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A Reduced Model for Microbial Electrolysis Cells

Dina Aboelela, Moustafa Aly Soliman, Ibrahim Ashour

Abstract: Microbial electrolysis cells (MECs) are breakthrough technology of cheap hydrogen production with high efficiency. In this paper differential-algebraic equation (DAE) model of a MEC with an algebraic constraint on current was studied, simulated and validated by implementing the model on continuous-flow MECs. Then sensitivity analysis for the system was effectuated. Parameters which have the predominating influence on the current density and hydrogen production rate were defined. This sensitivity analysis was utilized in modeling and validation of the batch-cycle of MEC. After that parameters which have less influence on MEC were eliminated and simplified reduced model was obtained and validated. Finally, MEC energy productivity was maximized by optimization of operating conditions.

Keywords: hydrogen production, optimization, sensitivity analysis, validation.

I. INTRODUCTION

Nowadays energy consumption is increasing rapidly as the modern life style relies on energy. Most of the needed energy is generated from nonrenewable resources such as fossil fuel which cause drastic climate change due to the emissions of pollutants such as CO_x , NO_x , SO_x , C_xH_y , ash, and other organic compounds as combustion products. Consequently, One of the biggest defies in the near future is to obtain new sustainable power sources which are environment friendly to replace the traditional energy which have limited resources and deleterious environmental impact [1].

Most promising fuel to substitute the fossil fuel is hydrogen as it has energy content of 122 kJ/g [2] which is 2.75 times greater than hydrocarbon fuels. It is environment friendly, colorless, tasteless, odorless, light and non-toxic. When it is utilized as fuel, the only combustion product is water [3]. Hydrogen can be produced by biological processes which is clean and feasible methods as it is operated at ambient temperature and pressure with minimal energy consumption [4].

One of these biological processes is Microbial Electrolysis Cells (MEC) which is a state of art technology for energy recovery from organic waste and biomass residue, where microorganisms are utilized to catalyze electrochemical oxidation-reduction reactions which produce hydrogen. Although MEC technique still under development, it is clear

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Ibrahim Ashour, Minia University, Faculty of Engineering, Department of Chemical Engineering, Minia 61519, Egypt. Email: Ibrahim.ashour@gmail.com that it has tremendous potential as it requires energy input less than water electrolysis and has efficiency greater than fermentative hydrogen production [5-8].

In the MEC systems, bacteria oxidize organic matter, which releases protons into solution and electrons to anode [9]. Then the released electrons to anode flows through an external electrical circuit to the cathode where they react with the protons to form hydrogen.

For instance, if a substrate of (1 M) acetate is used, the MEC reactions will be:

Anode: CH3COO⁻ + $4H_2O$ 2HCO₃⁻ + $9H^+$ +8e⁻ E anode = -0.28 V (NHE) Cathode: $8H^+$ + 8e⁻ 4H₂ E cathode= -0.42 V (NHE)

The design of MEC prevent production of methane in anode chamber by applying small quantity of electric energy. Also to enhance hydrogen gas production, cathode chamber has to be kept free of oxygen. Selection of anode materials, microorganisms and efficient design are the key factors of success of the MEC process [10]. Figure 1 shows the schematic diagram of MEC [11].

Microbial electrolysis is endothermic reaction (with negative change in enthalpy - Δ H). The theoretical minimum required voltage in MEC is 0.14 V however minimum actual applied voltage in MEC is 0.3 V due to the high internal resistance in MEC systems. Even though the energy requirements in MEC is less than the energy requirements in electrolysis cell because exoelectrogens reduces the energy requirements of the reaction.

In the studied case, only 0.6 - 1.0 Volts were applied to produce the same amount of hydrogen, which can be produced from water electrolysis with applying about 1.8 - 2.0 Volts [12, 13].

In this study, enhancement the performance of MEC will be studied by modelling the MEC using MATLAB then simplifying DAE using sensitivity analysis then optimizing the operating condition to obtain the maximum energy production.



