A Simple Microbial Fuel Cell Model for Improvement of Biomedical Device Powering Times

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***Abstract*— This study describes a Matlab based Microbial Fuel Cell (MFC) model for a suspended microbial population, in the anode chamber for the use of the MFC in powering biomedical devices. The model contains three main sections including microbial growth, microbial chemical uptake and secretion and electrochemical modeling. The microbial growth portion is based on a Continuously Stirred Tank Reactor (CSTR) model for the microbial growth with substrate and electron acceptors. Microbial stoichiometry is used to determine chemical concentrations and their rates of change and transfer within the MFC. These parameters are then used in the electrochemical modeling for calculating current, voltage and power. The model was tested for typically exhibited MFC characteristics including increased electrode distances and surface areas, overpotentials and operating temperatures. Implantable biomedical devices require long term powering which is the main objective for MFCs. Towards this end, our model was tested with different initial substrate and electron acceptor concentrations, revealing a four-fold increase in concentrations decreased the power output time by 50%. Additionally, the model also predicts that for a 35.7% decrease in specific growth rate, a 50% increase in power longevity is possible.**

I. Introduction

Microbial Fuel Cells (MFC) have been recognized as a promising technology capable of using microorganisms to break down organic substrates for the generation of electricity. Typically they are composed of two-chambers with bacteria, electrode and substrate in the anode chamber and a chemical electron acceptor and electrode in the cathode chamber, separated by a proton exchange membrane (PEM) as illustrated in Fig. 1 [1].

Bacteria will break down the organic substrate, releasing electrons to a mediator or intermediary electron acceptor and any other chemicals including Hydrogen atoms. The mediator transfers the electron to the anode electrode where it can pass through an electrical circuit and appear in the cathode electrode. The hydrogen atom diffuses through the membrane, and unites with the electron and the final electron acceptor in the cathode chamber as shown in Fig. 1 [2].

Implantable biomedical devices require battery replacement after several years, often at a cost and risk to patients due to the need for surgery. Recharging Radio Frequency (RF) technologies are often uncomfortable and require regular mains power plug in. If the organic substrates were taken from the blood or through injection, implantable MFCs could provide a perpetual battery for biomedically implantable devices [3].

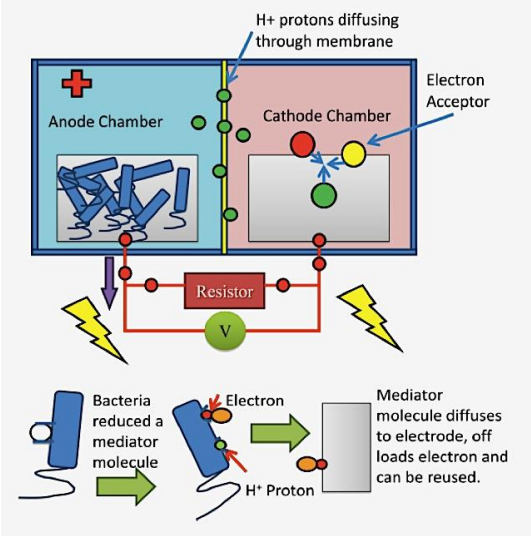

Figure 1. Internal Operation of a MFC.

A study by Rezaei et al found that increased substrate particle size increases power longevity however the power output time for this study was only ~25 days, suggesting that improvements could be made [4]. To increase power source output time, it is often suggested to increase capacity and decrease the rate of power usage.

In this paper, a Matlab based MFC model is shown for suspended cells, focusing on the anode chamber. The model incorporates substrate and electron acceptor limited microbial growth, calculation of chemical concentrations and fundamental electrochemical calculations for electrical outputs.

The model is tested to ensure it imitates certain MFC behaviours. The model is then tested with increasing substrate and electron acceptor conditions and decreased microbial growth rate, and assessing the affect on power output time. The model predicts that for a 35.7% decrease in specific growth rate, a 50% increase in power longevity is possible and that for a fourfold increase in initial concentrations, a 50% decrease in power longevity is observed.

II. Modeling Method

The model is broken up into three main sections, which takes into account microbial growth, 1) production secretion 2) chemical concentrations and 3) electrochemical reactions. Each has its own set of calculations, which contributes to the

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final calculation of outputs including voltage, current and power. All calculations and plotting is done with Mathworks Matlab.

