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Review article

Models for Microbial Fuel Cells: A critical review

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HIGHLIGHTS

- Mechanisms, advantages, drawbacks, and applications of different MFC models are discussed.
- Mechanism-based and Application-based taxonomy of MFC models is presented.
- Different modeling approaches to the MFC are reviewed.

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ABSTRACT

Microbial fuel cells (MFCs) have been widely viewed as one of the most promising alternative sources of renewable energy. A recognition of needs of efficient development methods based on multidisciplinary research becomes crucial for the optimization of MFCs. Modeling of MFCs is an effective way for not only gaining a thorough understanding of the effects of operation conditions on the performance of power generation but also becomes of essential interest to the successful implementation of MFCs. The MFC models encompass the underlying reaction process and limiting factors of the MFC. The models come in various forms, such as the mathematical equations or the equivalent circuits. Different modeling focuses and approaches of the MFC have emerged. In this study, we present a state of the art of MFCs modeling; the past modeling methods are reviewed as well. Models and modeling methods are elaborated on based on the classification provided by Mechanism-based models and Application-based models. Mechanisms, advantages, drawbacks, and application fields of different models are illustrated as well. We exhibit a complete and comprehensive exposition of the different models for MFCs and offer further guidance to promote the performance of MFCs.

1. Introduction

Microbial Fuel Cells (MFCs) have received an extensive attention in the recent years as a novel source of renewable energy. The MFC regarded as a direct bio-electrochemical reactor realizes a conversion of chemical energy in microorganism to electricity, treats the organism as the substrate and utilizes the microbial redox reaction to generate electricity directly [1]. The power generation principle and the application of MFCs have resulted in comprehensive studies [2–6]. Bacteria provide the catalyst to oxidize the substrate in the anaerobic anode and electrons are transferred as the reaction production to the anode electrode, through an external circuit to the aerobic cathode where the reduction reaction is carried out and combines reductant to produce the water molecules, as shown in Fig. 1 [5].

According to the electrons transferred to the anode surface in different ways, the MFCs can be classified into the direct MFCs (conduction based) and indirect MFCs (mediators based). On the basis of the existence of proton exchange membrane (PEM), the MFCs are divided into two-chamber MFCs and single chamber MFCs. As the new biomass power generation energy, MFCs are capable of not only replacing the traditional fossil fuel and reducing the impact on environment but also achieving the sustainability of water resources with the wastewater as substrate used and simultaneous electricity power generation [7,8]. However, there are several hurdles remaining for MFCs to be widely adopted. The main drawback in the MFCs operation is the low power output, which limits the performance of MFCs to drive electronic devices. The power output of MFCs cannot reach the high-power level as well as the industrial application occasions of the other renewable

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Nomenclature

a,b	The coefficient of Tafel equation
$\mu_{a/m}$	Growth rate for anodophilic/methanogenic biomass
η_a	Anode overpotential
S_{d0}	Influent substrate concentration
η	Overpotential
$S_{a/d}$	Concentration of electron acceptor/donor
α	Charge transfer coefficient of anodic reaction
K_{sa}	Half velocity rate constant for electron acceptor
$\alpha_{a/m}$	Biomass retention parameter
K_{sd}	Half velocity rate constant for electron donor
V_a	Volume of anode chamber
$K_{d,a/m}$	Decay rate for anodophilic/methanogenic biomass
U	The local potential
K_{dec}	Decay constant for acetate utilisers
D	Dilution rate
$\phi_{a/i}$	Volumetric fraction of active/inactive biomass
A_m	Cross-section area of membrane
v	Advective velocity of biofilm matrix
A_F	Surface area of the biofilm
r_{res}	The rate of endogenous respiration
R	Ideal gas constant
r_{ina}	The rate of inactivation of active biomass
T	Temperature
k_{bio}	Biofilm conductivity
$D_{ED,f}$	Diffusion constant for electron donor
M_{total}	Mediator fraction
$X_{f,a/i}$	Density of active/inactive biomass
M_{red}	Reduced mediator fraction
n	Number of electrons transferred
$S_{E/B}$	Concentrations at electrode surface/bulk liquid
F	Faraday constant
I	Current
Y	Bacterial yield
i	Current density
q_{max}	Maximum substrate consumption rate
i_0	Exchange current density
$q_{a/m}$	Substrate consumption rate by anodophilic/methanogenic biomass
i_l	Limiting current density
$q_{s,B/F}$	Net reaction rates of reaction in bulk/biofilm
$R_{solution}$	Resistance of solution
$q_{s,E}$	Electrochemical rates of solute component
$R_{membrane}$	Resistance of membrane
x	Concentration of biomass
$R_{A/B}$	Resistance of anode/cathode
$x_{a/m}$	Concentration of anodophilic/methanogenic biomass
$R_{min/max}$	Lowest/Highest observed internal resistance

energy, such as solar power, wind power, nuclear power, and others. Furthermore, the costly materials of electrode and catalyst result in reducing the economic competitive abilities compared with other sources of energy [9]. Therefore, how to improve the power generation performance and find inexpensive electrode and catalyst materials are the pronounced challenges present in the applications of MFCs.