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Figure 1: Schematic diagram of MEC

II. MATERIALS AND METHODS

Pinto [14-16] developed model equations which simulate the bio catalytic reactions of MEC which is catalyzed by anodophilic and methanogenic bacteria. Then the model was modified to obtain dynamic model which simulate the production of electricity and hydrogen rapidly and effortless. This model assumed that the acetate is the only organic substance in the feed wastewater and both anodophilic and methanogenic bacteria population are present. For the simplicity the modelling of biofilm growth, biofilm is splitted to two different layers with assumption that the distribution of microorganisms in each layer is homogeneous. The first biofilm layer which grow on the anode is considered to be composed of anodophilic and acetoclastic methanogenic microorganisms. Anodophilic microorganisms are able to use the anode as electron acceptor while acetoclastic methanogenic microorganisms produce methane. The involvement of an intracellular mediator was assumed in the mechanism of charge transfer from acetate to the anode. The second biofilm layer which grow on the cathode is considered be composed of hydrogenotrophic methanogens to microorganisms, which transform hydrogen produced to methane.

The main assumptions to construct the model are the following [14, 15]:

1. Acetate is the only organic substance in the feed wastewater.

2. The acetate is homogenously mixed in the anodic cell and the change of concentration in the biofilm is ignored.

3. Microbial populations is equally spread in the biofilm and retention of biomass because of biofilm evolution is illustrated.

4. Intracellular electron transfer mediator is considered to be constant in anodophilic microorganisms.

5. No Biomass growth is considered in the anodic liquid as hydraulic retention times used for MEC operation is very short.

6. Immediate release of produced gases.

7. Instant gas transfer from liquid to gas phases is assumed.

8. Adjustment pH and temperature to keep them constant during the operation.

a) Microbial populations

Three microbial populations are responsible for acetate and intracellular mediator conversion as follows:

1. Anodophilic microorganisms:
$$C_2H_4O_2 + 2H_2O + 4 M_{ox}$$

$$+ 2H_2O + 4 M_{ox} \qquad 4 M_{red} + 2CO_2$$
$$4 M_{red} \longrightarrow 4 M_{ox} + 8e^{-} + 8H^{+}$$

Where M_{red} and M_{ox} are anodophilic intracellular mediator in the reduced and oxidized forms, respectively.

2. Acetoclastic methanogenic microorganisms:

 $C_2H_4O_2 \longrightarrow CH_4 + CO_2$

3. Hydrogenotrophic methanogenic microorganisms:

$$CO_2 + 4H_2 \longrightarrow CH_4 + 2H_2O$$

b) Material balances

Material balances equations for continuous flow MEC with equal inlet stream and outlet stream flow rates are:

$$\frac{dA}{dt} = -q_a x_a - q_m x_m + D(A_0 - A)$$
(2.1)

$$\frac{dt}{dt} = -q_a x_a - q_m x_m + D(A_0 - A)$$
(2.1)
$$\frac{dx_a}{dt} = \mu_a x_a - K_{da} x_a - \alpha_1 x_a$$
(2.2)

$$\frac{dx_m}{dt} = \mu_m x_m - K_{dm} x_m - \alpha_1 x_m \tag{2.3}$$

$$\frac{dx_h}{dt} = \mu_h x_h - K_{dh} x_h - \alpha_1 x_h \tag{2.4}$$

Where the acetate concentration in the feed stream is A_0 and acetate concentration in the anodic compartment is A in $[mg-A L^{-1}]$; the concentration of anodophilic, acetoclastic, and hydrogenotrophic microorganisms are x_a , x_m , and x_h respectively in [mg-x L⁻¹]; the time is t in [d]; acetate consumption rates of the anodophilic and acetoclastic microorganisms are q_a, and q_m respectively in [mg-A mg-x⁻¹ d^{-1}]; the growth rates of anodophilic, acetoclastic, and hydrogenotrophic microorganisms are μ_a , μ_h , and μ_m respectively in $[d^{-1}]$; the dilution rate is D in $[d] = F_{in}/V$, the feed flow is F_{in} in [L/d], the anodic compartment volume is V in[L]; decay rate is K_d in [d⁻¹], while the dimensionless biofilm retention constants for layers 1 and 2 are a₁, a₂ respectively.

