



Modeling the performance of enzymatic glucose fuel cells



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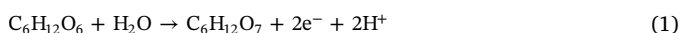
ABSTRACT

A mathematical model is developed to study the transient performance of a mediatorless membraneless enzymatic glucose fuel cell. The concentration profiles of glucose across the cell is seen to decrease across the cell with increasing time indicating the consumption of glucose in the enzyme layer. The concentration of hydrogen ions across the cell is seen to decrease with increasing time indicating the consumption of hydrogen ions at the cathode. The potential drop across the cell is found to play a role in the concentration profiles of hydrogen ions across the cell. The concentration of the enzyme is found to play an important role in determining the glucose concentration and hydrogen ion concentration across the cell. The anodic current density is found to be a strong function of the enzyme concentration. Modeling results are compared with polarization curves from experimental data and found to compare well with experimental data.

1. Introduction

Enzymatic glucose fuel cells have been in the news for quite some time now. These fuel cells use glucose as a fuel and enzymes as biocatalysts to convert chemical energy into electrical energy. Enzymes are proteins that catalyze chemical reactions. Enzymes [1] like glucose oxidase are typically used to oxidize glucose on the anode. Similarly, an enzyme like laccase could be used to reduce oxygen on the cathode. Two basic mechanisms for enzyme electrocatalysis are studied in literature: Direct Electron Transfer (DET) and Mediated Electron transfer (MET) [1]. In DET, the enzyme is immobilized directly on the electrode surface. This allows the electrons to tunnel directly from the electrode surface to the enzyme. However, MET needs a mediator species that shuttles the electrons between the electrode and the enzymes. Very little modeling work is available in the area of enzymatic glucose fuel cell particularly those that study the transport of the species between the anode and the cathode. The following reactions are seen to happen in a glucose fuel cell [2,3]:

At the anode:



At the cathode:



Overall cell reaction:



The maximum theoretical fuel cell potential for a glucose fuel cell is around 1.256 V [2,3]. However, typical operating glucose fuel cells operate at an open circuit potential of 0.7–0.8 V (owing to over potential losses). Scott Barton [1] has looked at the various types of models which can be used to describe enzymatic glucose fuel cells. Basu et al. [2] have modeled the performance of an anion exchange membrane direct glucose fuel cell, where they postulated that the increase in the anionic conductivity of the ionomer and glucose concentration increases the performance of the fuel cell up to a limit. Debika [3] has attempted to model batch type direct glucose cell by considering activation, ohmic and concentration overpotentials. Rubin [4,5] proposed a simple theoretical analytical model to study the performance of an enzymatic membraneless glucose fueled fuel cell with Direct Electron Transfer mechanism. The study of steady state performance of the fuel cell as a function of hydrogen ion concentration across the cell was also carried out. Yin Song [6] has developed a mathematical model to study effect of microelectrode arrays on the performance of enzymatic bio fuel cells. Osman [7] has modeled the performance of bio fuel cell with an air breathing cathode. Annepu [8] had developed a mathematical model to study the performance of a direct glucose fuel cell dividing the fuel cell into five compartments. Rajendran [9] has written a review article which studies the modeling of nonlinear processes in enzymatic biofuel cell. Saranya [10] has developed a mathematical model using homotoperturbation method to solve nonlinear equations in enzymatic glucose fuel cells. Rajendran [11] had developed an approximate

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Nomenclature

C_{H^+}	concentration of hydrogen ions
C_G	concentration of glucose
D_{H^+}	hydrogen ion diffusion coefficient
D_{cG}	diffusion coefficient of glucose
E_T	volume enzyme concentration
L	thickness of the enzyme layer
K_{cat}	kinetic enzyme reaction rate constant for glucose oxidation

K_m	Michaelis Menten constant.
Δv^*	dimensionless voltage drop across the cell
Δv	dimensional voltage drop across the cell
l	distance between anode and cathode
y	stoichiometric coefficient
z	coordinate direction normal to the anode (m)
t	time(min)
K_c	reaction rate constant at the cathode for the oxygen reduction reaction
O_2	concentration of oxygen

analytical solution for nonlinear diffusion equations in a mono enzymatic biosensor involving Michaelis Menten kinetics. Malinidevi [12] had developed a model to study the reaction and diffusion of enzymes immobilized in an artificial membrane. However, there is a lot of study left to be done in the field of enzymatic glucose fuel cells. We have tried to simulate the transient behavior of an enzymatic membraneless, mediatorless glucose fuel cell in this paper.

