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Analysis and Prediction of Microbial Fuel Cell Behaviour Using MLP and SVRA

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ABSTRACT

Background

Microbial fuel cell (MFC) is a device for simultaneous wastewater treatment and clean energy production. In this study, different amounts of yeast extract (1, 2, 3, 4, or 5 g/L) were varied and the MFC performance was measured in terms of power generation, COD removal and coulombic efficiency.

Methods

The first part of this study examined a dual chamber MFC with varying volumes of yeast extract for power output, COD removal, and coulombic efficiency. Soft computing approaches were utilized in the second part of the study to estimate MFC performance, and multilayer perceptron (MLP) with varied numbers of hidden layers was used to improve model accuracy. The method was next implemented in MATLAB software using 70% and 30% of the dataset for training and testing purposes of the system, which was validated with the traditional support vector regression (SVR) estimation method.

Findings

The experimental results have shown that the MFC4 (4 g/L yeast extract) had the highest catalytic activity and produced the maximum power (308 mW/m²). Comparing the experimental results and soft computing model proved that MFC behaviour can be predicted 5.1819 times more accurately using MLP compared with traditional SVR.

Keywords: microbial fuel cell; power generation; chemical oxygen demand removal; multilayer perceptron; support vector regression.

ABBREVIATIONS

Full name	Abbreviation
Correlation Coefficient	CC
Coulombic Efficiency	CE
Chemical Oxygen Demand	COD
Cyclic Voltammetry	CV
Extreme Learning Machine	ELM
Feedforward Neural Network	FFNN
Genetic Algorithm	GA
Microbial Fuel Cell	MFC
Multilayer Perceptron	MLP
Mean Square Error	MSE
Oxygen Reduction Reaction	ORR
Proton Exchanged Membrane	PEM
Root Mean Square Error	RMSE
Scanning Electron Microscopy	SEM
Solid Oxide Electrolyser Cell	SOEC
Support Vector Machine	SVM
Support Vector Regression	SVR

1. INTRODUCTION

Through continued global industrialization, carbon dioxide emissions are expected to increase by more than 60% by 2030. Additionally, about half of the wastewater is discharged without treatment [1]. A microbial fuel cell (MFC) is a device that transfers energy produced by microorganisms into electrical energy. This approach simultaneously results in energy production and wastewater treatment [2-4]. In addition to the aforementioned benefits, an MFC can also be used in bioremediation. One of the valuable advantages of an MFC is that it can operate in high chemical oxygen demand (COD) and salinity, as well as variable pH [5, 6]. Other wastewater treatment options have several requirements including membranes, ion exchange, upflow anaerobic organisms, and are not self-reliant. MFCs are emerging as a viable choice for sustainable energy production and wastewater treatment, especially as resources deplete, water gets scarcer, and the planet warms [7, 8]. Generally, a MFC comprises a cathode and anode separated by a proton exchange membrane (PEM) [9, 10]. Unfortunately, while MFC performance has improved in recent years, power generation and organic degradation remain relatively low [11]. While several studies have examined how the PEM and cathode catalysts influence the performance of an MFC, few focus on media composition. Santoro et al. [12] conducted a study on how the surface of an electrode affects the attachment of bacteria. They found that while the attachment of microorganisms makes the electrode surface less hydrophobic, their water content becomes similar after a short time, producing the same voltage. In other words, the surface of the electrode basically affects bacterial attachment but has no long-term effect on electrical output.

Soft computing methods have recently been developed in different fields, including materials microstructure, manufacturing, and energy production [13-15]. As such, these methods have gained tremendous interest within various industries. Machine learning-based models are designed and developed using the experimental datasets of the process and are often more accurate than the classical models [16]. Ogaji et al. [17] conducted one of the pioneering studies using machine learning in roll forming technology to analyze the effectiveness of the fuel cell using multilayer perceptron (MLP) using various

hyperparameters, such as hidden layers, neurons, activation function, and training methods. Unfortunately, when compared to standard methodologies such as linear regression, their proposed soft computing strategy produced similar accuracy. Nazari [18] estimated how the PEM of the fuel cell influences the output voltage using gene expression programming. Garg et al. [19] used multi-gene genetic programming, feedforward neural network (FFNN), and support vector regression (SVR) to model the performance of an MFC. They intended to predict the output voltage of an MFC before and after start-up using temperature and ferrous sulfate concentrations, but their model was time-consuming and inappropriate for real-time applications. Tardast et al. [20] used MLP to estimate bioelectricity production with glucose as electron donors, demonstrating higher prediction power with a correlation coefficient (CC) of 0.99. Unfortunately, a substantial amount of data is required for training proposed algorithms before they can be used in real-world applications. An extreme learning machine (ELM) [21] was used for the calculation of the Solid Oxide Electrolyser Cell (SOEC) performance using volume percentage and operating voltage of H₂, CO₂, and H₂O. Despite having a lower computing load, their proposed method did not properly analyze all of the parameters in the SOEC's performance, such as pressure, flow rate, temperature, and materials. Tsompanas et al. [22] used FFNN with a topology of 4-10-1 to estimate the MFC voltage under different conditions. However, the training process of their proposed method was time-consuming and could only be implemented in narrow applications. Chen et al. [23] suggested a hybrid soft computing model incorporating wavelet analysis, ELM, and a genetic algorithm (GA) to assess the impact of relative humidity, load current, hydrogen pressure, and temperature on proton exchange for an MFC for electric vehicles. While the experimental results demonstrate the efficiency of their proposed method compared to traditional methods such as Elman and relevance vector machine, real-world application is lacking. Vichard et al. [24] used an echo state network to extract the proton exchange of the MFC's degradation prediction and aging laws. Zhang et al. [25] proposed a data-driven soft computing model using SVR to optimize porous media flow field geometry in PEM fuel cells. Recently, Dwivedi et al. [26] reviewed the recent research in the area of MFCs and the implementation of soft computing methods to increase the performance of these practical environment-friendly applications. Nguyen

et al. [27] proposed the deep learning method combining MLP and GA to develop a three-dimensional Multiphysics model for a microfluidic MFC.

In this study, various media were tested within MFCs in the first stage of this research to quantify power density, current density, electrocatalytic activity, and system performance. Five distinct MFCs were established with variable quantities of yeast extract (MFC1, MFC2, MFC3, MFC4, and MFC5), and several MFC performance characteristics were measured. Next, the computational efficiency and accuracy were targeted simultaneously using the data generated to develop a highly accurate soft computing method for estimating electric current (I) produced in an MFC based on yeast extract concentration. Then, MLP was used to extract a highly efficient prediction model for MFC performance with a lower computational load for real-time applicability. The model was investigated using different hyperparameters (hidden layers and the number of neurons) to reach the best possible solution. Finally, a traditional soft computing method, SVR, was employed to prove the efficiency of the proposed method in points of lower error and higher CC. Here, MFCs with different amounts of yeast extract, one of the most important media components, were assembled and MFC performance (activity of biocatalyst, catalytic activation) was measured. This work expands our understanding of the parameters that influence MFC performance and opens up new avenues for MF commercialization and application.

2. MATERIALS AND METHODS

2.1.MFC Configuration

The MFC was built of two chambers, which are separated by Nafion 117 as a PEM. The PEM allows only protons to pass through, and the electrons pass through the external circuit to reach the anode [28]. Then, electricity will be produced in the cathode chamber through the oxygen reduction reaction process. The schematic of the MFC is shown in Fig. 1. In the anode chamber by utilizing organic substrates, carbon dioxide will be produced and at the cathode, by ORR, water was produced.