A. Substrate Limited Growth of Bacteria in a Batch Chemostat

Microbial growth is calculated based on a Continuously Stirred Tank Reactor (CSTR) model, which takes into account inflows and outflows of bacteria and chemicals [5-6]. The calculation of bacterial cells is as follows:

$$\frac{\mathbf{dC_c}}{\mathbf{dt}} = \boldsymbol{\mu_{max}}\mathbf{C_c}\frac{\mathbf{C_1}}{\mathbf{K_1+C_1}} - \mathbf{K_d}\mathbf{C_c} \quad (1)$$

Where C_c is the concentration of cells (grams/litre), μ_{max} is the maximum specific growth rate (grams/liter/hour), c_1 is the concentration of substrate (grams/liter), K_1 is the Half-Velocity Constant of limiting substrate (Dimensionless) and K_d is the cell death constant. The degradation of substrate is found by:

$$\frac{dC_1}{dt} = -\frac{1}{Y_1}\cdot\mu_{max}\cdot C_c\cdot\frac{C_1}{K_1+C_1} \quad (2)$$

Y_1 is the substrate to cell yield coefficient. The use of electron acceptor can be calculated by:

$$\frac{dC_2}{dt} = -\frac{1}{Y_2}\cdot\mu_{max}\cdot C_c\cdot\frac{C_1}{K_1+C_1} \quad (3)$$

Y_2 is the electron acceptor to cell yield coefficient. Equations (1) to (3) are solved simultaneously with Matlab's 'ode23' differential equation solver.

B. Product Secretion and Chemical Concentrations through Microbial Stoichiometry

Microbial stoichiometry allows us to understand the flow of different amounts of chemicals throughout the MFC being up taken and secreted by bacteria, both to monitor the chemicals and for their use in other parts of the model [7-8].

We first have a synthesis equation, describing the creation of a microbial cell from substrate acetate as follows:

$$5C_2H_3O_2 + 2NH_3 + 26H^+ + 26e^- \rightarrow 2C_5H_7O_2N + 6H_2O \quad (4)$$

The second equation, which describes the microbial cell's reactions, including electron transfer to electron acceptor, whilst living, is the respiration equation as follows:

$$C_2H_3O_2 + 2H_2O + 7Fe^{2+} \rightarrow 2CO_2 + 7H^+ + 7Fe^{3+} \quad (5)$$

These two equations are then linked via yield terms describing how many microbial cells are created per amount of substrate, and combined together. The third equation is the endogenous respiration equation, which describes a microbial cells death and breakdown of the cell as follows:

$$C_5H_7O_2N + 8H_2O \rightarrow NH_3 + 5CO_2 + 20H^+ + 20e^- \quad (6)$$

Yield terms and endogenous death rates used in the model are based on S. oneidensis modelling in a chemostat reactor conducted by [9]. Each chemical species in equations (4) to (6) has its own differential equation of the form:

$$\frac{dU_i}{dt} = Y_{Uri}C_c r_g + (Y_{Udi}K_d C_c) \quad (7)$$

Where U_i is the concentration of the ith chemical species, Y_{Uri} is the stoichiometric coefficient of the ith chemical species during respiration, C_c is the microbial concentration, r_g is the microbial growth rate, and determines the chemical reaction rate, Y_{Udi} is the stoichiometric coefficient of the ith chemical species during death and K_d is the death constant, representing the proportion of the microbial population that dies [7-8]. This forms a system of differential equations which is solved and plotted in Matlab, using the 'ode23' function.

The calculation of current is calculated using the Butler-Volmer equation as follows:

$$i = i_0\left[\frac{C_0}{C_0^*}\exp\left(\frac{-\alpha\eta F}{RT}\right) - \frac{C_r}{C_r^*}\exp\left(\frac{(1-\alpha)\eta F}{RT}\right)\right] \quad (8)$$

Where i_0 is the exchange current density, i is the current density (A/m^2), C_0 is the concentrations of the oxidized chemical species (moles), C_0^* is the initial concentration of oxidized chemical species (moles), α is the charge transfer coefficient (dimensionless), η is the activation overpotential (volts), F is the Faraday constant (electric charge per mole), R is the universal gas constant (JK^{-1}mol^{-1}), T is the absolute temperature (Kelvin), C_r is the concentration of reduced chemical species (moles/liter) and C_r^* is the initial concentration of reduced chemical species (moles/liter). Chemical concentrations are calculated within the microbial stoichiometry section, whilst the overpotentials are further discussed [10-12].

The cell voltage is calculated from the following equation:

$$E_{cell} = (E_A - \eta_{an-act} - \eta_{an-conc}) + (E_C - \eta_{cath-act} - \eta_{cath-conc}) - \eta_{ohm} \quad (9)$$

E_A is the anode electrode voltage, η_{an-act} is the anode activation overpotential, $\eta_{an-conc}$ is the anode concentration overpotential, E_C is the cathode electrode potential, $\eta_{cath-act}$ is the cathode activation overpotential, $\eta_{cath-conc}$ is the cathode concentration overpotential and η_{ohm} is the sum of the internal and external ohmic resistances [10].

