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A Generalized Model for Complex Wastewater Treatment with Simultaneous Bioenergy Production Using the Microbial Electrochemical Cell

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ABSTRACT

The objective of this study was to construct a novel model to be applied in a general manner to simulate microbial electrochemical cells (MXCs); for both microbial fuel cell (MFC) and microbial electrolysis cell (MEC). The liquid bulk was modeled based on the organic matters degradation to acetate via the anaerobic digestion process. Biofilm simulation was established based upon one-dimensional distribution and the dynamical electron transfer was completed by means of the conduction-based mechanism. We, for the first time, introduced biofilm local potential modeling for MEC simulation with general and simplified linear boundary conditions. The MFC-related part of the model was evaluated based on the experimental results from a gluconic acid-fed MFC with various simulated variables of liquid bulk and biofilm such as, bulk concentrations, distributions of microbial volume fractions and local potential in the biofilm, and biofilm thickness. The MEC-related part of the model with simplified linear boundary condition was assessed by the MEC experimental data fed with potato wastewater as the complex substrate. The MEC performance as an energy carrier generator was characterized based on the hydrogen production rate evolution, the variations of microbial distributions, and methane production at different applied potential differences. In addition, polarization characteristics were simulated and discussed based on the experimental results. These valuations showed that the presented model is successfully able to predict both MFC and MEC performance.

1. Introduction

Microbial electrochemical cells (MXCs) are recognized as a modern technology to directly utilize bioenergy stored in organic substances, especially in wastewater. Bacteria have the main role as a biocatalyst in these systems. They oxidize materials in the anode compartment and produce electrons [1]. Electrons can be transferred to the anode surface by the mediator-based mechanism or by the conductive biological nanowires or conduction-based pathway [2], then they depart across an external circuit to the cathode electrode where an oxidant (usually oxygen) is reduced. Electrical current generation can be implemented through a microbial fuel cell (MFC). Hydrogen production through an MFC is not thermodynamically possible, so by excluding the oxidant (oxygen) in the cathode and using an additional power supply in the circuit, it is possible to convert produced protons spontaneously to hydrogen as an energy carrier on the cathode surface [3]. This process is conducted in a device called the microbial electrolysis cell (MEC). In respect to significant environmental concerns and the potential toxicity of organic substances in wastewater, MXCs represent a promising candidate as a cost-effective and efficient method for degradation of organic content of wastewater.

Several experiments have been conducted to evaluate MXCs main performance as a current or hydrogen generator fed with different organic matters [4,5]. Evaluation of these systems, especially in the system scale-up and design, requires more comprehensive knowledge about electrochemical and biochemical reactions and syntrophic interactions among a plethora of bacteria which participate in these reactions. Anaerobic digestion and electrogenesis are two primary steps in bioelectrochemical systems. The objective of anaerobic digestion is to transform organic materials to end products of liquid and gases through a variety of bioconversions including hydrolysis, acidogenesis, acetogenesis and methanogenesis [6]. One of the economical and appropriate solutions to investigate the microbial behavior and to comprehend the bioelectrochemical interactions in both MFCs and MECs is mathematical modeling.

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Nomenclature

A	surface area (m^2)
b	inactivation, endogenous respiration and detachment constant (day^1)
C	suspended microorganism concentration ($kgCOD_X\,m^{-3}$) or cathodic hydrogenotrophic methanogens concentration (g-HM m^{-2}-cathode)
D	diffusion coefficient ($m^2\,day^{-1}$)
E_{KA}	half maximum rate potential (V)
f_e^0	fraction of energy-generating electrons (dimensionless)
J_s	mass flux ($kgCOD_S\,m^{-2}\,day^{-1}$)
K	Monod half-saturation constant ($kgCOD_S\,m^{-3}$)
K_{bio}	biofilm conductivity ($S\,m^{-1}$)
n	number of electrons transferred (mole- mol^{-1}-H_2)
Q	volumetric rate ($m^3\,m^{-3}$-anolyte day^{-1})
q	substrate consumption rate in the liquid bulk ($kgCOD_S\,day^{-1}$) or in the biofilm ($kgCOD_S\,kgCOD_X^{-1}\,day^{-1}$)
r	inactivation and endogenous respiration rate (day^{-1})
S	substrate concentration ($kgCODS\,m^{-3}$)
V_1 *and* V_2	constants of the linear applied potential-related function
v	advective velocity ($m\,s^{-1}$)
$V_{a,b}$	anode compartment liquid volume (m^3)
X	biomass density ($kgCOD_X\,m^{-3}$)
Y	biomass ($kgCOD_X\,kgCOD_S^{-1}$) or (g-HM mol^{-1}-H_2) and acetate/methane ($kgCOD_S\,kgCOD_S^{-1}$) yield coefficients
Y_C	dimensionless cathode efficiency
$Y_{(CH_4/H_2)}$	methane production yield coefficient (m^3-$CH_4\,m^{-3}$-H_2)
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})
μHM	hydrogenotrophic methanogens specific growth rate (day^{-1})
τ	time conversion factor ($s\,day^{-1}$)
ϕ	microorganism volume fraction in the biofilm (dimensionless)