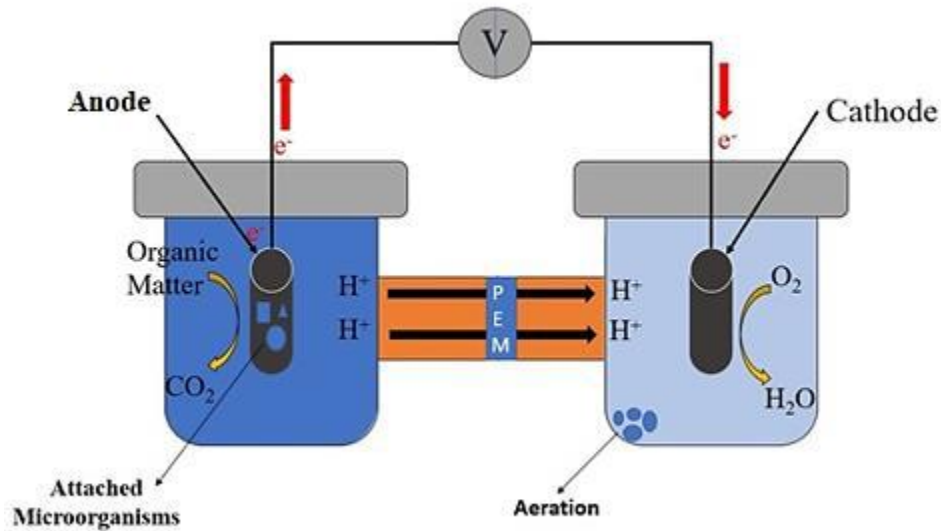


Figure 1. The schematic of an MFC.

2.2. Media

For the media, 5 g/L of glucose was used as the carbon source, and variable amounts of yeast extract were used as the nitrogen source (1, 2, 3, 4, and 5 g/L), with additional components as previously described [29] so the media had the COD of 50'000 ppm and the pH of the cathode and anode is neutral (6.5-7). The anode and cathode had an equal volume of 300 ml. Carbon paper was used as the electrode in both the anode and cathode. The cathode electrode was covered by 0.5 mg/cm² Platinum. The electrode's area was 12 cm² and the MFCs were operated at room temperature. Palm oil mill effluent (POME, Selangor, Malaysia) was used to inoculate the MFC.

2.3. Analysis and Calculation

A voltammeter measures the produced voltage in each second, and the current and voltage can be calculated as below:

$$I = \frac{V}{R} \quad (1)$$

$$P = V \times R \quad (2)$$

where I shows the voltage, and R is the resistance connected to the system. The COD reagents (high range) were used to measure the COD. A sample was taken from the anode chamber to find the COD and then diluted 10-fold in water. Then, 2 mL of the sample was added to the high-range COD vials and heated to 150 oC. Finally, a spectrophotometer was used to measure COD [30]. For finding the COD removal in a cycle, one sample at the first and another sample at the end of cycle (it almost takes 72 hours) were take and the difference of them reported the COD removal (ΔCOD).

This formula can calculate the system's columbic efficiency (CE) as follows:

$$CE = \frac{M \int_0^t I dt}{F b V_{an} \Delta COD} \quad (3)$$

where M is the molecular weight of oxygen, and F is the Faraday number. The number of transferred electrons per mole of oxygen is $b = 4$. The change of COD is shown by ΔCOD and V_{an} is the volume of the anode [31].

2.4.Support Vector Regression

Cortes and Vapnik [32] introduced a support vector machine (SVM), which can be categorized as a supervised learning technique. SVM can handle classification and regression data known as SVR. The objective of SVM is to find the best decision hyperplane to maximize distances between two sample classes on both sides of the hyperplane while retaining good generalization ability. SVM is suitable for small-sized and nonlinear data and can be used in various fields, such as approximation. The data set can be represente using linear regression as follows:

$$D = \{(x^1, y^1), (x^2, y^2), \dots, (x^n, y^n)\}, x \in \mathbb{R}^m, y \in \mathbb{R} \quad (4)$$

where x and y are the attribute and labels of the linear function, while:

$$f(x) = \langle w|x \rangle + b \quad (5)$$

The regression function can be found as follows:

$$\min \phi(w, \xi) = \min \left(\frac{1}{2} \|w\|^2 + C \sum \xi_i^- + \xi_i^+ \right) \quad (6)$$

where w and C are the support vector and cost for adjusting the training model. Also, ξ_i^- and ξ_i^+ are the slack variables for eliminating errors. In SVM, the Loos function is used to reduce the error between the label and prediction data and achieve satisfactory results. The ε -insensitive loss function was used in this paper, as shown below:

$$L_\varepsilon = \begin{cases} 0 & \text{for } |f(x) - y| < \varepsilon \\ |f(x) - y| - \varepsilon, & \text{otherwise} \end{cases} \quad (7)$$

Then, Eq. (6) should be solved with the subjection of:

$$y_i - w \cdot x_i - b < \varepsilon + \xi_i^- w \cdot x_i + b - y_i \quad (8)$$

$$\varepsilon + \xi_i^- w \cdot x_i + b - y_i < \varepsilon + \xi_i^+ \xi_i^- \quad (9)$$

with consideration $\xi_i^+ \geq 0$.

The solution of Eq. (6) can be shown in the following form:

$$\max \left(-\frac{1}{2} \sum_{i=1}^l \sum_{j=1}^l (\alpha_i - \alpha_i^*) (\alpha_j - \alpha_j^*) \langle x_i, x_j \rangle \right) + \sum_{i=1}^l \alpha_i (y_i - \varepsilon) \alpha_i^* (y_i + \varepsilon) \quad (10)$$

where α_i^* and α_i are the Lagrange multipliers with the following constraints:

$$\sum_{i=1}^l (\alpha_i - \alpha_i^*) = 0 \quad (11)$$

$$0 \leq \alpha_i^*, \alpha_i \leq C, i = 1, \dots, l \quad (12)$$

Karush-Kuhn-Tucker conditions should be followed to solve Eq. (10). The mapping function Ψ is employed to map the nonlinear data into the feature space for improved regression.

2.5. Multilayer Perceptron

MLP in this study consists of one to three hidden layers with a combination of input and output layers. In addition, except for input nodes, the nonlinear activation function is employed for neurons. MLP is used in the interaction of the supervised learning method to solve issues with both classification and regression purposes. The network indexes (weights and biases) are extracted during the training process of the network using the dataset for inputs (yeast extract g/L and electric current mA/m²) and output (power generation mW/m²) with minimizing the error. The backpropagation method is used inside the MLP structure to relate the optimal value of the biases and weights to the system's error [33]. The system error is the difference between the output of the main system (target) and the output of the MLP (obtained) using MSE or RMSE, etc., techniques. Backpropagation is the learning mechanism used, which is stochastic gradient descent with a backward pass of the various biases and weights through the MLP. The output node, j , in the data point, n , during the learning process (backpropagation) can be calculated as:

$$e_j(n) = T_j(n) - O_j(n) \quad (13)$$

where O and T are the obtained and targets value of the system.

The minimization of the error is used to extract the weights of the neurons throughout the entire output of the systems as follows:

$$\varepsilon(n) = \frac{1}{2} \sum_j e_j^2(n) \quad (14)$$

Then, the following formula can be used to calculate the variation of the weight based on the gradient descen technique as follows:

$$\Delta w_{ij}(n) = -\eta \frac{\partial \varepsilon(n)}{\partial v_i(n)} O_j(n) \quad (15)$$

where η and v_i are the learning rate and induced local field, respectively. η should be selected to converge the response quickly and without overfitting. The following is a simplified form of the weights for the induced local field for output neurons:

$$-\frac{\partial \varepsilon(n)}{\partial v_i(n)} = e_j(n) \phi' \left(v_j(n) \right) \quad (16)$$

where ϕ' is the constant value against weight, it is an induced local field known as the activation function's derivative. Inside the hidden node, calculating the fluctuation of the weights is difficult. However, the weight's derivative can be shown as:

$$-\frac{\partial \varepsilon(n)}{\partial v_i(n)} = \phi' \left(v_j(n) \right) \sum_k -\frac{\partial \varepsilon(n)}{\partial v_k(n)} w_{kj}(n) \quad (17)$$

It should be noted that the weight variation based on Eq. (15) inside the hidden node depends on the k th output layer weight. As a result, the output layer weights are affected by the hidden layer weight change determined by the activation function derivative.