According to the two phase biofilm growth model, formation and retention of biofilm in each layer is considered [14]. The biofilm retention constant can be calculated from the following equation assuming stationary phase as thickness of the biofilm reaches the steady state [14, 15].

$$\alpha_1 = \frac{(\mu_a - k_{da})x_a + (\mu_m - k_{dm})x_m}{(x_a + x_m)} \text{ if } x_a + x_m \ge x_{max1} \quad (2.5)$$

$$\alpha_1 = 0$$
 otherwise

 α_2

 α_2

$$= \mu_m - K_{dh} \text{ if } x_h \ge x_{max2}$$
(2.6)
= 0 otherwise

Where the maximum possible biomass concentration of the biofilm layer 1 or 2 is (X_{max}) in [mg-x L⁻¹].

The rate of methane production in biofilm layers 1 and 2 can be calculated from the following balance equations:

$$Q_{CH4-1} = Y_{CH4} q_m x_m V$$
(2.7)

$$\mathbf{Q}_{\mathrm{CH4-2}} = \mathbf{Y}_{\mathrm{H2/CH4}} \,\mathbf{Y}_{\mathrm{h}} \,\boldsymbol{\mu}_{m} \,\mathbf{x}_{\mathrm{h}} \,\mathbf{V} \tag{2.8}$$

For MEC, the rate of hydrogen production is calculated from the following equation:

$$Q_{H2} = Y_{H2} \left(\frac{l_{MEC}}{m F} \frac{R T}{P} \right) - Y_h \mu_h x_h V$$
(2.9)

Where the methane yield is Y_{CH4} in [mL-CH₄ mg-A⁻¹];

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the dimensionless cathode efficiency is Y_{H2} ; the yield of methane from hydrogen is $Y_{H2/CH4}$ in[mL-CH₄ mg-H₂⁻¹]; the MEC current is I_{MEC} in [A]; the yield rate for hydrogen consuming methanogenic microorganisms is Y_h in [L mg-x⁻¹ d⁻¹]; the Faraday constant is F in [A d mole⁻⁻¹]; the ideal gas constant is R in [L atm K⁻¹mol⁻¹]; the MEC pressure is P in [atm]; while the MEC temperature is T in [K].

• Intracellular Material Balances of Anodophilic Microorganisms

For each anodophilic microorganism balance equations as following:

$$\begin{split} \mathbf{M}_{\text{Total}} &= \mathbf{M}_{\text{red}} + \mathbf{M}_{\text{ox}} \\ \frac{dM_{ox}}{dt} &= -Y_M \ q_a + \frac{\gamma \ I_{MEC}}{V \ X_a \ mF} \end{split} \tag{2.10}$$

Where the oxidized mediator fraction per anodophilic microorganism is M_{ox} in [mg-M mg-x⁻¹]; the reduced mediator fraction per each anodophilic microorganism is M_{red} in [mg-M mg-x⁻¹]; the total mediator fraction per microorganism is M_{Total} in [mg-Mmg-x⁻¹]; the MEC current is I_{MEC} in [A]; the mediator yield is Y_M in [mg-M mg-A⁻¹]; the mediator molar mass is g in [mg-M mol med⁻¹], while the number of electrons transferred per mol of mediator is m in [mol-e⁻ mol med⁻¹].

c) Kinetic Equations

Kinetics equations using multiplicative Monod are:

$$\mu_a = \mu_{maxa} \frac{A}{K_{Sa} + A} \frac{M_{OX}}{K_{M} + M_{OX}}$$
(2.12)

$$\mu_m = \mu_{maxm} \frac{A}{Ksm+A} \tag{2.13}$$

$$q_a = q_{maxa} \frac{A}{Ksa + A} \frac{M_{OX}}{K_M + M_{OX}}$$
(2.14)

$$q_m = q_{maxm} \frac{A}{Ksm+A} \tag{2.15}$$

Where the maximum growth rate is μ_{max} in $[d^{-1}]$; the maximum acetate consumption rate is q_{max} in [mg-A mg-x⁻¹d⁻¹], while the half-saturation (Monod) constant is K in [mg-A L⁻¹mg-M L⁻¹].

