Design of neural network model-based controller in a fed-batch microbial electrolysis cell reactor for bio-hydrogen gas production

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Abstract. One of major challenge in bio-hydrogen production process by using MEC process is nonlinear and highly complex system. This is mainly due to the presence of microbial interactions and highly complex phenomena in the system. Its complexity makes MEC system difficult to operate and control under optimal conditions. Thus, precise control is required for the MEC reactor, so that the amount of current required to produce hydrogen gas can be controlled according to the composition of the substrate in the reactor. In this work, two schemes for controlling the current and voltage of MEC were evaluated. The controllers evaluated are PID and Inverse neural network (NN) controller. The comparative study has been carried out under optimal condition for the production of bio-hydrogen gas wherein the controller output is based on the correlation of optimal current and voltage to the MEC. Various simulation tests involving multiple set-point changes and disturbances rejection have been evaluated and the performances of both controllers are discussed. The neural network-based controller results in fast response time and less overshoots while the offset effects are minimal. In conclusion, the Inverse neural network (NN)-based controllers provide better control performance for the MEC system compared to the PID controller.

1. Introduction
Microbial electrolysis cells (MEC) used for wastewater treatment are a novel and promising renewable energy technology that can produce H\textsubscript{2} while the treatment is being performed. It is a new bio-electrochemical process that is capable of producing hydrogen gas [1]. Currently, several studies of the MEC system have been reported in the literature. One important and interesting phenomenon of the MEC model is a competition between anodophilic and methanogenic microorganisms to consume the substrate in the anode compartment [2, 3]. Competition among these microbial populations has severe...
effects on the performance of the MEC bioreactor. An initial study of this system used a model involving competition among anodophilic, methanogenic acetoclastic and hydrogenotrophic methanogenic microorganisms in the biofilm as reported by Pinto et al. [4]. Others have reported improvements in the modeling and simulation of a two-chamber microbial fuel cell [5], conduction-based modeling of the biofilm anode of a microbial fuel cell, analysis of a microbial electrochemical cell using the proton condition in biofilm model [6] and a multi-population model of a microbial electrolysis cell [7]. Picioreanu et al. [8] provided detailed descriptions of the mathematical model for microbial fuel cells with anodic biofilms and anaerobic digestion. The model was based on evaluation of the effect of pH and electrode geometry on microbial fuel cell performance.

Bio-hydrogen production process in the MEC is a nonlinear and highly complex system due to the microbial interaction. Its complexity makes MEC system difficult to operate and control under optimal conditions. However, these problems can be alleviated using an integrated process system engineering approach, which involves process modeling and control simultaneously. Artificial neural networks (ANNs) are one of the most effective techniques and powerful tools to be used in modeling of complex processes and unknown systems. ANNs are able to cope with non-linear process between input and output variables without the requirement of explicit mathematical representation. In the process control system, ANNs have been widely used when conventional control techniques did not give good performance [9, 10].

In the literature, several studies and investigations on the modeling of biohydrogen production using ANN approach is reported. For example, El-Shafie [11], use ANNs to successfully predict hydrogen yield with the following input: initial medium pH, initial glucose concentration and reaction temperature. Sridevi et al. [12] studied the Back propagation NNs modelling of biodegradation and fermentative biohydrogen production using distillery wastewater in a hybrid upflow anaerobic sludge blanket reactor. The hydrogen production profile in batch studies was simulated using ANN by Nasr et al. [13]. The ANN inputs were the initial pH, initial substrate, biomass concentrations, temperature, and time. A model was trained, tested and validated to predict the hydrogen production profile. However, none of these studies in the literature involve neural network based controller for biohydrogen gas production in the MEC.

This study focuses on the comparative controller performance in a feedback control approach for the MEC fed-batch reactor, where the comparative study between PID and neural network model-based controller are discussed. The performance and assessment of these PID and neural network controller for tuning and rejection of the load disturbances and noise will be discussed. The requirements for a good controller for optimal H2 gas production are also highlighted in this work. Where, better control system for optimum bio-hydrogen gas production can be achieved.