3. RESULTS AND DISCUSSIONS

3.1. Scanning Electron Microscopes

Scanning electron microscopy (SEM) allows observation of microbial attachment on the surface of the anode. Attachment to the anode depends on several factors, such as the topology of the surface, shear forces on the microorganisms, hydration forces, surface chemistry, and the community of microorganisms present in the wastewater. SEM revealed dense biofilm growth on the anode, with a mix of rod-shaped bacilli and spherical cocci morphologies of varying sizes (Fig. 2). While SEM alone cannot determine the specific types of the microorganisms present beyond morphology, recent work examining the metagenomic community structure of an MFC biofilm indicated that the community was primarily composed of three phyla, Proteobacteria, Firmicutes, and Bacteroidetes, consistent with the human gastrointestinal tract [34]. As wastewater was used

as the source of microorganisms, it is expected that the observed biofilms are likely composed of a similar mixture of phyla and electricity generation clarified that most of the microorganisms are exoelectrogenics [35].

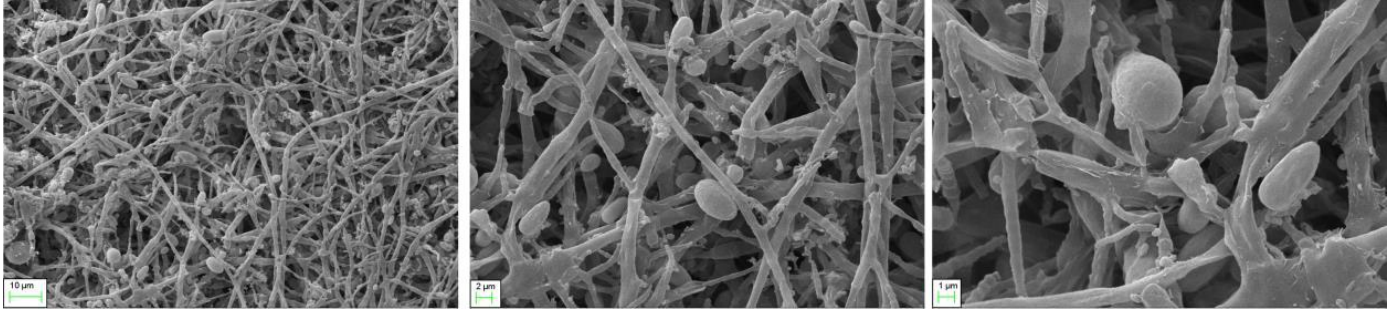


Figure 2. The attachment of microorganisms on the electrode surface.

3.2. Power Density

Power density results are shown in Fig. 3. As observed, the maximum power density generated by MFC1 is 170 mW/m², while 266.6, 308, and 287 mW/m² for MFC2, MFC3, and MFC4, respectively. The maximum power density for an MFC fed with 5 g/L yeast extract is 144 mW/m², which is the lowest of any MFC evaluated. The results show a clear increase in power generation with increasing yeast extract from 1 g/L to 4 g/L, but a sharp decline with 5 g/L yeast extract.

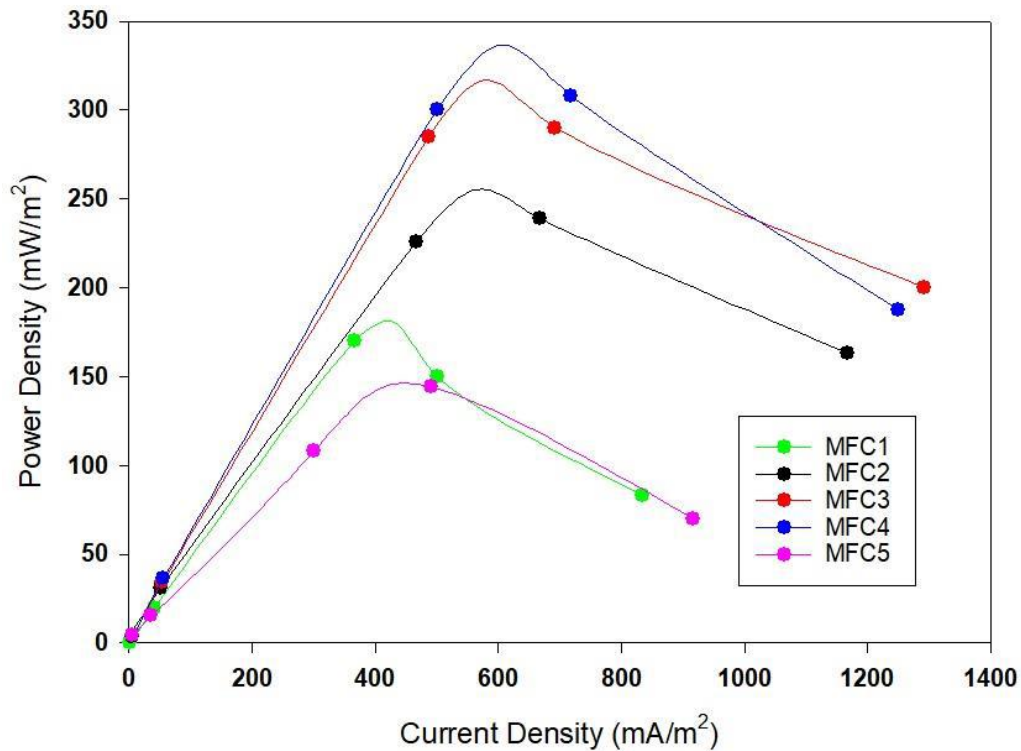


Figure 3. The power density versus current density.

The polarization curve is shown in Fig. 4. The slope of the line voltage versus current density shows the system's resistance. Fig. 4 depicts a lag in MFC1 and MFC5, which represents the time required for microbial attachment to the anode and growth. MFC2, MFC3, and MFC4 have shorter latency, whereas MFC5 has quite a large lag. The resistance for MFC1 is about 324 Ω , and MFC5 is about 365 Ω . The resistance for MFC2, MFC3, and MFC4 are 200, 240, and 130 Ω . MFC4 has the lowest internal resistance, while MFC5 has the highest. The result of internal resistance correlates with the inhibition effect in MFC5, and its internal resistance is higher than even MFC1. MFC4 has the lowest internal resistance with a high difference from the other MFCs, producing the highest power density due to higher growth and maturation of microorganism that caused easier transport of electrons to the anode electrode surface and more protons to the cathode.

