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A novel model for predicting bioelectrochemical performance of microsized-MFCs by incorporating bacterial chemotaxis parameters and simulation of biofilm formation

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ABSTRACT

Bacterial transport parameters play a fundamental role in microbial population dynamics, biofilm formation and bacteria dispersion. In this study, the novel model was extended based on the capability of microsized microbial fuel cells (MFCs) as amperometric biosensors to predict the cells' chemotactic and bioelectrochemical properties. The model prediction results coincide with the experimental data of *Shewanella oneidensis* and chemotaxis mutant of *P. aeruginosa* bdlA and pilT strains, indicating the complementary role of numerical predictions for bioscreening applications of microsized MFCs. Considering the general mechanisms for electron transfer, substrate biodegradation, microbial growth and bacterial dispersion are the main features of the presented model. In addition, the genetic algorithm method was implemented by minimizing the objective function to estimate chemotaxis properties of the different strains. Microsized MFC performance was assessed by analyzing the microbial activity in the biofilm and the anolyte.

1. Introduction

Microbial fuel cells (MFCs) are one of the novel platforms for utilizing bioenergy from organic substrates particularly in wastewater resources by using electrogenic microorganisms as biocatalysts [1]. The ability of microorganisms to utilize a wide range of organic materials, particularly found in wastewater, as electron donors demonstrates the unique advantages of these systems over conventional wastewater treatment and/or bioenergy generators [2]. In addition, other applications such as biosensors and chemostat assays have accelerated interest in and developments of this technology in recent years [3].

Regarding MFC applications [4–6], any variations in the concentration of organic compounds as well as the microbial population are directly proportional to the output current. Thus, MFCs as amperometric biosensors have proven to be a valid and novel alternative to conventional biosensors for screening biological processes [7].

The intrinsic advantages of microsized MFCs such as cost and time-efficiency, high reproducibility, and exquisite control over experimental parameters make them a powerful platform for the investigation of biochemical phenomena [8–10].

With regard to the importance of mathematical modeling as complementary knowledge in understanding the different bioelectrochemical processes in MFCs and designing the high-performance system [11], the configuration of numerical methods in microsized MFCs can provide an genuine approach for studying biochemical processes.

According to previous published studies on MFC modeling, the foundation of conventional MFC models faced the main limitation that they could not be implemented to simulate the initial state of biofilm formation [12–14]. The development of next generation model of microorganisms distribution on the basis of assumptions of the initial dispersal and their suitableness was assessed based on the predicted results with the final experimental data of sustained situations (i.e. the current evolutions [11,15] and/or polarization curves [12–14]). Neither the mechanisms of biofilm attachment to the anode nor the distribution of planktonic bacterial cells in the anolyte solution were considered in all previous MFC models. Therefore, to consider the free-swimming bacterial cells' dispersions, interactions, and attachments in the form of biofilm, as well as the bioelectrochemical reactions of exoelectrogenic bacteria, more comprehensive kinetics of bacterial chemotaxis should be added to the previous models.

In this study, the prediction of bacterial transport parameters as the key characteristics of microbial population dynamics and biofilm formation [16] as a means understand the mechanisms of the suspended microorganisms' distribution in the anolyte and the improvement of previous MFC models, was implemented numerically. The presented

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Nomenclature

A	Surface area (cm^2)
b_{ina}	Inactivation constant (min^{-1})
b_{res}	Endogenous respiration constant (min^{-1})
D	Diffusion coefficient ($cm^2\ min^{-1}$)
E_{KA}	Half maximum rate potential (V)
E^0	Standard reduction potential for the mediator couple (V)
E	Sensing molecule concentration (mmol)
F	Faraday's constant (96480 C $mole^{-1}$)
f_e^0	Fraction of energy-generating electrons (Dimensionless)
I	Current (mA)
i_0	Exchange current density ($mA\ cm^{-2}$)
J_s	Substrate mass flux ($gCOD_S\ cm^{-2}\ min^{-1}$)
J	Current Density ($mA\ cm^{-2}$)
K	Monod half-saturation constant ($gCOD_S\ cm^{-3}$)
k_d	Dissociation constant (mM)
L_b	Thickness of liquid concentration boundary layer (cm)
M	Mediator concentration (mM)
N	Number of electrons transferred ($mole^-\ molH_2$)
Q	Substrate consumption rate ($gCOD_S\ gCOD_X^{-1}\ min^{-1}$)
Q	Volumetric inlet flow rate ($cm^3\ min^{-1}$)
R	Inactivation and endogenous respiration rate (min^{-1})
R	Universal gas constant ($J\ mol^{-1}\ K$)
R_m	Membrane resistance(kΩ)
S	Substrate concentration ($gCOD_S\ cm^{-3}$)
T	Temperature (K)
V	Electrical Potential (V)
$V_{a,c}$	Anode compartment liquid volume (cm^{-3})
X	Biomass density ($gCOD_X\ cm^{-3}$)
Y	Biomass yield coefficient ($gCOD_X\ gCOD_S^{-1}$) or mediator yield coefficient ($mmol_M\ gCOD_S^{-1}$)
Z	Coordinates of biofilm and anode compartment (cm)