Subscript

a	active biomass
Ac	acetate
AM	acetoclastic methanogens
anod	anode
app	applied potential difference
bulk	liquid bulk
cat	cathode
cell	fuel cell
CH_4	methane
Demanded H_2	demanded hydrogen
det	detachment
E	electrogenic microorganism
ext	external
f	biofilm
H_2	hydrogen
HM	hydrogenotrophic methanogens
i	inactive biomass
ina	inactivation
l	liquid
max	maximum
ohm	ohmic
Produced H_2	produced hydrogen
res	endogenous respiration
S	substrate
surface	liquid/biofilm interface
WW	wastewater
X	biomass

Different viewpoints have governed the development of MFCs models. With regard to the electrochemical, biochemical and transport phenomena equations, the dynamic behavior of the system, biofilm characteristics as a pure or mixed-culture, and considering operational parameters such as anolyte and catholyte properties are the main factors that have been used to construct simple to complex MFCs mathematical models. A simple mediator-based model with suspended cells was investigated by Zhang and Halme [7]. The main application of this model was to understand the basic concepts in an MFC with restricted applicability. Actually, both suspended and attached microorganisms in the form of biofilm can play important roles in MFCs, especially when a wastewater containing a mixture of substrates and a multi-species biocatalyst engaged in the bioconversions, are used.

Picioreanu et al. [8] introduced an anodic biofilm-based model with a soluble redox mediator and liquid bulk modeling as well as some later extended forms [9,10] were proposed based on a more complex anaerobic digestion modeling and including influence of some other variables such as pH on the MFC performance. Although the physical and biochemical behavior through the general mass balancing were implemented in this model allowing it to be brought under a mixed-culture MFC, due to several unknown model parameters and heavy mathematical calculations, its applications were limited in the range of simple substrates and it could not be performed on a complex wastewater feed [11]. Oliveira et al. [12] proposed a simple model with rapid implementation and computations to describe the effect of some operational conditions such as temperature and substrate concentration on the MFC performance. It was one-dimensional model coupled with transport phenomena consist of heat, charge and mass transfer as well as biofilm modeling. But it cannot describe the dynamic behavior of MFC and microbial population and acetate was only used as the substrate in the model simulations. In another research by Kato Marcus et al. [13], a new approach of the electroactive bacterial oxidation kinetics was derived as the Nernst-Monod expression. This equation is a dual-limitation Monod kinetics and was established on the conduction-based mechanism by which electrons are transferred in a conductive biofilm. In their model, active and inactive biomass distributions in the biofilm were modeled, but a liquid bulk simulation was not included and the microbial community was only considered as a pure culture comprising two clusters; active and inactive biomass, moreover the anode potential was assumed to be poised. To describe the competition between methanogenic and electrogenic microorganisms, Pinto et al. [14] governed a time-dependent model with the uniform distribution of bacteria in the anode chamber, a constant pool of intercellular mediators and acetate as the only substrate. Sedaqatvand et al. [15] developed a general anode potential status including the different overpotentials to extend the Marcus' conduction-based model [13], they also estimated the design parameters of a single chamber MFC fed with dairy wastewater as a complex wastewater [16], but the