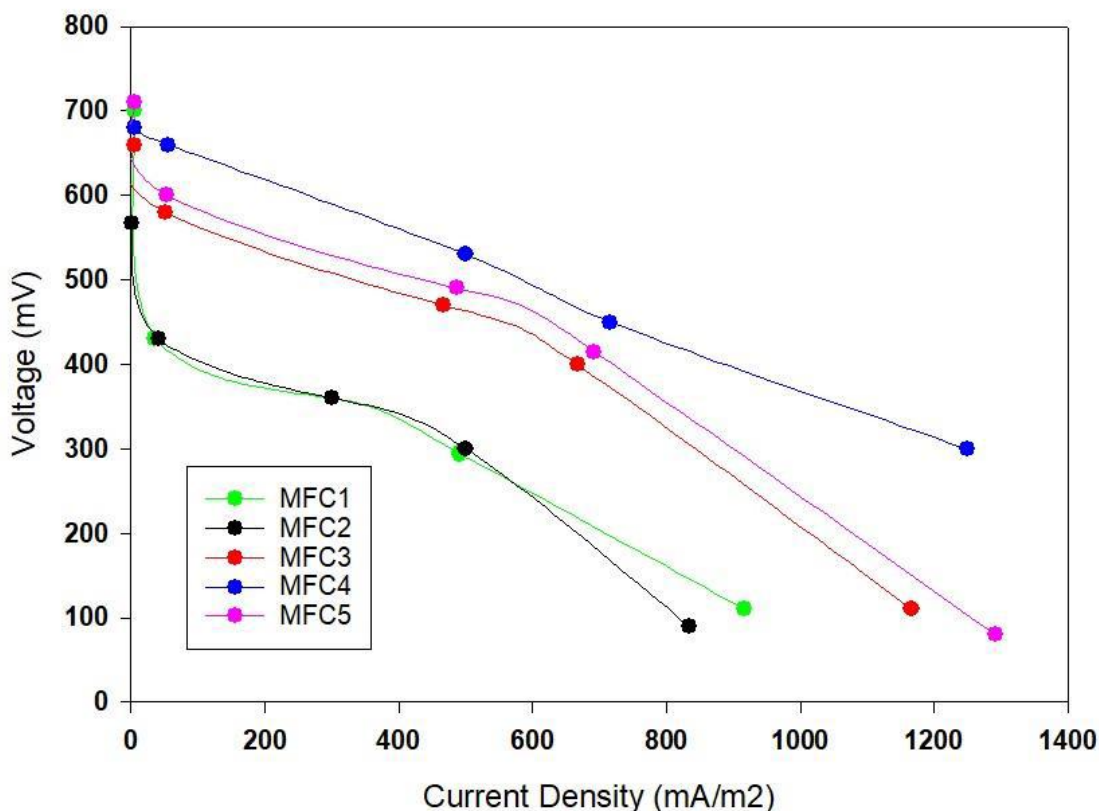


Figure 4. The polarization curve of the MFCs.

3.3. *Electrocatalytic Activity*

Voltammetry tests were performed to measure the current produced by each MFC (Fig. 5). Cyclic voltammetry (CV) detects the activity and the initiation of electron transfer. The oxidation peaks can be observed on the top side of the graph. The peak position and height are directly related to the catalytic activity. According to the CV data, MFC4 had the highest peak. These results suggest that the microorganisms get activated with lower energy and produce a high current. MFC2 and MFC3 show almost the peaks in the same place and same height. MFC1 shows a clear peak with lower current production. These findings show that while all of the MFCs demonstrated catalytic activity, MFC4 produces a larger current with less energy.

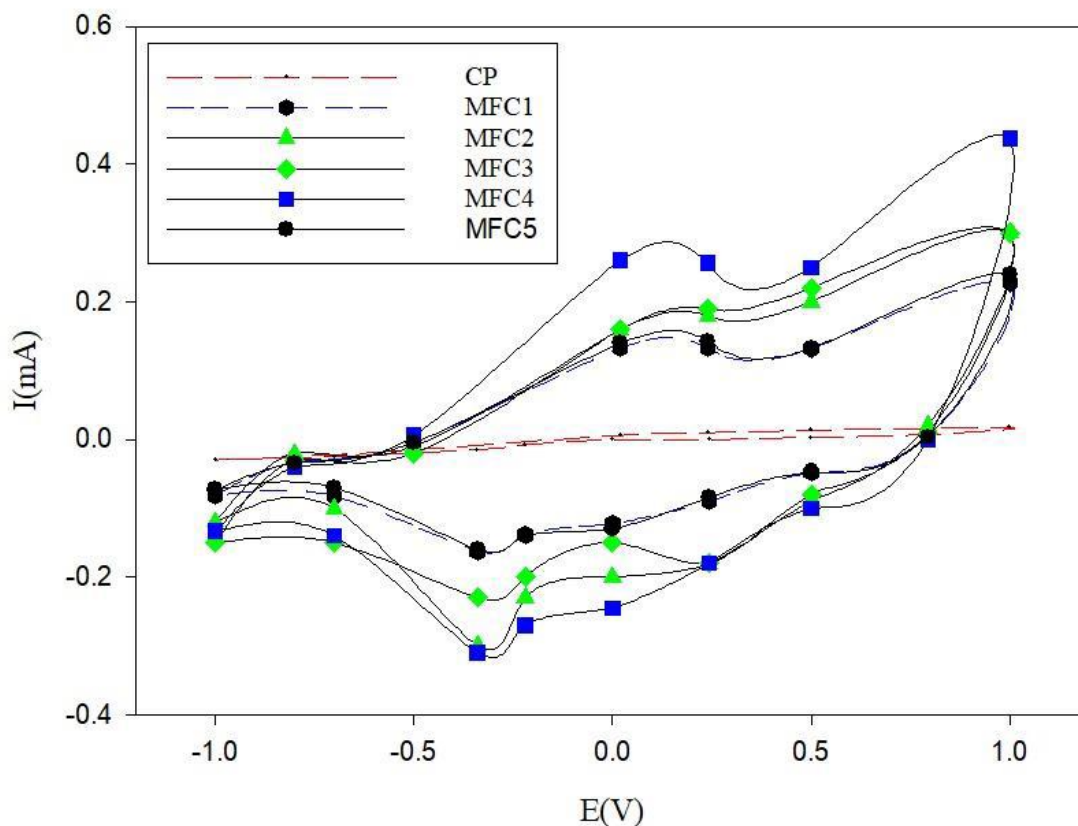


Figure 5. The cyclic voltammetry of different attached microorganisms.

3.4. Chemical Oxygen Demand Removal and Coulombic Efficiency

Fig. 6 depicts the COD removal and CE of MFC systems as a result of the catalytic activity of microorganism in wastewater. The figure demonstrates that most of the MFC systems have high COD removal. MFC3 and MFC4 had the highest COD removal by 70%, while MFC5 could remove the COD only by 49%. At the same time, MFC3 and MFC4 showed high catalytic activity based on CV. The lowest CE (29%) belongs to MFC5, and the highest CE (50%) is for MFC4. This could be due to the attachment of some microorganisms to the surface of the electrode that utilize the organic compounds present but do not produce protons and electron and thus have no role in CE.

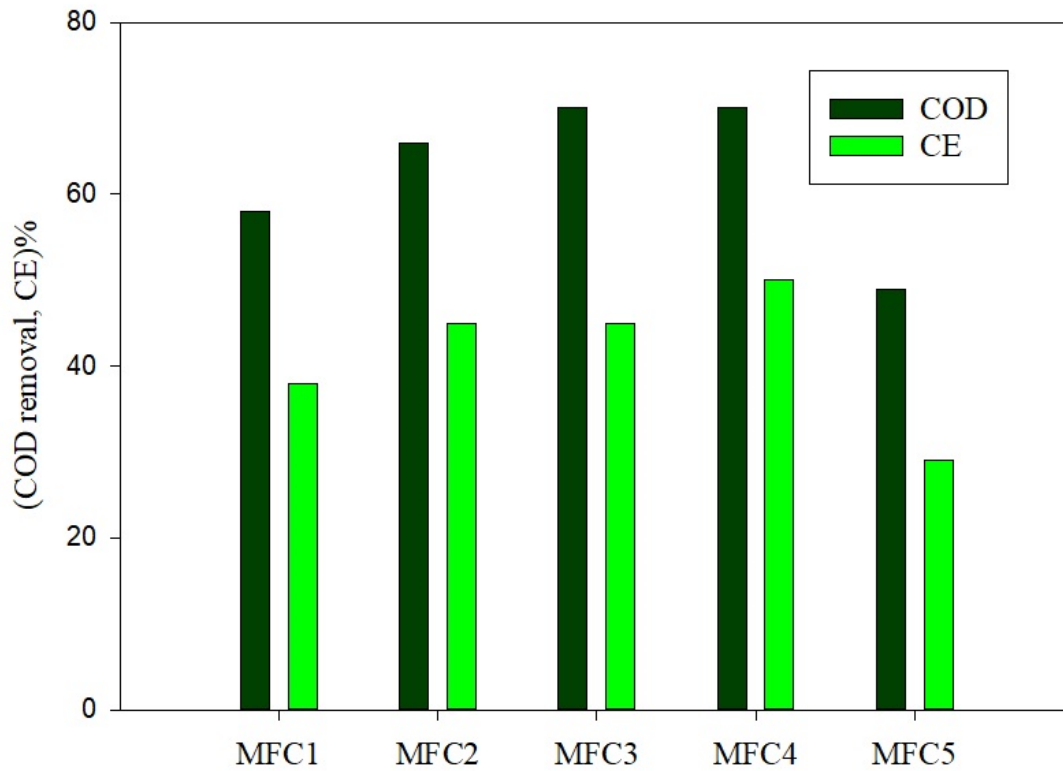


Figure 6. COD removal and CE of different MFCs.