2. Mathematical model
The model equations presented here are based on multi-population MEC models, and the following modifications were made to modify the model proposed by Pinto et al. [4] for our case study:

1. The model here is modified for a fed-batch reactor; the Pinto model assumed a continuous system.
2. In this proposed model, the biofilm formation and retention consists of two-phase model biofilm growth, anodic biofilms (Layer 1) and a cathode biofilm population (Layer 2). The Pinto model uses three phases, an outer biofilm layer (Layer 1), an inner biofilm (Layer 2) and cathode biofilms (Layer 3). Using the two-phase model will be more practical and easier to apply in a real plant.
3. This proposed model involves metabolic activities of methanogenic acetoclastic, and methanogenic hydrogenophilic microorganisms without involving the fermentation used in the Pinto model. We assume that it is very difficult to observe two different processes simultaneously in the same reactor, such as fermentation and the bio-electrochemical process [7].

2.1. Mass balances for the MEC system
The dynamic mass balance equations for the components S, Xa, Xm, Xh and Mox in the reactor system are given below as follows:

```latex
\textbf{Mass balances for the MEC system}
\textbf{S, Xa, Xm, Xh and Mox in the reactor system are given below as follows:}
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where $S$ is the substrate concentration, $x_a$, $x_m$, and $x_h$ are the concentration of the anodophilic, acetoclastic, and hydrogenotrophic microorganisms, respectively; $M_{ox}$ is the oxidized mediator fraction per electricigenic microorganism; and $Q_{H_2}$ is the hydrogen production rate (mL/day). Detailed parameter descriptions are provided in Table 1.

2.2. Electrochemical process

The MEC voltage can be calculated using the theoretical values of electrode potentials by subtracting the ohmic, activation, and concentration losses. Resistance to the flow of ions in the electrolyte and electrode during the MEC operation generates ohmic losses. These partial resistances consist of the counter-electromotive force ($E_{CEF}$), activation loss ($\eta_{act}$), concentration loss ($\eta_{conc}$), and ohmic loss ($\eta_{ohm}$). Each of these polarizations has different magnitudes for different current density degrees. At low current densities, activation losses are dominant due to reaction-energy barriers at the electrode-electrolyte interface that need to be overcome to start the reaction. At high current densities, the reactant and product diffusion limitations lead to high concentration losses. Finally, ohmic losses increase linearly with current due to electron and ion conduction at the electrodes and electrolytes, contact resistance across each material’s interface, and interconnections to electrodes. Therefore the following electrochemical balance can be written as follows:

$$\eta_{ohm} = R_{int}I_{cell}$$
$$-E_{applied} = E_{CEF} - \eta_{ohm} - \eta_{conc} - \eta_{act}$$
$$\eta_{conc,A} = \frac{RT}{mF} \ln \left( \frac{M_{Total}}{M_{red}} \right)$$
$$\eta_{act,C} = \frac{RT}{mF} \sinh^{-1} \left( \frac{I_{MEC}}{A_{sur,A} I_0} \right)$$
$$I_{MEC} = \frac{E_{CEF} + E_{applied} - \frac{RT}{mF} \ln \left( \frac{M_{Total}}{M_{red}} \right) - \eta_{act,C}(I_{MEC})}{R_{int}}$$
$$I_{MEC} = \frac{E_{CEF} + E_{applied} - \frac{RT}{mF} \ln \left( \frac{M_{Total}}{M_{red}} \right) - \eta_{act,C}(I_{MEC})}{R_{int}}$$
value if $E_{\text{applied}}$ is smaller than the sum of $\eta_{\text{conc}}$, $\eta_{\text{act}}$, and $E_{\text{CEF}}$, only non-negative values of $I_{\text{MEC}}$ were considered. The detailed characterization, operation and constant parameters used in these simulation studies are listed in Table 1.

### Table 1. Values of kinetic parameters used for the simulation studies.

| Symbols | Description | Value |
|---------|-------------|-------|
| $\mu_{\text{max},m}$ | The maximum growth rate of the acetoclastic methanogenic microorganism | 0.3 $d^{-1}$ |
| $\mu_{\text{max},a}$ | The maximum growth rate of the anodophilic microorganism | 1.97 $d^{-1}$ |
| $\mu_{\text{max},h}$ | The maximum growth rate of the hydrogenotrophic microorganism | 0.5 $d^{-1}$ |
| $q_{\text{max},a}$ | The maximum reaction rate of the anodophilic microorganism | 13.14 mg-A mg-x$^{-1}$ d$^{-1}$ |
| $q_{\text{max},m}$ | The maximum reaction rate of the acetoclastic methanogenic microorganism | 14.12 mg-A mg-x$^{-1}$ d$^{-1}$ |
| $K_{S,a}$ | The half-rate (Monod) constant of the anodophilic microorganism | 20 mg-A L$^{-1}$ or mg-M L$^{-1}$ |
| $K_{S,m}$ | The half-rate (Monod) constant of the acetoclastic methanogenic microorganism | 80 mg-A L$^{-1}$ or mg-M L$^{-1}$ |
| $K_M$ | Mediator half-rate constant | 0.01 mg-M L$^{-1}$ |
| $K_h$ | Half-rate constant | 0.001 mg L$^{-1}$ |
| $Y_{H_2}$ | The dimensionless cathode efficiency | 0.9 [dimensionless] |
| $Y_h$ | The yield rate for hydrogen consuming methanogenic microorganisms | 0.05 [ml-H$_2$: mg-x$^{-1}$ d$^{-1}$] |