The activation overpotentials can be calculated by the Nernst equation as follows:

$$\eta_{act} = \frac{RT}{n\alpha F}\ln\left(\frac{i}{i_0}\right) \quad (10)$$

Where R is the universal gas constant (JK^{-1}mol^{-1}), F is the Faraday constant (Cmol^{-1}), T is the absolute temperature (Kelvin), i is the current density (A/m^2), i_0 is the exchange current density (A/m^2) taken as 2 x 10^{-4} A/m^2 [10], n is the number of moles involved in the reaction and α is charge transfer coefficient taken as 0.5 [11-12].

The ohmic resistance for the solution is calculated by $\eta_{ohm} = -i \times R_{sol}$ where R_{sol} is the solution resistance between anode and cathode electrodes and is calculated by $R_{sol} = (d_m/k_m) + (d_c/k_{sol})$ where d_m is the membrane thickness (meters), k_m membrane electrical conductivity (Ohms$^{-1}\Omega^{-1}$),

d_e is the distance between the anode and cathode electrodes (meters), k_{sol} is the solution electrical conductivity (Ohms$^{-1}\Omega^{-1}$) [6].

For simplification, since a chemostat, continuously stirred tank reactor (CSTR) mode is used, concentration overpotentials normally occurring at the bulk solution-electrode interface are set to zero, and concentration overpotentials are not calculated. Additionally, we focus on the reactions occurring in the anode chamber, and therefore assume a value for the cathode reactions as follows [6, 10]:

$$V_c = E_C - \eta_{cath-act} = 0.68V \quad (11)$$

Leaving our equation as:

$$E_{cell} = (E_A - \eta_{an-act}) + V_c - \eta_{ohm} \quad (12)$$

The anode electrode voltage is again calculated by the Nernst equation as follows:

$$E_A = E^0 - \frac{RT}{nF} lnQ \quad (13)$$

Q is the reaction quotient calculated by $Q = C_rC_h/C_o$ where C_r is the concentration of reduced mediator; C_h is the hydrogen concentration and C_o is the oxidized mediator concentration [10-12].

III. Testing and Results

When the model was programmed with Matlab, testing was then conducted on the Microbial Fuel Cell to ensure its outputs matched previous studies. Following this, variables for extending the power longevity of MFCs were implemented and tested with the model.

A. MFC Properties

To test the model, different conditions from previous MFC studies were placed on our MFC model. The first test is the increasing of distances between electrodes, which creates a drop in power density [13]. Typically a change in operating temperatures should also lead to a higher power density [14]. Thirdly, an increased electrode surface area has in the past provided a higher current output [13]. Finally, overpotentials should be calculated, which have particular effects on the overall outputs [1-2].

A change in electrode distance from 1cm to 10cm resulted in an increased internal resistance of the simulated MFC from 20Ω to 23.61Ω. This is primarily composed of a change in resistance from 0.4Ω to 4Ω due to a greater amount of solution between the electrodes. There is also a greater distance for the compounds to travel from the anode electrode, through the membrane and to the cathode electrode. This observation is consistent with previous literature, with a decreased maximum power density of 0.72 mW/m^2 to 0.61 mW/m^2.

The operating temperature of the model was further tested to determine if changes were similar to published literature. Increases from 20°C to 40°C resulted in a decrease in anode voltage of 1.4mV, giving a decrease power density of 0.002mW/m^2. The effect the temperature has on the anode is consistent, though this is not the case for the power density.

Increases in electrode surface areas greatly increase the space for electrons to be transferred to and capture. Graphite felt was chosen for its large surface area of typically 610cm^2, whilst a reticulated vitreous carbon electrode has a smaller surface area of 61cm^2. Consistent with previous data, the maximum current for the reticulated vitreous carbon was calculated to be 0.88mA, whilst for graphite felt it was 0.08mA.

The various overpotentials, excluding concentration overpotentials, were calculated as per the equations in the Methods section, at the maximum current point. Fig. 2 shows the polarisation curve for each of the overpotentials.

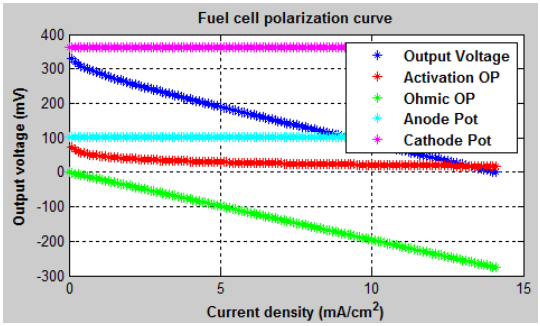

Figure 2. Calculated Overpotentials for the MFC Model.