3.5. Soft Computing Study

Initially, the dataset should be normalized to reduce the complexity of the system. The normalized data can be calculated as follows:

$$n_{x_i} = \frac{x_i - \underline{x}}{\overline{x} - \underline{x}} \quad (18)$$

where, $\underline{x}$ and $\overline{x}$ are functions to extract the minimum and maximum values from the dataset. Also, n_{x_i} represents the normalized input data for the i th item. Table 1 shows the mean square error (MSE) and root mean square error (RMSE) between the actual and predicted power generation of the MFCs using different numbers of hidden layers (1-3) and neurons (1-5). MSE and RMSE are calculated after 100 trials of the network to reach the most stable error. Based on the represented results, the hyperparameters of the number

of layers = 2 and the number of neurons = 4 is the most efficient model to reach the highest accuracy. In addition, if the search range is low, then the lower computation load of the system can simultaneously be satisfied.

Table 1. MSE and RMSE between the actual and predicted power generation of MFCs using MLP with different numbers of hidden layers and neurons.

i	Number of Layers	Number of Neurons	MSE (100 Trials)	RMSE (100 Trials)
1	1	1	1.62e+08	1.275e+04
2	1	2	2.109e+08	1.452e+04
3	1	3	2.347e+08	1.532e+04
4	1	4	1.019e+08	1.010e+04
5	1	5	9.808e+07	9.904e+03
6	2	1	8.884e+07	9.426e+03
7	2	2	3.205e+08	1.790e+04
8	2	3	1.520e+08	1.233e+04
9	2	4	8.046e+07	8.970e+03
10	2	5	1.181e+08	1.087e+04
11	3	1	2.020e+08	1.421e+04
12	3	2	2.928e+08	1.711e+04
13	3	3	2.621e+08	1.619e+04
14	3	4	2.995e+08	1.731e+04
15	3	5	1.129e+08	1.062e+04

Fig. 7 (a) & (b) shows the regression of the investigated SVR and MLP during the training and testing stage (all datasets). Fig. 7 depicts the actual and expected power generation of an MFC using vertical and horizontal

axes. During all data processes (including testing and training), the R-square of SVR and MLP is -0.88884 and 0.96987, respectively. These results demonstrate the higher efficiency of the MLP in predicting the power generation of an MFC compared with SVR.