| $m$ | The number of electrons transferred per mol of H$_2$ | 2 mol-e$^-$ mol-H$_2$$^{-1}$ |
| $P$ | The anode compartment pressure | 1 atm |
| $M_o$ | Oxidized mediator fraction | 800 mg-M mg-x$^{-1}$ |
| $\beta$ | The reduction or oxidation transfer coefficient | 0.5 [dimensionless] |
| $A_{\text{sur}}$ | The anode surface area | 0.01 m$^2$ |
| $i_0$ | The exchange current density in reference conditions | 0.005 A m$^{-2}$ |
| $E_{\text{CEF}}$ | The counter-electromotive force for the MEC | -0.35 V |
| $E_{\text{applied}}$ | The electrode potentials | 0.80 V |
| $K_{d,a}$ | The microbial decay rates of the anodophilic microorganism | 0.04 $d^{-1}$ |
| $K_{d,m}$ | The microbial decay rates of the acetoclastic methanogenic microorganism | 0.01 $d^{-1}$ |
| $K_{d,h}$ | The microbial decay rates of the hydrogenotrophic microorganism | 0.01 $d^{-1}$ |
| $Y_M$ | The oxidized mediator yield | 34.85 mg-M mg-A$^{-1}$ |
| $\gamma$ | The mediator molar mass | 663400 mg-M mol$_{\text{med}}$$^{-1}$ |
| $V_r$ | The anodic compartment volume | 10 l |

3. Design of Neural Network Controller

The basic direct neural network model used for the controller concept refers to the inverse form of the process. Inverse neural network model with feed-forward structure is used directly as elements within the feedback loop. The diagram of the neural network inverse model based control strategy implementation to control the MEC Current ($I_{\text{MEC}}$) controlled in Fed-batch Microbial Electrolysis Cell Reactor is shown in Fig. 1. From the figure, it can be seen that the inverse model acts as the controller and provides the current control action with respect to certain current and past values of the process variables. In this case, the neural network model is trained to predict the required manipulated variable i.e. Electrode potential ($E_{\text{applied}}$) and to bring the process to the set-point i.e. MEC current ($I_{\text{MEC}}$).
3.1 Training and validation data

The inputs and the outputs of the neural network are fed through a moving window approach. The model is made of 14 input and one output nodes, the input nodes consist of data for substrate (S), anodophilic microorganisms (xa), acetoclastic microorganism (xm), ammonium nitrogen (xn), oxidized mediator fraction (mox), MEC current (imec) and the one output node is electrode potentials (Eapplied) and past and current data for S i.e. S(t), S(t-1), xa i.e. xa(t), xa(t-1), xm i.e. xm(t), xm(t-1), xn i.e. xn(t), xn(t-1), mox i.e. mox(t), mox(t-1), imec i.e. imec(t), imec(t+1), imec(t-1) and output node is the electrode potentials (Eapplied).

The training of a neural network is done in conjunction with the back-propagation algorithm. The back-propagation pass is used to calculate the derivatives and the errors of every neuron in the network. The back-propagation algorithm learns to recognize and reproduce patterns in an iterative process whereby its weights are adjusted in order to minimize a selected error criterion. Data for training the neural network in the simulation work are obtained by solving the ordinary differential equations (ODE) utilizing the MATLAB 2011a software. Two sets of data have been prepared for training the neural network model and one is used for cross validation purposes in order to test the validity of the trained neural network models. The three training data sets are switched between each other during the training session in order to improve system identification by the neural network models [14]. The validation for neural network inverse based model are shown in Figure 2.

3.2 Forward and inverse modeling

The procedure of training a neural network to represent the dynamics of the system is referred to as forward modeling. Forward modeling refers to training the neural network model to predict the plant output, imec(t+1). In this case, connections between layers, or weights, are changed during training in order to minimize the error between the actual plant output and the predicted output from the neural network model. The input to the network consists of present and past value of S, xa, xm, xn, mox, imec and Eapplied values. The desired network output is the future imec(t+1) values. Those input and output values are fed into the network in the moving window approach. From these training exercises, the neural network architecture produced is a 14 nodes input layer, 28 nodes of hidden layer and a 1 output layer system. The activation function utilized is the sigmoidal function in both the hidden and output layer. The forward model can be expressed mathematically as a function of inputs to the model as shown below:
Inverse modeling refers to the training of the neural network in predicting the input to the plant given past data of the inputs and outputs together with the desired output. The inverse model is used directly as the controller within the feedback loop. Similar to the forward modeling methodology two training data sets were used, those were switch from one to the other during training to improve the identification process. In determining the inverse model to use as the controller, the network architecture and activation functions that were chosen are similar to the forward model. For this inverse model, the two-layered feed-forward network that has 14 input nodes, 24 hidden nodes and 1 output node is used. During training the network is fed with the required future value, \(I_{\text{MEC}(t+1)}\), together with the present and past input and outputs to predict the current input or control action, \(E_{\text{applied}(t)}\) as seen in Fig. 3. The inverse model can be expressed mathematically as a function of inputs to the model as shown below:

\[
E_{\text{applied}(t)} = f \left( S(t), S(t-1), x_{a(t)}, x_{a(t-1)}, x_{m(t)}, x_{m(t-1)}, x_{h(t)}, x_{h(t-1)}, Q_{H2(t)}, Q_{H2(t-1)}, M_{ox(t)}, M_{ox(t-1)} \right)
\]  

The data sets generated for the training and validating, transfer functions and method of training the inverse model used are similar to the forward model. The architecture of the inverse model can be seen in Figure 3.
Figure 3. The inverse model architecture for Microbial Electrolysis Cells.

Figure 4 shows the inverse modeling of MEC current to be used as training data. From the result, it can be seen that the artificial neural network accurately tracks the inverse dynamics of the MEC system.

**4. Neural Network Controller Scheme**

In this section, the performance of the basic neural network controller is discussed. The performance of the controller was investigated through studies of nominal operating condition, constant set-point and multiple set-point tracking study for testing the performance of process by loading internal disturbance. The variation in disturbance was generated by changing the counter-electromotive force (nominal value of 0.35 V).

4.1 Constant set-point

In this work, we performed set-point tracking study when the $I_{MEC}$ current was maintained at approximately the nominal optimal operation value of 0.16 A. Fig. 5 shows the process and controller...
response when using the conventional PID-ZN method and neural network model-based controller for single set-point performance under nominal operating conditions. The controller performs well and is successful in managing the process to follow the given set point. However, the PID (tuned with the Z-N method) gave a higher overshoot and more oscillations than the neural network model-based controller. This is also evident in the behavior of the manipulated voltage of the electrode potential applied for both cases.

![Graph 1](image1.png)

**Figure 5.** Comparison of PID-ZN and neural network model-based controller for constant setpoint.

**4.2 Disturbances rejection**

Figure 6 shows the comparison of the control performance of the PID-ZN method and neural network model-based controller for constant setpoint with disturbances in the MEC system. The disturbance considered in this study was generated through changes in the counter-electromotive force (V). Based on these results, the performance of this controller is generally acceptable and the neural network model-based controller gave smoother responses in the MEC system.

![Graph 2](image2.png)
4.3 Multiple set-point tracking study

Figure 7 shows the comparison of PID-ZN and neural network model-based controller for multiple setpoint tracking study. The controller performs well and is successful in managing the process to follow the given set point changes to keep up around at 0.11 A, 0.16 and 0.20 A, respectively. From these figures, we can see that neural network model-based controller can provide better control of the MEC system compared with the Ziegler-Nichols tuning method. It can be seen that the controller performs reasonably well when responding to deviation, but it becomes sluggish when responding to large deviations in the process response. However, the controller is also capable of following the time-varying characteristic of the process in most conditions.
5. Conclusions
In this paper, the optimal control design for MEC with various simulation tests involving single set-point study, multiple set-point changes and disturbance rejection was achieved using the neural network model-based controller. Various simulation tests have been evaluated and the performances of both controllers were discussed. A Ziegler–Nichols tuning method has been used to design the PID controller, while the neural network controller has been designed from the inverse response of the forward MEC model. The neural network-based controller results in fast response time and less overshoots while the offset effects are minimal. In conclusion, the neural network (NN)-based controllers provide better control performance for the MEC system compared to the PID controller.

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