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Short communication

# Constructed mathematical model for nanowire electron transfer in microbial fuel cells

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## HIGHLIGHTS

- Mathematical models for nanowire electron transfer mechanism in MFCs was performed.
- *G. sulfurreducens* and *S. oneidensis* were employed as microorganisms in MFCs.
- MFC performance was observed in terms of power generation and biofilm thickness.
- Computational models were in accordance to the experimental results.
- The study proved feasibility of integration of MFC with computational technology.

## ARTICLE INFO

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Power generation
Biofilm thickness

## ABSTRACT

Microbial fuel cell (MFC) technology is being given immense esteem in the scientific community for its capability of transforming organic waste directly into electricity through electrochemical reactions occurring at the microbial catalyzed anode, and microbial or abiotic cathode The microbes in a MFC transfer the electrons to the electrode through various electron transfer mechanisms and among them, nanowire transfer mechanism is the most significant one. The purpose of this study was to design and develop mathematical models for predicting the nanowire electron transfer mechanism. Results obtained from the experiments and simulations are found to be well in agreement with each other. These evidences prove that electron transfer mechanisms do occur in the microbial biofilm of the MFCs. In addition, these results imply that the f electron transfer mechanism may lead to an increase in power generation from the MFC. Biofilms with thicknesses of 2 μm and 1 μm have enhanced a current density increase of 86% and 73% respectively than that of 3 μm thick biofilms. Thus, it was observed that the biofilm thickness had a very less influence on the performance of MFC and these results can contribute to the development of MFC in the field of energy generation.

## 1. Introduction

Microbial fuel cells (MFCs) are bio-electrochemical transducers that can utilize the chemical energy in the organics and convert it into electrical energy with the aid of microbes. The microbes transfer the electrons to the electrode through various electron transfer mechanisms. However, the electron transfer mechanism plays an important role in maximizing the microbe to electrode interaction and helps provide an understanding of how such systems operate in the MFC [1]. Researchers have proposed three kinds of extracellular electron transfer (EET) mechanisms (Fig. 1). The first transfer mechanism uses direct electron transfer between electrons carriers in the bacteria and the solid electron acceptors [2]. The mechanism is carried out by the presence of outer-membrane (OM) cytochromes that can interact directly with the solid surface to carry out respiration [3,4]. The second transfer mechanism employs electron shuttle between bacteria and electrode. The mediated electron transfer (MRT) has redox mediators involved in the shuttling of electrons between bacteria and electrode [3,4]. The third type of mechanism uses nanowire conductive transfer between bacteria and electrode. The nanowire is likely a solid conductive or semi-

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**Nomenclature**

| | |
|---|---|
| $\gamma_s$ | a conversion factor from mass of substrate to coulombs |
| $q_{max}\ X_f$ | the maximum specific rate of substrate utilization and the concentration of active biomass in the biofilm |
| $L_{fa}$ | the biofilm thickness active in EET |
| $j_{max}$ | Current density |
| F | Faraday constant |
| R | Ideal gas constant |
| T | MFC temperature |
| $\kappa_{bio}$ | the conductivity of the solid conductive matrix |
| $j_0$ | the exchange current density |
| $\alpha$ | the electron-transfer coefficient |
| $A_{surface}$ | Electrode surface of area |
| $c_{red}$ | Reduction concentration |
| $c_{ox}$ | Oxygen concentration |
| $b_{ina}$ | Inactivation decay coefficient for active biomass |
| $b_{det}$ | The detachment rate |
| Y | the true yield |
| $q_{max}$ | Maximum specific rate of ED utilization |
| $b_{res}$ | Endogenous decay coefficient for active biomass |
| $\kappa$ | The ionic conductivity of the membrane |
| $\delta^M$ | is membrane thickness |

conductive material for electron transfer [2]. Moreover, it has been reported to accept electrons form iron (II) oxidation reaction in the solid transfer matrix [3,4]. Thus, the solid conductive matrix is likely to act as a semi-conductor rather than a conductor. In accordance to the above mentioned references, the EET mechanism can provide an understanding of power generation and the performance of microorganisms and their interaction with the electrodes. Thus, this perspective can be applied for influencing the MFC performance.