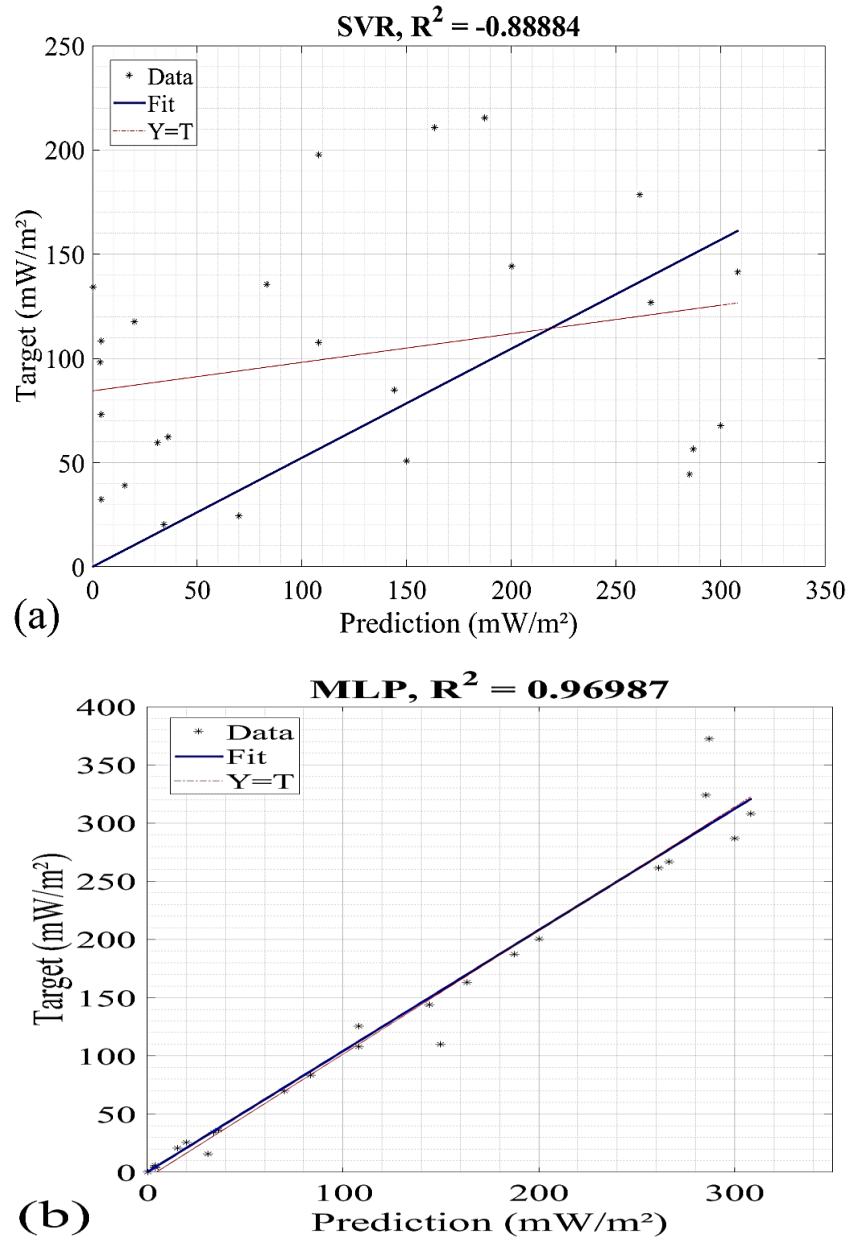
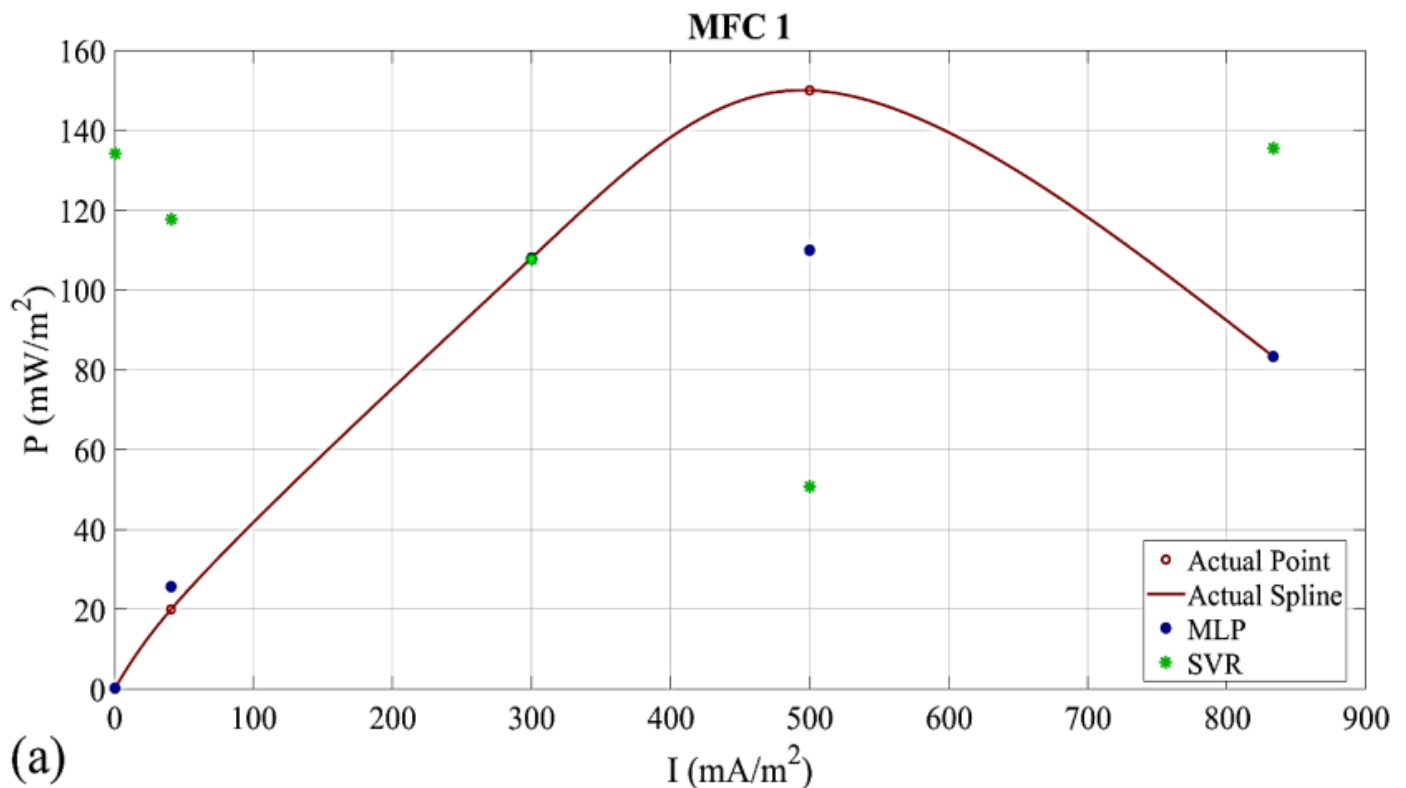
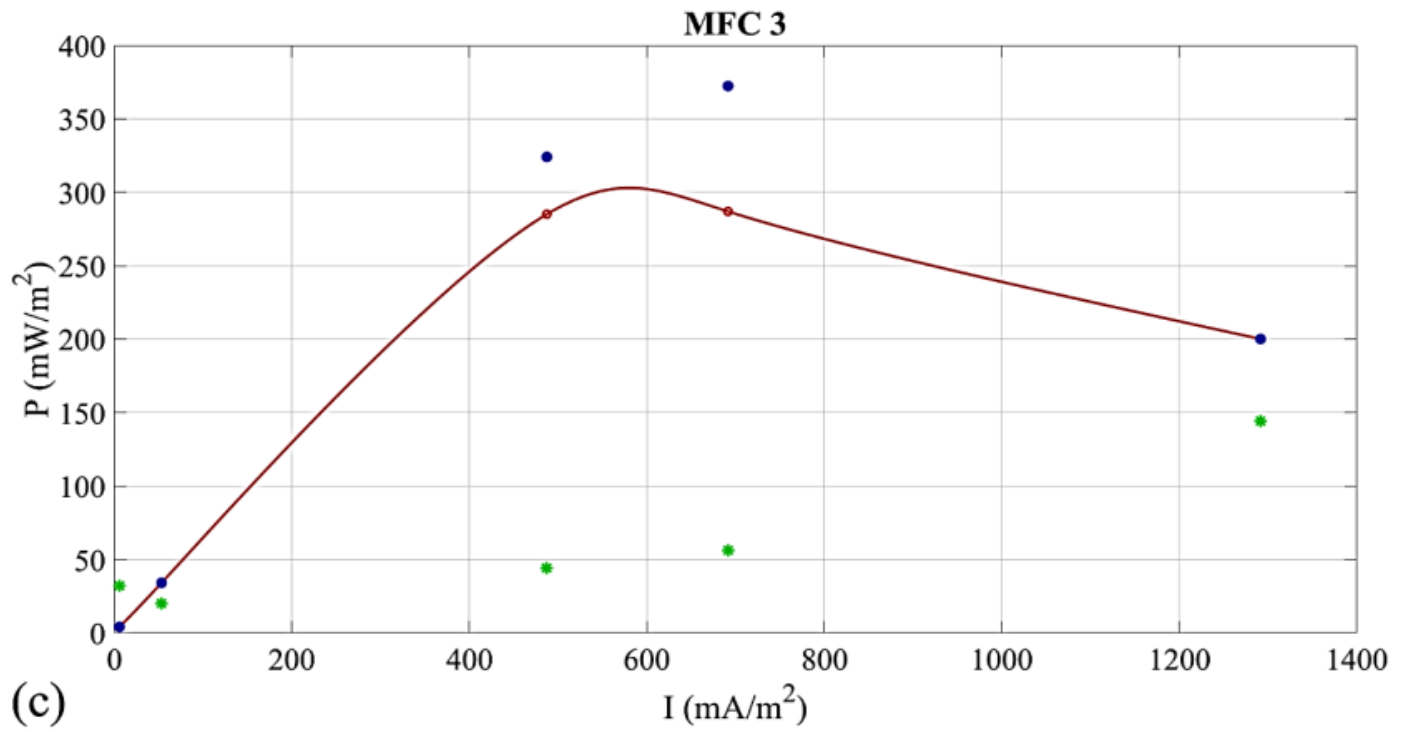
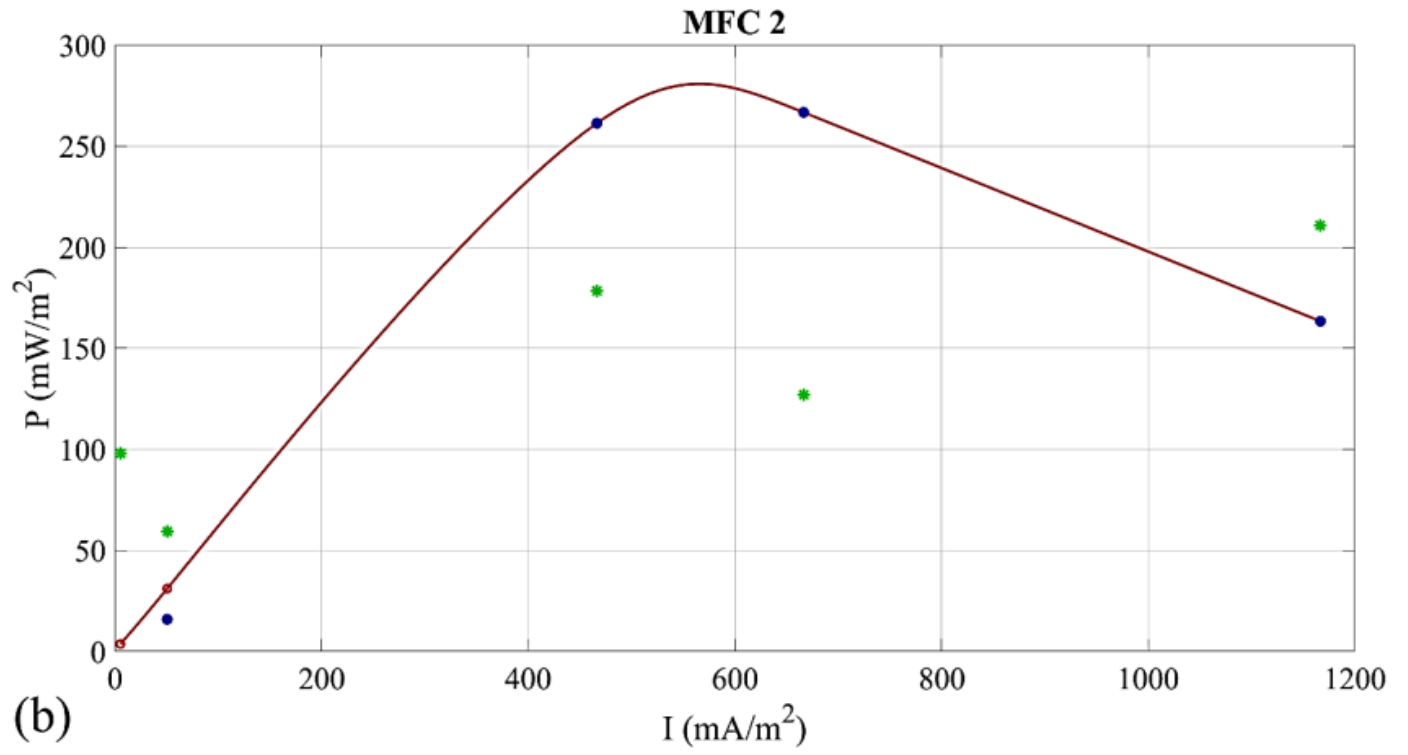