d) Electrochemical equations

The current can be calculated from the following algebraic equation whose derivation can be found in Pinto et al. (2010).

$$I_{MEC} = \frac{E_{CEF} + E_{applied} - \frac{RT}{mF} \ln\left(\frac{M_{Total}}{M_{red}}\right) - \eta_{act,c}(I_{MEC})}{R_{int}} (2.16)$$

Where the counter electromotive force is E_{CEF} in (V); the electrode potentials is $E_{applied}$ in (V); activation loss as a result of activation energy and electrochemical reactions is $\eta_{act,c}$ in (V) and the internal resistance is R_{int} in (Ω) can be calculated from the following equation.

$$\mathbf{R}_{\text{int}} = \mathbf{R}_{\text{min}} + (\mathbf{R}_{\text{max}} - \mathbf{R}_{\text{min}}) \boldsymbol{e}^{-K_R X_a}$$
(2.17)

Where the lowest observed internal resistance is R_{min} in $[\Omega]$; the highest observed internal resistance is R_{max} in $[\Omega]$; the constant which determines the curve steepness is K_R in [L mg-x⁻¹].

III. METHODOLOGY

This section will be concerned with developing a comprehensive simulation methodology for MEC model. Figure 2 summarizes the simulation algorithm for MEC model. The simulation study of MEC models have been carried out by using MATLAB differential algebraic solver "ode15s". In the beginning all parameters, DAE, initial

conditions, time of process and electrode potential were defined. Then the model was solved. The output results was considered as base case. After that sensitivity analysis was carried out to determine which parameters have the greatest effect on model, the sensitivity study was conducted on all the parameters of MEC one by one by changing one of the parameter, while the other parameters were left without any change. The sensitivity results were utilized to validate another model with some modification in parameters. Also sensitivity analysis results are used for model reduction of the DAE and obtain simplified equation. Finally the electric potential required to maximize energy productivity is found out.



Figure 2: Algorithm for MEC model development

IV. RESULTS AND DISCUSSION

A. CASE STUDY

The previous mentioned model was applied on a case study of Pinto [14-16] with adjusting some parameters to verify the model, the initial conditions in the case study was 1800; 100; 100; 100 and 0.03 mg/l of substrate, anodophilic, acetoclastic, hydrogenotrophic and oxidized mediator respectively. The following figures are representing the obtained results of different concentrations:

Figure 3a shows the behavior concentration of substrate. It was noticed that a fast decrease of the concentration of the substrate (S) happens at the first duration of the reaction until 1.2 day when the concentration became 630 mg/l, as it was decomposed by hydrogenotrophic microorganisms. Then concentration gradually increased for the rest of experiment time until it reached 900 mg/l at the end of the experiment, as the rate of decomposition decreases.

Figure 3b shows the behavior of anodophilic (xa) microorganisms. It was noticed that a fast increase in the concentration of anodophilic microorganisms (xa) happens in the first day of the experiment until concentration reached 400 mg/l, then the concentration increase slows down until it became constant in the fifth day at the concentration 510 mg/l till the end.

Figure 3c shows the behavior of acetoclastic (xm) microorganisms.



Published By: Blue Eyes Intelligence Engineering 1726 & Sciences Publication It was noticed that the concentration of acetoclastic microorganisms (xm) increased rapidly at the start of the experiment until 1.2 day and reached 130 mg/l, then it started to decrease slowly until it reached 0.188mg x/l in the eighth day and remained constant at this value for the rest of experiment. The low population of the acetoclastic methanogenic microorganisms means that the rate of methane formation was reduced in the anode biofilm layer 1 and the rate of formation of H₂ at cathode layer 2 was increased.