B. Decreased Growth and Reaction Rates

When the maximum specific growth rate parameter of the model was altered from 0.28 cells per hour, to 0.1 cells per hour, the maximum amount of cells calculated to be within the MFC changed from 0.08 moles per litre, to 0.06 moles per litre and the time at which each of these peaks occurred was 15.48 hours and 32.72 hours respectively. This result is also reflected in the concentrations of substrate and electron acceptor for the faster growth rate, whereby the bacteria consumed the substrate and electron acceptor faster than with the slower growth rate. Data is not shown.

This increase in growth time translates to an increase in power longevity. Measuring the current output, we noted that the peak for the faster growth rate is 10.11mA at 1.24 hours, and for the slower growth rate 11.47mA at 3.21 hours. Likewise, the time at which the current drops below 2mA for the faster growth rate is less than 5 hours, whereas for the slower growth rate it is greater than 10 hours (Fig. 3.)

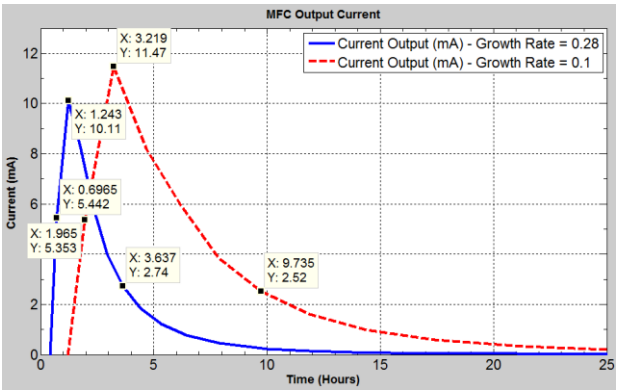

Figure 3. MFC Calculated Output Current for a growth rates of 0.28 and 0.1 cells per hour. Slowing the growth rate increases power output time.

C. Increased Initial Conditions

When the initial concentrations of substrate and electron acceptor were varied from between 0.03mM for substrate and 0.02mM for the electron acceptor to 2, 3 and 4 times the original amounts, increases in cell concentrations were observed, in shorter amounts of time with each increase. Concentrations of substrate and electron acceptor followed a similar trend, being consumed faster with each increase. Most importantly, the output current both decreased in its peak value and power longevity with increases in initial concentrations (Table 1).

TABLE I. INITIAL CONCENTRATIONS TEST RESULTS

Initial Conc.		Max Cell Conc. (moles per liter)	Power Output Time (Hours)	Max Current (mA)
Substrate (mM)	Electron Acceptor (mM)			
0.03	0.02	0.08	4.43	10.11
0.06	0.04	0.11	1.64	8.19
0.09	0.06	0.14	1.51	7.19
0.13	0.08	0.17	1.47	6.51

IV. DISCUSSION AND CONCLUSION

Testing of our MFC model was generally consistent with laboratory MFC observations. In particular we noted that, increases in electrode distance resulted in decreased power density and increases in electrode surface area resulted in increased power density.

Interestingly, data for the changes in temperature was not entirely consistent with other predicted models. A study by Liu et al found that increases in temperature resulted in increased power densities [14], which is not consistent with our model findings. Closer inspection of their data showed that the drop in power density results from lower temperatures at higher current densities at the cathode electrode.

Temperature affects the Nernst and activation overpotential equations, which indirectly affects the power density through the anode voltage. This resulted in a change in anode voltage and on power density for our model. For simplification, as with many models, our model's focus was on the anode chamber [6, 10], thus our inconsistent decreased power density results.

Plots for electrochemical overpotentials are difficult to generate in real time laboratory based MFCs. Modeling these reactions with well known electrochemistry equations provides both further proof and insight into voltage losses in MFCs. In particular we note that the activation overpotentials appear to have their greatest affect in the lower current densities, but do have an overall affect. We also identified a critical need to lower ohmic overpotentials, which has the single greatest effect on the output of the MFC.

Often when attempting to increase the power longevity of devices, we increase their capacity. In the case of a MFC however, we hypothesized that by increasing the initial concentrations of substrate and electron acceptor in an MFC, the power longevity would be decreased due to the bacteria growing to their maximum population faster. This would deplete their substrate faster. Results from the described model prove this very point. It was found that for a decrease in growth rate of 35.7%, we see an increase in power longevity of over 50%, as well as an increase in peak output current.

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