaches, respectively. ANN models for these cases showed good results regardless of the water sample used (domestic or brewery wastewater). Namely, the problem of determining the minimum measurement time required for a sufficiently accurate determination of the BOD_5 was solved. Rapid acquisition of BOD_5 values can offer benefits for wastewater monitoring and treatment. This will enable us to react faster, take necessary actions promptly, and identify optimal treatments under changing needs. In turn, it will help to reduce costs and assist in being compliant with legal requirements to maintain BOD_5 under certain levels.

For future work, more complex neural network methods will be explored. The goal will be to identify if it is possible to further improve the performance and reduce the number of monitoring hours. One such network is the Transformer network used for time series forecasting (Li et al. 2019) which has shown strong results. It identifies local relationships from the given sequence, while also maintaining long-term memory dependencies. The Transformer network can be adapted for both direct and indirect BOD_5 predictions.

References

Kingma, D.P., Ba, L.J., 2015. Adam: a method for stochastic optimization. The 3rd International Conference on Learning Representations (ICLR2015), San Diego.

Lóránt, B., Gyalai-Korpos, M., Goryanin, I., Tardy, G.M., 2019. Single chamber air–cathode microbial fuel cells as biosensors for determination of biodegradable organics. Biotechnol Lett 41, 555–563. https://doi.org/10.1007/s10529-019-02668-4

Pal, S.K., Mitra, S., 1992. Multilayer Perceptron, Fuzzy Sets, and Classification. IEEE Trans. Neural Netw. 3, 683–697. https://doi.org/10.1109/72.159058

Rabaey, K., Verstraete, W., 2005. Microbial fuel cells: novel biotechnology for energy generation. Trends Biotechnol 23, 291–298. https://doi.org/10.1007/s10529-015-1929-7

Sedaghat, M., Kiomarsiyan, A., 2019. Applying MLP-ANN as a novel and accurate method to estimate gas density. Pet. Sci. Technol. 37, 2128–2133. https://doi.org/10.1080/10916466.2018.1482324

Srivastava, N., Hinton, G., Krizhevsky, A., Sutskever, I., Salakhutdinov, R., 2014. Dropout: A simple way to prevent neural networks from overfitting. J. Mach. Learn. Res.15(1), 1929–1958.

Tardy, G.M., Lóránt, B., Gyalai-Korpos, M., Goryanin, I., 2021. Microbial fuel cell biosensor for the determination of biochemical oxygen demand of wastewater samples containing readily and slowly biodegradable organics. Biotechnol Lett 43, 445–454. https://doi.org/10.1007/s10529-020-03050-5

Wang, Y., Gao, W., 2018. Prediction of the water content of biodiesel using ANN-MLP: An environmental application. Energy Sources, Part A: Recovery, Utilization, and Environmental Effects 40(8), 987–993. https://doi.org/10.1080/15567036.2018.1468510

Yang, H., Zhou, M., Liu, M., Yang, W., Gu, T., 2015. Microbial fuel cells for biosensor applications. Biotechnol Lett 37, 2357–2364. https://doi.org/10.1007/s10529-015-1929-7

Yilmaz, I., Kaynar, O., 2011. Multiple regression, ANN (RBF, MLP) and ANFIS models for prediction of swell potential of clayey soils. Expert systems with applications 38(5), 5958–66. https://doi.org/10.1016/j.eswa.2010.11.027

Yoosefzadeh-Najafabadi, M., Earl, H.J., Tulpan, D., Sulik, J., Eskandari, M., 2021. Application of machine learning algorithms in plant breeding: predicting yield from hyperspectral reflectance in soybean. Frontiers in plant science 11, 2169. https://doi.org/10.3389/fpls.2020.624273

Zhang, C., Pan, X., Li, H., Gardiner, A., Sargent, I., Hare, J., Atkinson, P. M., 2018. A hybrid MLP-CNN classifier for very fine resolution remotely sensed image classification. ISPRS Journal of Photogrammetry and Remote Sensing 140, 133-144. https://doi.org/10.1016/j.isprsjprs.2017.07.014

Li, S., Jin, X., Xuan, Y., Zhou, X., Chen, W., Wang, Y.X. and Yan, X., 2019. Enhancing the locality and breaking the memory bottleneck of transformer on time series forecasting. Advances in neural information processing systems, 32.