Figure 3d shows the hydrogen production rate. It was noticed that the rate increased rapidly until it reached 200 ml/d on the first day, then decrease until it reached 170 ml/d in the sixth day and became constant until the end of the experiment at an applied voltage of 1.3 V.



Figure 3: (a) Behavior of substrate concentration for base case and model reduction, (b) Behavior of Anodophilic concentration for base case and model reduction, (c) Behavior of Acetolastic concentration for base case and model reduction, (d) Behavior of H₂ production for base case and model reduction.

B. Sensitivity analysis on MEC parameters

Sensitivity analysis of the fed-batch MEC reactor was conducted by Azwar [17, 18] who studied the effect of the change in different parameters on hydrogen production rate and the MEC current $I_{\mbox{\scriptsize MEC}}.$ Results are summarized as follows.

Effect of the maximum growth rate of the hydrogenotrophic microorganism $(\mu_{max, h})$ on the I_{MEC} current and the hydrogen production rate was studied. In this study the maximum growth rate of the hydrogenotrophic microorganism was varied between $0.3 \le \mu_{\text{max, h}} \le 0.9$ (d-1). It was noticed that maximum growth rate of the hydrogenotrophic microorganism is directly proportional with the rate of hydrogen production and it has noticeable effect on I_{MEC} current.

Then the change in initial concentration of the anodophilic microorganisms (x_{ao}) between 0.1, 0.5, 1.0, and 1.5 mg/l, effect on the hydrogen production rate and the I_{MEC} current was studied and the study showed that the initial concentration has a great influence on hydrogen production rate and the $I_{\mbox{\scriptsize MEC}}$ current. As its concentration increases the rate of hydrogen production and the I_{MEC} current increases since the start of analysis until 2nd day.

After that the effect of change in initial concentration of the hydrogenotrophic microorganism in the range from $1 \le x_{ho} \le$ 15mg/l was studied on the performance. It was noticed that the high initial concentration of hydrogenotrophic microorganism leads to high hydrogen production rate, on the other hand it has only minor effect on IMEC.

The effect of change in anodic compartment volume was studied, the results showed that increasing the volume of anodic compartment increases the hydrogen production rate but it does not have any effect on current I_{MEC} .

The Effect of change in the maximum growth rate $(\mu m,m)$ by acetoclastic methanogenic microorganism was studied in the range from 1.5 \leq $\mu_{m,\ m}$ \leq 3.0 h and the study showed that maximum growth rate only has effect in the initial start of the process and minor effect on current IMEC and the rate of hydrogen production.Sensitivity analysis was conducted by Dudley [19] on the main parameters of MEC batch-cycle reactor, and it was found that $\mu_{max,\,a},\,q_{max,\,a},\,K_{S,a},\,K_{M},$ and Y_{M} have greatest effect on the current density in the study.

The increase of $\mu_{max,a}$, $q_{max,a}$, and Y_M , increases the current density. Specially in the beginning of the process the effect of $q_{max,a}$, and Y_M was very noticeable. The effect of Y_M decays with the time. On the other hand the increase of $q_{max,a}$, causes the increase of current density in the first 25 hours then it causes it to decrease. In this paper, a preliminary sensitivity analysis on the model, operating and design parameters was conducted on all the parameters one by one by changing one of the parameter, while the other parameters were left without any change. This analysis used the local relative sensitivity analysis method [20], to determine the change in calculated hydrogen production rate as a ratio to the changes in the parameters. With utilizing the following equation for each parameter, x_i

$$T_j = \frac{P(t, x_j + \delta x_j) - P(t, x_j)}{\delta x_j} * \frac{x_j}{P(t, x_j)}, j = 1, \dots, 6 \quad (2.18)$$

Where the time dependent sensitivity is T_i for the parameter j; the value of parameter j is x_i ; the change in x_i is x_i ; and the hydrogen production rate is P. the step of the change in this study is $\delta x = 0.01 x j$.