Greek

α_s	Sensing molecules production rate in liquid bulk (mmol $gCOD_X^{-1}\ min^{-1}$)
A	Sensing molecules production rate in biofilm (mmol $gCOD_X^{-1}\ min^{-1}$)
B	Redox transfer coefficient (Dimensionless)
Γ	Electron equivalence of substrate or biomass ($mole^{-1}$ gCOD)
η_a	Local electrical potential of the biofilm (V)
H	Over potential (V)
K	Biofilm or Solution conductivity ($mS\ cm^{-1}$)
Λ	Sensing molecules degradation rate (min^{-1})
μ_0	Random mobility Coefficient ($cm^2\ min^{-1}$)
μ	Fixed rate of bacterial stickiness (Dimensionless)
N	Cell swimming speed ($cm\ min^{-1}$)
χ_0	Chemotactic sensitivity coefficient in biofilm ($cm^2\ min^{-1}$)
X	Chemotactic sensitivity coefficient in liquid bulk ($cm^5\ min^{-1}$)

Subscript

A	Electron acceptor
act	Activation
anode	Anode compartment
b,bio,f	Biofilm
bulk	Liquid bulk
conc	Concentration
D	Electron donor
ext	External
in	Inlet
ina	Inactivation
int	Internal
L	Liquid
ox	Oxidized
ohm	Ohmic
red	Reduced
res	Endogenous respiration
S	Suspended
sol	Solution

model considered a general manner of both electron transfer mechanisms (including conduction based and mediator based), bacterial growth and substrate biodegradation by both biofilm and anolyte microorganisms. The microsized MFCs as a high throughput system provide a promising capability for investigating the metabolic parameters by means of their effects in current production that represent the rate of bacteria respiration.

2. Model formulation

The current study was directed towards a mathematical description of the bioelectrochemical and chemotaxis properties of biocatalysts in microsized MFCs. The model equations of the system, from the substrate biodegradation equations to the microorganisms' distribution equations, are presented in Sections 2.1 to 2.7. Later, the experimental data of *Shewanella oneidensis* (*S. oneidensis*) and genetically engineered genes of *Pseudomonas aeruginosa* (*P. aeruginosa*) as biocatalysts in the microsized MFCs were used to study, the effects of the chemotactic and phenotypic characteristics of these microorganisms.

2.1. Substrate and mediator mass balance

By considering the acetate as a usable substrate for electrogenic microorganisms, the mass balance equation of acetate oxidation and mediator reduction as the final electron acceptor is considered in the following Eqs. (1,2) [17].

$$C_2H_4O_2 + 2H_2O + 4M_{ox} \rightarrow 4M_{red} + 2CO_2 \quad (1)$$

$$4M_{red} \rightarrow 4M_{ox} + 8e^- + 8H^+ \quad (2)$$

where M_{ox} and M_{red} are the oxidized and reduced forms of the mediators, respectively. As shown in Eq. (1), each mole of acetate reduces four moles of the oxidized mediators. Therefore, to balance the consumption rate of the mediators, this stoichiometry coefficient was used [15]. The total amount of mediators is a function of the microbial concentration in liquid bulk. The mass balance of these two forms is dependent on the rate of oxidation in the cell and reduction on the anode surface. This relation is described as:

$$\frac{dM_{ox}}{dt} = -Y_M q_s + \frac{\rho_M}{V x_s}\frac{I_s}{mF} \quad (3)$$

$$M_{Total} = M_{red} + M_{ox} \quad (4)$$

where q_s is the rate of substrate consumption by the suspended microorganisms in the anolyte ($gCOD_s\ cm^{-3}\ min^{-1}$); Y_m denotes the oxidized mediator yield ($mmol_M\ gCOD_S^{-1}$); V represents the anode chamber volume (cm^3); x_s represents the suspended microorganisms concentration in liquid bulk ($gCOD_x\ cm^{-3}$); I_s denotes the current produced by the