Figure 7. The regression of the data during all data (training and testing) for power density (mW/m^2) using (a): SVR; (b): MLP.

Fig. 8 depicts the target and predicted power generation of MFCs for training and testing datasets using SVR and MLP. The redline was generated by interpolating the recorded power generation during the experiments with the spline interpolation technique. As shown in Fig. 8, the RMSE between the actual and predicted power generation of MFC1 using SVR and MLP are 89.4879 and 18.0897 (mW/m²), 87.6237 and 9.5476 (mW/m²) for MFC2, 151.8677 and 42.0045 (mW/m²) for MFC3, 132.6438 and 5.8921 (mW/m²) for MFC4, and 70.8608 and 8.2370 (mW/m²) for MFC5, respectively. Based on the data shown in Fig. 8, the CC between actual and predicted power generation for MFC1, MFC2, MFC3, MFC4, and MFC5 using SVR is -0.7621, 0.6393, 0.3848, 0.3497, and 0.3223. Finally, CC between actual and predicted power generation for MFC1, MFC2, MFC3, MFC4, and MFC5 using MLP are 0.9671, 0.9998, 0.9887, 0.9994, and 0.9927, as show in Fig. 8.





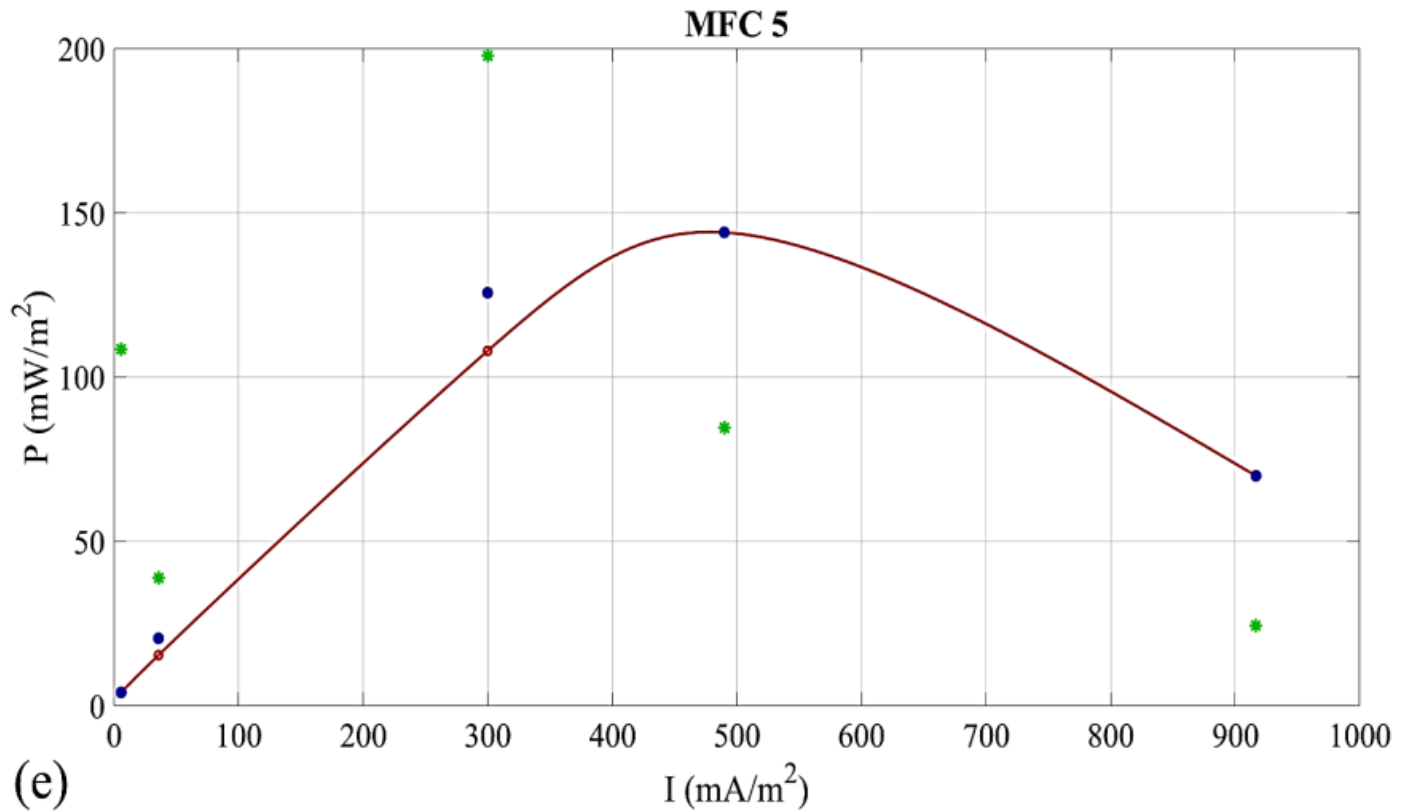
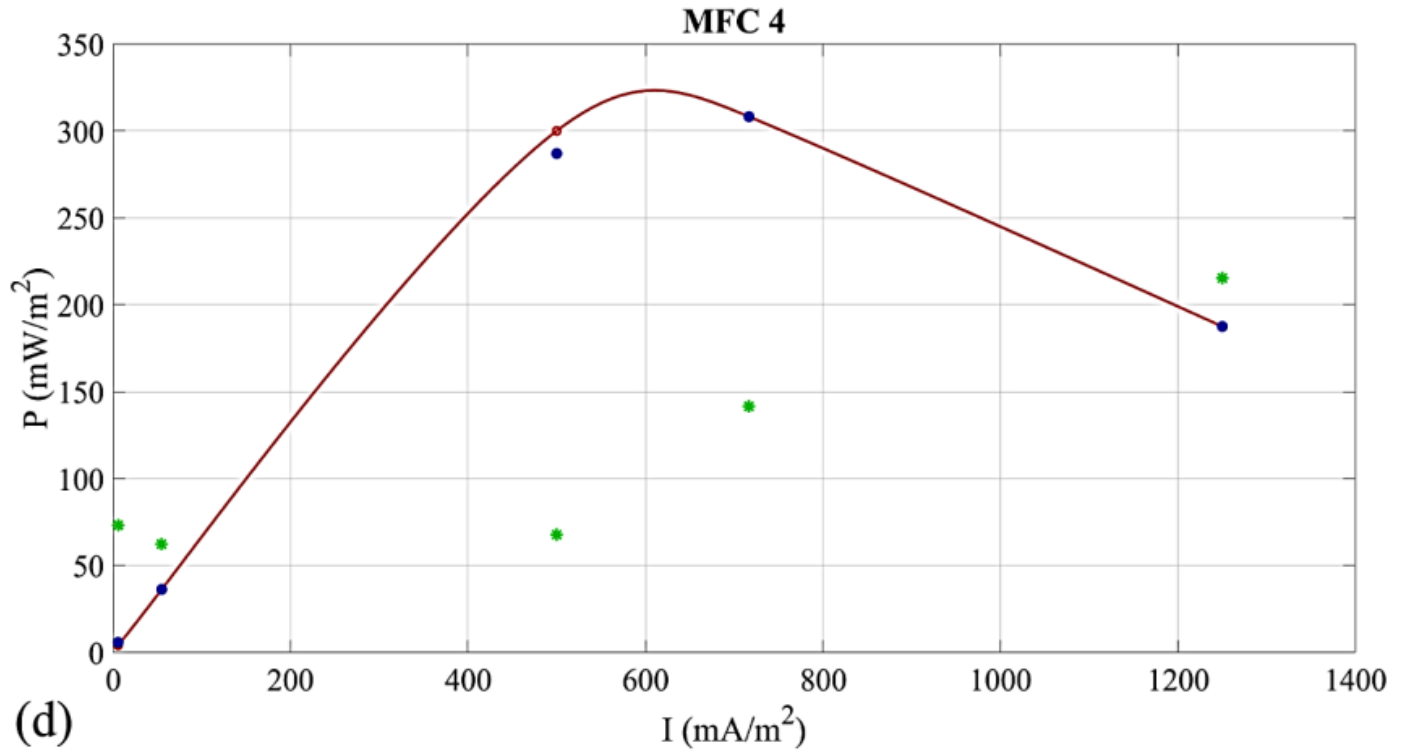