1. Model Parameters

1.1. Maximum growth rate

The results of sensitivity analysis for the maximum growth rates and reaction rates effect on hydrogen production are shown in Figure 4a it is clear that anodophilic, hydrogenotrophic microorganism maximum growth rates $(\mu_{m,a} \text{ and } \mu_{m,h})$ and $\mbox{ anodophilic microorganism maximum }$ reaction rate (qmax,a) are effectual parameters, whereas acetoclastic methanogenic microorganism maximum growth rate (µm,m) and acetoclastic methanogenic microorganism maximum reaction rate $(q_{max,m})$ are not affecting on hydrogen production.

1.2. Half-rate

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The results of sensitivity analysis for the half rates effect on hydrogen production are displayed in Figure 4b it is clear that the curve steepness (K_R) and mediator half-rate constant (K_M) are effectual parameters, whereas the anodophilic (KSa),



acetoclastic (K_{Sm}) methanogenic microorganism half-rate constant, the anodophilic (K_{da}) and acetoclastic (K_{dm}) methanogenic microorganism microbial decay rates and are not affecting on hydrogen production.

1.3. Operating Parameters (Electrode potentials and Mediator fraction)

The results of sensitivity analysis for operating parameters on hydrogen production are displayed in Figure 4c it is clear that applied voltage (E_{app}), MEC temperature (T) and pressure (P) are effectual parameters, whereas total mediator weight percentage (M_{Total}), incoming flow (F_{in}) and counter electromotive force (E_{CEF}) are not affecting on hydrogen production.

2. Design Parameters

The results of sensitivity analysis for anodic compartment volume and anode surface area effect on hydrogen production are displayed in Figure 4d it is clear that anodic compartment volume and anode surface area (V and A) are effectual parameters, due to the increase of organic compounds in the system available.



Figure 4: Relative sensitivity of H2 production with respect to: (a) maximum growth rates and reaction rates (b) half rate and decay rates, (c) operating parameters, (d) Design Parameters.

C. MEC Validation

After the sensitivity analysis study the effectual parameters of MEC were defined, this results were utilized in order to fit the data prediction model of Pinto [14] with experimental results of one batch acetate fed MEC by Hongqiang [21].

Some of the parameters in Pinto [14] model were adjusted as shown in Table 1. While the remaining parameters were kept the same as shown in appendix. The obtained simulation results were similar to the actual experimental results.

The results of simulation were compared to the experimental data as shown in Figures 4 and 5. It was noticed that the maximal current reached at 0.013A and the H₂ production rate reached 110.9 ml/d.



Figure 4: Model validation of MEC current based of Hongqiang data



Figure 5: Model validation of H2 production rate based of Hongqiang data

D. Model Reduction

The sensitivity results were utilized to simplify the MEC equations as follow:

Assume that k_{da} , k_{dm} , k_{dh} , k_{sa} and k_{sm} equal zero. The following simplified equations (6.1 -6.14) can be obtained:

$$\mu_{a} = \mu_{\max a} \frac{M_{OX}}{K_{M} + M_{OX}} \tag{6.1}$$

$$\mu_{\rm m} = \mu_{\rm maxm} \tag{6.2}$$

$$q_{\rm a} = q_{\rm maxm} \tag{6.3}$$

$$q_{a} = q_{\max a} \frac{q_{A}}{K_{M} + M_{OX}}$$
(6.3)

$$q_a = q_{maxm}$$
(6.4)
If $x_c + x_m < x_{max}$

$$M_{a} = M_{ox}$$

$$\frac{dt}{dt} = -q_{\max a} \frac{1}{K_M + M_{OX}} x_a - q_{\max m} x_m + D(A_0 - A) \quad (6.5)$$

$$\frac{dx_a}{M_{OX}} = 0 \quad (6.5)$$

$$\frac{d\mathbf{x}_{a}}{dt} = \mu_{\max a} \frac{\mathbf{x}_{OX}}{\mathbf{x}_{M} + \mathbf{M}_{OX}} \mathbf{x}_{a}$$
(6.6)

$$\frac{dx_m}{dt} = \mu_{maxm} x_m; x_m = x_{m,0} \exp(\mu_{maxm} t)$$
(6.7)

$$\frac{dt}{dt} = \mu_{\text{maxh}} x_{\text{h}}; x_{\text{h}} = x_{\text{h},0} \exp(\mu_{\text{maxm}} t)$$
(6.8)