The MFC is a complex and hybrid system that involves a number of bio-electrochemical coupling reactions, which leads to the strong non-linear characteristics and significant hysteresis properties and makes it difficult to control and optimize the power generation of MFCs directly. Furthermore, bacteria inoculation and performance measurement

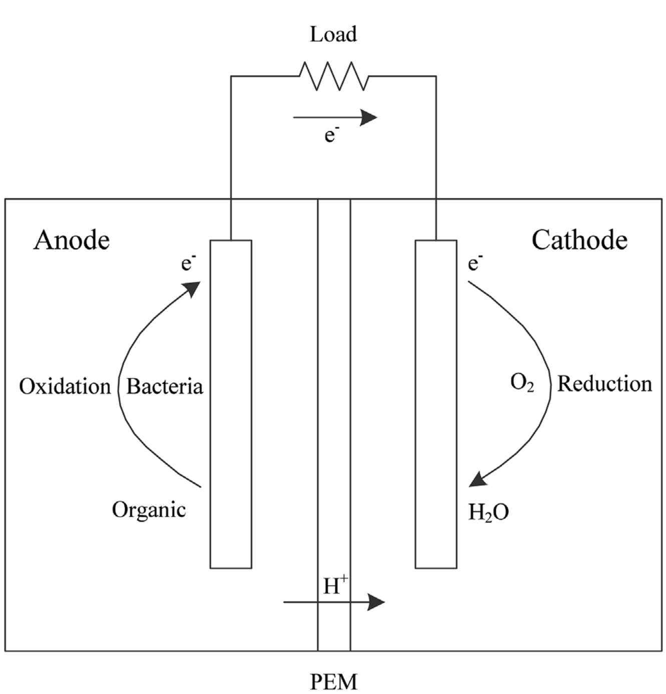

Fig. 1. Schematic diagram of MFCs (shown are two-chamber MFCs).

completed through experiments are time-consuming and uneconomic. Hence, considering mathematical models to understand the major influence factors of the whole system to distinguish the main bottlenecks and improve the power generation performance of MFCs arises as an efficient alternative to follow. The influential variables of the MFCs power generation performance can be obtained based on mathematical modeling. In general, the models primarily represent the chemical reaction process, mass transport process and electricity generation process of the cell. MFCs models have also been developed by considering the successfully implemented models for other fuel cells, such as the Direct Methane Fuel Cell (DMFC) [10], the Solid Oxide Fuel Cell (SOFC), the Anaerobic Digest Model No.1 (ADM1) [11], and others. MFCs models are applied to the online or offline mode on basis of different real-time data, which means these two models have independent application areas. However, both models exhibit the same key objectives of providing sound prediction abilities as well as robustness. Adhering to different modeling objectives, the models for MFCs can be divided into the full-cell models discussing reactions of both the anodic and cathodic compartment, and the half-cell models focusing on a specific compartment considering the anode or cathode as the limiting factor of MFCs [12]. With the development of MFC modeling, conflicting aspects between the exhaustive expressing degree and practical application have appeared in different models. Many efforts have been directed to the fields related with MFCs modeling.

Zhang and Halme [13] proposed a dynamic mathematical model for an MFC with added-mediator to transfer electrons. The process of modeling ignored the cathodic reactions and incorporated the classical electrochemical reactions in the anode chamber, including the consumption of substrate, the potential, and the current calculation and so on. With the novel understanding of the electron transfer mechanism, Kato Marcus et al. [14] modeled the conduction-based MFC that applied the biofilm to transferring the electrons to the anode without mediator, that is biofilm-anode, for the first time and evaluated, the limitation element caused by biofilm in MFCs. Based on the mediator-less MFCs, the biofilm models have been added to MFCs models. Picioreanu et al. [15] developed the first computational biofilm model of an MFC to investigate that the bacteria accumulated at the anode surface to form the biofilm and the variation of thickness of biofilm. The