Figure 8. The actual and predicted power generation (mW/m²) based on current density (mA/m²) during all data (training and testing) using SVR and MLP for (a): MFC1; (b): MFC2; (c): MFC3; (d): MFC4; (e): MFC5.

Fig. 9 depicts the difference in power generation between real and predicted MFCs using SVR and MLP. Based on the results in Fig. 9, the MLP has a lower prediction error than the SVR. The RMSE between the actual and predicted dynamic viscosity using MLP reduced by 5.1819 times compared with SVR.

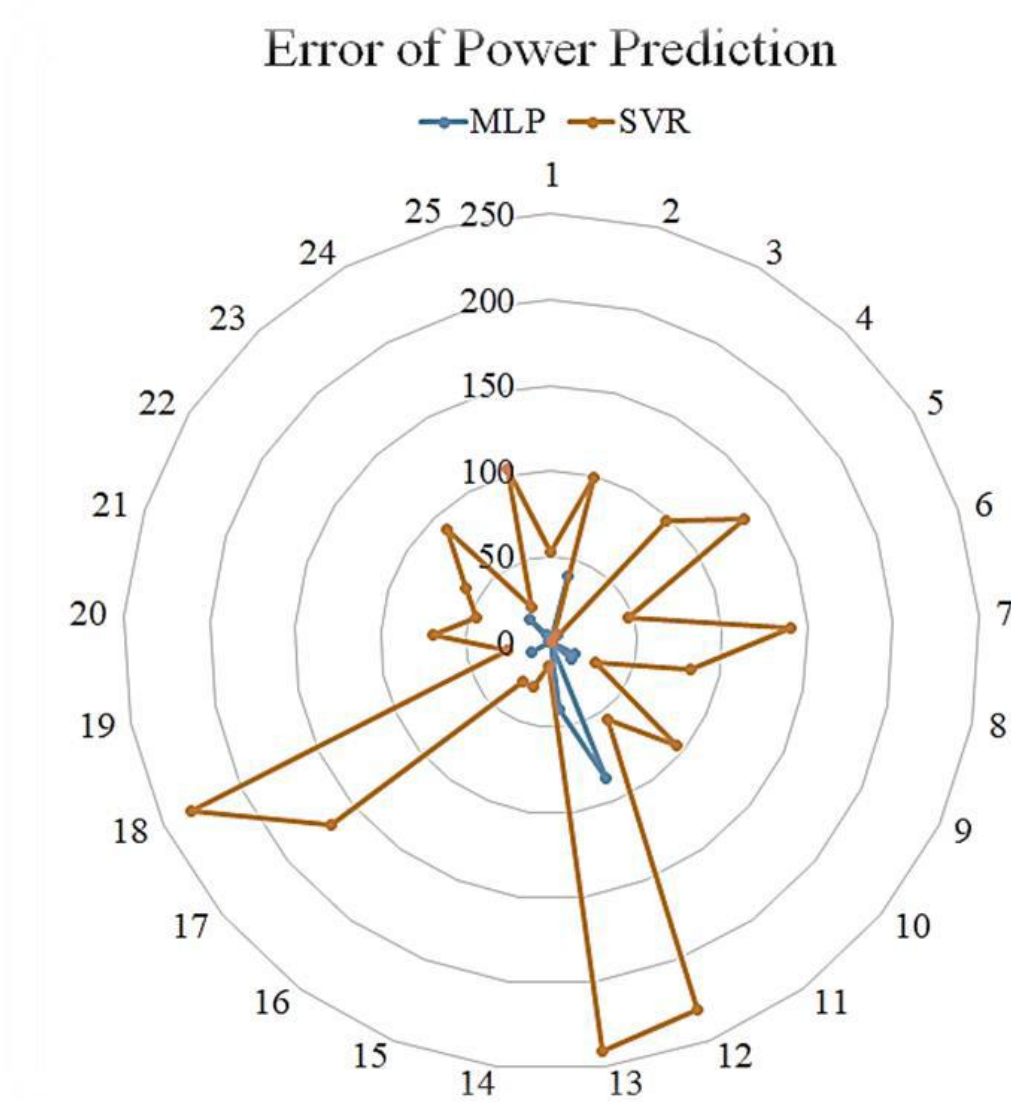


Figure 9. The error between the actual and predicted power generation of MFCs using SVR and MLP with consideration of all datasets.

Overall, the MFCs have been studied in terms of power generation. Also, the polarization curves of them were found for calculating the internal resistance. SEM photos have shown the attachment of dense layers of different variants of microorganisms. Furthermore, MLP outperforms SVR as the classic machine learning method in terms of computing the power generation of MFCs.

4. CONCLUSION

An MFC is a breakthrough innovation that generates power from organic waste using microorganisms. However, due to the high capital cost and uncertainty of MFC performance, this technology has not been commercialized. This paper measured how different yeast extract concentrations, the main nitrogen source for microbial growth in our MFCs, influenced MFC power density. As expected, we observed differences in MFC performance based on this parameter, with disadvantages for the highest amount of yeast extract tested. We found that MFC4 had the highest power density while MFC5 had the lowest. MFC3 had the highest level of COD removal, whereas MFC5 and MFC1 had the lowest. A soft computing method was utilized to forecast the power generation of MFCs based on yeast extract (g/L) and current density (mA/m²) based on our experimental data. The extracted dataset for 5 different amounts of yeast extract used in the MFCs was used to train and test the MLP to predict the power generation for other combinations of the systems. It should be noted that 70% and 30% are used for training and testing purposes of the algorithm. The proposed MLP model is validated with SVR as the traditional machine learning method candidate. It has been implemented in MATLAB software, and the results showed that MLP has sufficient prediction power (5.1819 times more accurate than traditional SVR) to be used for the calculation of power generation of MFC based on the concentration of yeast extract and the electric current produced.

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