If
$$x_h < x_{max,2}$$
, $x_h = x_{max,2}$ if $x_h > x_{max,2}$

$$0 = -Y_M q_{maxa} \frac{M_{OX}}{KM + M_{OX}} + \frac{\gamma I_{MEC}}{\gamma X_a m F}$$
(6.9)

From this equation;

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d/

$$I_{MEC} = V x_{a} m F Y_{M} q_{maxa} \frac{M_{OX}}{\gamma(KM + M_{OX})}$$

a m F Y_M q_{maxa} $\frac{1}{\gamma}$ < 0.2909V x_a Y_M q_{maxa} (6.10)

$$\frac{dx_a}{dt} = \gamma \mu_{\text{maxa}} I_{\text{MEC}} / (V \text{ m F } Y_M q_{\text{maxa}})$$
(6.11)

If
$$x_a + x_m > x_{max1}$$

$$\frac{\mathrm{d}\mathbf{x}_{a}}{\mathrm{d}\mathbf{t}} = \frac{\mu_{\max} - \mu_{\max}}{\mathbf{x}_{\max,1}} \mathbf{X}_{a} \mathbf{X}_{m}$$
(6.12)

$$\frac{dx_{m}}{dt} = -\frac{\mu_{maxa} - \mu_{maxm}}{x_{max,1}} x_{a} x_{m}$$
(6.13)

And its solution

And

$$\frac{x_{a}}{x_{max1}} = \frac{x_{a0} e^{(\mu_{maxa} - \mu_{maxm})t}}{(x_{max1} - x_{a0}) + x_{a0} e^{(\mu_{maxa} - \mu_{maxm})t}}$$
(6.14)

Validation for the simplified equations was accomplished on the case study. By implementing these equations, the results in Figure 3 were obtained. It is noticeable that the reduced model results are exactly the same as the base case model results.

MEC optimization to maximize energy gain Е.

In this section, study of maximization of hydrogen production and minimization of energy requirements by selecting the optimum operating conditions was conducted.

The easiest method to increase the hydrogen production (Q_{H2}) is applying higher energy to the cell as hydrogen production is directly proportional to energy applied (E_{app}) . Unfortunately this will not maximize MEC energy productivity. As MEC productivity function is the difference between the H₂ energy (in watts) and the applied energy.

MATLAB function fminsearch which is based on Nelder Mead simplex method was used to obtain the maximum MEC productivity by manipulating the applied energy. The optimization results showed that maximum MEC productivity is 0.0024 W, which was obtained when the produced energy as hydrogen was 0.0143 W and the applied energy was 0.0119 W and potential of 1.0105 V.

V. CONCLUSIONS

In this study MEC model was studied and validated. Then sensitivity analysis of this model was conducted, and the effective parameters were defined, It was noticed that the parameters which has the highest effect on the cell are $\mu_{m,a}$, $\mu_{m,\,h},\,q_{m,a}$, $K_M,\,K_R,\,T,\,P,\,V,\,A$ and $E_{app}.$ These results were utilized to reduce the model and obtain simple equations. These simple equations were used for validating experimental results. After this optimization of the operating parameters of MEC was accomplished. In the future work combination of (MEC) and microbial fuel cell (MFC) will be studied.

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0.6 V	300 mL	0 mL d ⁻¹	$0.01 \ mL-H_2mg-x^{-1} \ d^{-1}$	0.77	0.5 d ⁻¹	-0.034 V	0.0065 m ²	0.2 L mg-x-1	15 Ω	400	5460

Table 1: Changing parameter for validation

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