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One-dimensional Conduction-based Modeling of Bioenergy Production in a Microbial Fuel Cell Engaged with Multi-population Biocatalysts

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ABSTRACT

Anaerobic digestion processes and the conductive electron transfer approach were used to describe the bioenergy production processes in a microbial fuel cell (MFC), respectively. The present model is a far more completed form of conduction-based modeling which is able to predict performance of an MFC fed with complex substrates and inoculated with multi-population culture. One-dimensional spatial distributions of the different microorganisms, as biocatalysts of processes and intermediates produced in the different steps of the anaerobic digestion processes in the biofilm, as well as the dynamic behavior of the anolyte including syntropic interactions among different groups of microorganisms to degrade organic materials and wastewater were simulated. In addition, a fast convergence and reliable numerical solution was proposed to increase the model's applicability for a variety of simple to complex substrates. Model validation was performed using experimental results from the MFCs fed with glucose, gluconic acid, xylose, arabinose, cellulose, protein and dairy wastewater. Also, MFC performance was assessed by analyzing the microbial activity in the biofilm as biocatalyst and characterizing the anolyte's features. The results obtained from the simulation were compared to some previous models, as well. The results show a promising pathway for modeling the complex nature of bioenergy production in the MFCs.
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1. Introduction

The microbial fuel cells (MFCs) are regarded as an energy harvesting effort coupled with renewable energy stored in organic substances and, in particular, in wastewater to generate power and simultaneously to treat wastewater. Bacterial oxidation of fermentable materials leads to electron generation. Generated electrons are transferred to the surface of the anode across the biofilm by a direct or mediated electron transfer mechanism [1]. Dependent upon the feed type as a complex mixture of substrates, a microbial consortium serves as biocatalyst and is used to oxidize organic matters during the anaerobic digestion process. Different steps of anaerobic digestion including hydrolysis of macromolecules, acidogenesis of hydrolysates, acetogenesis and methanogenesis are combined with bioelectrogenesis that occurs in an MFC [2]. A myriad of microorganisms as a monolithic population, which have adapted to and live in a specific growth medium, collaborate to decompose organic materials to the simpler liquid and gas products. Several modifications and investigations such as the effect of flow rate and inoculum [3], controlling methanogenesis activity [4,5], the effect of pH [6,7] as well as membrane and electrodes modifications [8–10], have experimentally been conducted to enhance and evaluate the performance of an MFC. In addition, the scale up of MFCs has been discussed in some studies [11,12]. From the other point of view, mathematical modeling tends to present a new and economical approach to assess MFCs. Based on the complexity of microbial behavior, biochemical and bioelectrochemical reactions and mass transports in the biofilm and the liquid bulk, different models have been proposed. The starting point of MFC modeling was established by Zhang and Halme [13]. That model was a simple model to comprehend the basic concepts of MFCs formulated based on the externally mediated electron transfer mechanism. Some mediator-based models have been developed to describe the MFC performance with considering both liquid bulk and biofilm simulation [14] and competition between methanogens and electrogens [15,16]. Acetate was deemed as the sole carbon source in most of the models to evaluate and validate the simulation [17,18]. Picioreanu et al. (2007) [14] developed a complex methodology to model an MFC based on redox mediators which is extendable to two and three dimensional simulations. Experimental evaluation of this model was conducted by an acetate fed-MFC (not a complex fed-one) inoculated with *Geobacter sulfurreducens*bacteria, which transfer electrons by nanowires, not mediators. In addition, in