2. Model development

Fig. 1 shows the schematic of a glucose fuel cell. The glucose is sent in from the anode. The conversion of glucose to hydrogen occurs across the enzyme layer indicated in the schematic. The rate of hydrogen production by the enzyme electrode (amount of hydrogen ions generated per unit time per unit volume) as a function of glucose concentration can be calculated from Michaelis Menten (MM) [4,5] model.

$$G_H = \frac{2V_{max} \cdot C_G}{K_m + C_{C_6H_{12}O_6}} \quad (4)$$

where G_H is the rate of production of hydrogen in the enzyme layer, C_G is the glucose concentration in the enzyme layer, V_{max} is given by $K_{cat}[E_T]$, where $[E_T]$ is the volume enzyme concentration [3,4], and K_m is the Michaelis-Menten constant.

2.1. Model assumptions

1) The glucose fuel cell is modeled as one entity instead of modeling individual components of the fuel cell.

2) The model assumes one-dimensional transport of hydrogen ions across the fuel cell.

3) The model assumes that the reaction of the glucose to form hydrogen occurs only in the enzyme layer (thickness of the enzyme layer is approximately 1mm) [4]. No reaction is assumed to occur at the interface of the substrate with the enzyme layer ($z = 0$). The incoming glucose concentration is assumed to be $1 \text{ mol} \cdot \text{m}^{-3}$. The thickness of the cell is assumed to be approximately 3 mm [4].

4) The model assumes that the unreacted glucose and hydrogen ions diffuse across the cell to the cathode. The unreacted glucose is assumed to react only at the anode and not at the cathode. The oxygen reduction reaction is assumed to take place at the cathode.

5) The model assumes that the transport of glucose is solely by diffusion (the effects of convection are neglected). The effects of the potential drop across the bio fuel cell on glucose transported is considered to be negligible (glucose is not a charged species).

6) The model assumes that both diffusion and migration (potential drop across the cell) play a role in the transport of hydrogen ions across the cell.

7) The effect of potential on the reaction kinetics at the anode and cathode is neglected.

8) The product of the rate constant for the cathodic reaction and oxygen concentration at the cathode was assumed to be a constant (i.e. the cathodic reaction is only a function of the hydrogen ion concentration at the cathode).

2.2. Transport equations

The transport equations for the glucose species across the cell is given by

$$\frac{\partial C_G}{\partial t} = D_{cG} \frac{\partial^2 C_G}{\partial z^2} - \frac{K_{cat} [E] \cdot C_G}{K_m + C_G}, \text{ for all } z \quad (5)$$

where K_{cat} is the rate constant for the glucose reaction in the enzyme layer, K_m is the Michaelis-Menten constant, C_G is the concentration of the glucose in the enzyme layer, $[E]$ is given by $L \cdot [E_T]$ where L is the thickness of the enzyme layer and E_T is the volume enzyme concentration [4,5].

The boundary conditions for the transport of glucose across the cell are given by

$$\text{At } z = 0, C_G = 1.0 \text{ mol} \cdot \text{m}^{-3} \text{ (for all } t) \quad (6)$$

$$\text{At } z = l, \frac{\partial C_G}{\partial z} = 0.0 \text{ mol} \cdot \text{m}^{-3} \text{ (for all } t) \quad (7)$$

The cell is initially filled with glucose solution, therefore, entire model domain is taken at a constant concentration value. Thus, the initial condition is simply given by

$$\text{At } t = 0, C_G = 1.0 \text{ mol} \cdot \text{m}^{-3} \text{ (for all } z) \quad (8)$$

Eq. (5) studies the concentration of glucose across the cell with the second term on the RHS indicating the glucose consumption term according to the MM (Michaelis Menten) model. Eq. (7) indicates that the flux of glucose does not change with distance at $z = l$.

The transport equations of the hydrogen ions across the cell is given by

$$\frac{\partial C_{H^+}}{\partial t} = D_{H^+} \frac{\partial^2 C_{H^+}}{\partial z^2} - y D_{H^+} \frac{\Delta v^*}{l} \frac{\partial C_{H^+}}{\partial z} + 2 \cdot \frac{K_{cat} [E] \cdot C_G}{K_m + C_G}, \text{ for } z < l \quad (9)$$

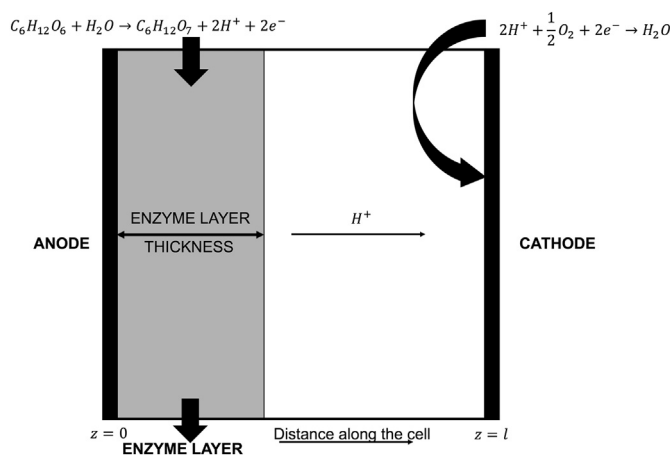


Fig. 1. Schematic of an enzymatic glucose fuel cell.

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