Many researchers have investigated the performance of MFCs by the experimental studies but only few researchers have focused on the development of models for the simulation of MFCs. Zhang et al. [5] have proposed one-dimensional MFC model and discussed the influence of substrate concentration on MFC performance. They have reported about biochemical and electrochemical processes in the MFCs. Oliveira et al. [6] have reported that they designed a one-dimensional model to predict current and voltage production. They have assumed conditions on the basis biochemical and electrochemical processes to develop computational models. In addition, they reported the concentration of substrate and temperature influence on the biofilm thickness and growth. Many researchers investigated the effect of a variety of carbon sources on MFC performance, but only few studies thoroughly focused on the kinetic analysis of the type and concentrations of substrate [7]. Pinto et al. [8] reported a model to describe the competition of anodophilic and methanogenic microorganisms in the MFC. The Marcus et al. [9] reported about the derived Nernst-Monod equation to describe electron-donor (ED) rate and ED concentration for the biofilm in the MFC. Alavijeh et al. [10] developed mathematical models for complex concentration and biocatalyst in a MFC and further explained its influence on the MFC biofilm. They have determined that the concentration of substrate was a key factor that directly influenced MFC performance. They reported that the power density increase was parallel to the increase of glucose concentration in the MFC. Katuri et al. [11] have designed the dynamic response model to describe the effect of different glucose concentrations in the MFC from 1 to 7 mM. They reported that the power density increase was parallel to the increase of glucose concentration in the MFC. However, these references have discussed about the effects of substrate concentration with the basis of different models. So, according to these reference, we have substantiated the electron transfer mechanism and its influence on the MFC. In addition, it is important to understand the control parameters in the MFC. Therefore, mathematical models were developed in the present study to discuss the effects of operational parameter like the substrate concentration on the MFC performance. In brief, numerous studies have been developed to discuss the influence of design parameters on MFC performance. Moreover, the research results found that the EET from microorganism to electrode surface is the main reason behind the MFC performance. The nanowire transfer mechanism is a type of electron transport mechanism in a microorganism that focusses on the role of out-membrane c-type cytochromes [12]. However, most of the microorganisms perform bacterial dissimilatory metal reduction during the nanowire electron transfer mechanism through the nanowire or conductive pili. The bacteria dissimilatory metal reduction produced electron acceptor Fe (III) to assist electron transfer through nanowire electron transfer mechanism from the microbe to the anode electrode of MFC [13]. Thus, this study was focused on designing mathematical models for EET mechanism in MFC. Numerous research reports have determined that in-depth understanding of the EET mechanism is very important for the evaluation of the electron transfer from microbe to electrode surface in the MFC. In addition, the MFC system would be influenced by the operational parameters. Mathematical model were evaluated for batch type MFCs with nanowire electron transfer mechanism in this study. The research purpose of this study was to design mathematical models for the investigation of nanowire electron transfer mechanism in batch type MFCs.

## FIGURES

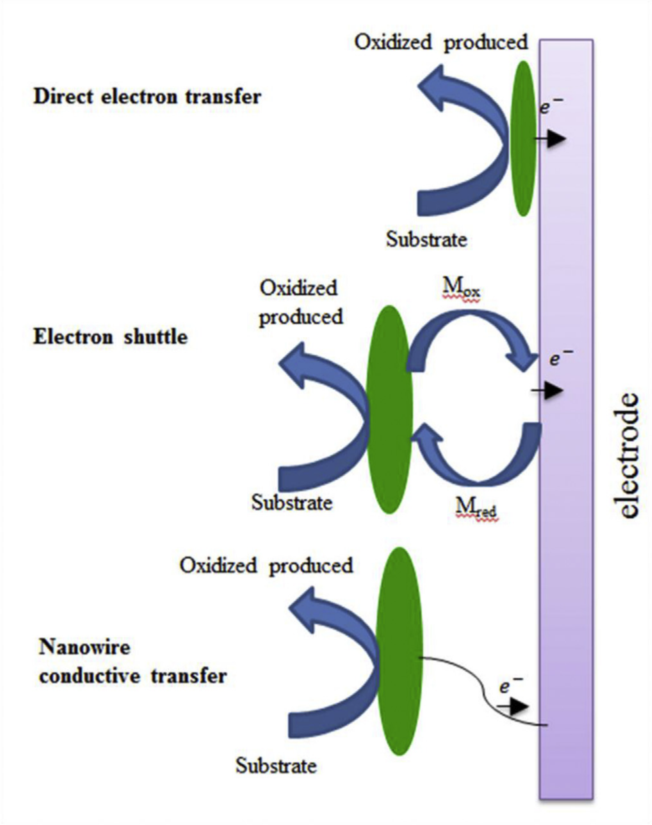

**Fig. 1.** The three kinds of extracellular electron transfer (EET) mechanisms.