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Nomenclature

A surface area (m^2)
b inactivation, endogenous respiration and detachment constant (day^1)
C suspended microorganism concentration ($kgCOD_X$ m^{-3})
D diffusion coefficient (m^2 day^{-1})
E_{KA} half maximum rate potential (V)
F Faraday's constant (Coulomb mole-$^{-1}$)
f intermediate production yield ($kgCOD_S$ $kgCOD_S{}^{-1}$)
f_e^0 fraction of energy-generating electrons (dimensionless)
I current (A)
j current density (A m^{-2})
J_s mass flux ($kgCOD_S$ m^{-2} day^{-1})
K Monod half-saturation constant ($kgCOD_S$ m^{-3})
k hydrolysis rate constant (day^{-1})
k_{bio} biofilm conductivity (S m^{-1})
L thickness (m)
MW molecular weight substrate consumption rate in the liquid
q bulk ($kgCOD_S$ day^{-1}) or in the biofilm ($kgCOD_S$ $kgCOD_X{}^{-1}$ day^{-1})
R universal gas constant (J mol^{-1} K^{-1}), electrical resistance (Ω) and net bioreaction rate ($kgCOD_S$ m^{-3} day^{-1})
r inactivation and endogenous respiration rate (day^{-1})
S substrate concentration ($kgCOD_S$ m^{-3})
T temperature (K)
t time (day)
V voltage or electrode potential (V)
v advective velocity (m s^{-1})
$V_{a,b}$ anode compartment liquid volume (m^3)
X biomass density ($kgCOD_X$ m^{-3})
Y biomass yield coefficient ($kgCOD_X$ $kgCOD_S{}^{-1}$)
z spatial longitudinal coordinate from the anode surface (m)

Greek
γ electron equivalence of substrate or biomass (mole-$kgCOD^{-1}$)
η local electrical potential of the biofilm (V)
μ net specific growth rate (day^{-1})
τ time conversion factor (s day^{-1})
φ microorganism volume fraction in the biofilm (dimensionless)

Subscript
a active biomass
Aa Amino acids
Ac acetate
AM acetoclastic methanogens
$anod$ anode
Bu butyrate
$bulk$ liquid bulk
cat cathode
$cell$ fuel cell
Ch carbohydrates
$C4$ butyrate/valerate-consuming microorganisms
det detachment
E electrogenic microorganism
ext external
f biofilm
Fa Fatty acids
H hydrogen
HM hydrogenotrophic methanogens
$hydr$ hydrolysis
i inactive biomass
ina inactivation
l liquid
Li lipids
$local$ local potential
max maximum
O_2 oxygen
ohm ohmic
Pr proteins
Pro propionate
net net
res endogenous respiration
S substrate
s surface
Su sugars
$interface$ liquid/biofilm interface
Va valerate
X biomass

another research [16], this model was improved with Anaerobic Digestion Model No. 1 (ADM1) [19] and simulation results were compared with a glucose-fed MFC experimental data [16]. In addition, Picioreanu et al. [20] extended the model to describe macro-scale phenomena in the anolyte with a micro-scale two-dimensional simulation of the biofilm. Moreover, charge balance and spatial pH distribution were considered. Three case studies were used to generally describe the variations of variables such as pH, substrate, biomass concentrations and electrical parameters; however, the model was not compared experimentally with a complex wastewater. The presented models by Picioreanu et al. were more realistic with regard to the MFC nature, but they were implemented in a long-running simulations [21]. Pinto et al. [15] proposed a simple mediator-based model including ordinary differential equations with a fast convergence solution. This model can be used for control and optimization of an acetate-fed MFC in continuous mode with considering acetoclastic methanogens growth, but it is not applicable for complex substrate-fed MFCs. Marcus et al. [22] proposed a new approach in MFC modeling, based on the foundation of conduction-based electron transfer through the conductive biofilm. This model presents a detailed description of the biofilm with a dynamic and one-dimensional distribution of acetate, active and inactive biomass. The electrical conduction and electron production in the biofilm were modeled by the Ohm's law and Nernst-Monod kinetics. It is the first conduction-based model and is obviously in the face of some restrictive deficiencies. Modeling with only constant anode potential (or poised one) and lack of experimental evaluation with a complex feed and multi-population biocatalysts as well as anolyte simulation are the main bottlenecks. Hence, some of the researchers developed more extended models based on the Marcus' key model. Merkey and Chopp [23] extended the Marcus' model to consider the geometry of biofilm growth in an MFC with multidimensional simulation. They modeled only the anode with constant potential and validated simulation results by an acetate-fed MFC. Sedaqatvand et al. [24] improved the previous conduction-based model [22] for the MFC fed with a complex feed, considering the variable anode surface potential. They considered that electron production occurs directly from dairy wastewater in a single step without simulating the anolyte and microbial community. In the proposed models by Jayasinghe et al. [25] and Korth et al. [26], Marcus' model was extended by considering intracellular and extracellular electron transfer. These models are

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