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Review

Modeling, optimization and control of bioelectrochemical systems

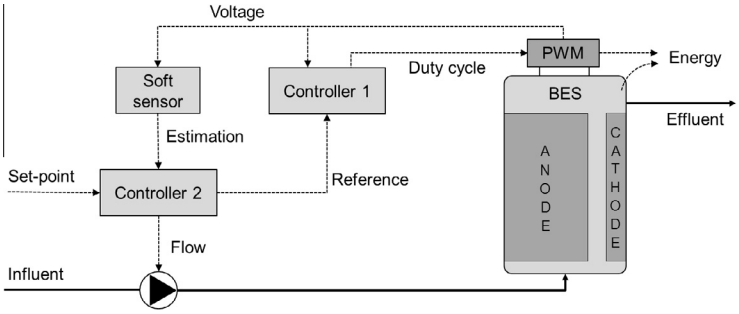
Dídac Recio-Garrido [a,b], Michel Perrier [a], Boris Tartakovsky [a,b,*]

[a] Département de Génie Chimique, École Polytechnique Montréal, C.P. 6079 Succ., Centre-Ville Montréal, QC H3C 3A7, Canada
[b] National Research Council of Canada, 6100 Royalmount Ave., Montréal, QC H4P 2R2, Canada

HIGHLIGHTS

- BES dynamic models and process control approaches are reviewed.
- Dynamic models can be used to optimize BES design and operation.
- Successful BES commercialization requires reliable process control strategies.

GRAPHICAL ABSTRACT



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ABSTRACT

Bioelectrochemical systems (BESs) such as Microbial Fuel Cells (MFCs) and Microbial Electrolysis Cells (MECs) are capable of producing energy from renewable organic materials. Over the last decade, extensive experimental work has been dedicated to exploring BES applications for combined energy production and wastewater treatment. These efforts have led to significant advancement in areas of BES design, electrode materials selection, as well as a deeper understanding of the associated microbiology, which helped to bring BES-based technologies within commercial reach. Further progress towards BES commercialization necessitates the development of model-based optimization and process control approaches. This work reviews existing MFC and MEC dynamic models as well as the emerging approaches for optimization and control.

Contents

* Corresponding author at: National Research Council of Canada, 6100 Royalmount Ave., Montréal, QC H4P 2R2, Canada. Tel.: +1 514 496 2664.
E-mail address: Boris.Tartakovsky@cnrc-ntc.gc.ca (B. Tartakovsky).

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1. Introduction

Human development is intricately linked both to energy and water availability. The International Energy Agency (IEA) estimates that energy production requires about 15% of world's total water consumption [1]. At the same time, significant amounts of energy are needed for wastewater treatment. With this respect, bioelectrochemical systems (BESs) such as Microbial Fuel Cells (MFCs) and Microbial Electrolysis Cells (MECs), which are capable of producing energy from wastewater, represent a promising new technology that could contribute to resolving this dilemma [2–4].

MFCs and MECs exploit the ability of anodophilic (exoelectricigenic) microorganisms for extracellular electron transfer and hence energy production through microbial oxidation of organic matter [5]. Both MFCs and MECs can operate using a wide variety of industrial and domestic wastewaters [6,7]. Typically, BESs consist of two electrodes connected by an external circuit [8] with the organic matter oxidation taking place at the anode and reduction reactions, such as oxygen reduction reaction in MFCs or hydrogen evolution reaction in MECs, taking place at the cathode. Detailed description of MFC and MEC principles of operation can be found in a number of reviews [3,8–10].

Extensive experimental work during the past decade has led to significant advancements in the understanding of BES microbial populations [3,5], materials [11,12], design and operation [13]. Yet, progress in MFC and MEC scale-up faces a number of challenges, mostly related to low volumetric performance and reactor instability [14,15]. With this in mind, model-based design, control and optimization approaches, which are used in bioprocess engineering [16], might be instrumental in furthering BES technologies towards commercialization. Previous reviews on MFC modeling include a number of modeling approaches [13,17,18]. These reviews, however, did not focus on fast process dynamics and the emerging area of BES real-time monitoring, control and optimization, which deals with unpredictable external disturbances and maximizing energy production. To address this gap, we review the existing MFC and MEC dynamic models, the existing control strategies and the energy harvesting configurations. Following this review, model-based methods for control and optimization of MFCs and MECs are discussed.

2. Dynamic modeling

The concept of a mediator-less MFC was only introduced about a decade ago [19,20] while the MEC concept is even more recent [21]. Accordingly, most of the research is dedicated to experimental studies, with only some studies dedicated to MFC modeling and even fewer to MEC modeling. Two approaches are commonly used in BES modeling. The bioelectrochemical modeling utilizes the knowledge of microbiology and bioelectrochemistry to describe microbial growth and carbon source consumption in BESs, while the approach of electrical equivalent circuit modeling describes BESs as electrical circuits to represent fast (milliseconds to seconds) electrical processes, while neglecting the relatively slow (minutes to days) dynamics of biomass growth and metabolism. A key assumption in the bioelectrochemical models is the mechanism by which the electron transfer from a carbon source to the anode is accomplished. Based on a number of recent experimental studies, direct electron transfer (involving either direct contact or the presence of conducting nanowires) and mediated electron transfer (via exogenous redox mediators or via secondary metabolites) are commonly accepted [10]. The following sections classify BES models based on the complexity of the mass balances (e.g. ideal mixing vs biofilm systems) and the complexity of the transport phenomena (e.g. one-dimensional vs three-dimensional biofilm) and microbial populations considered by the model.

2.1. Single-species ideal mixing modeling

A relatively simple approach to describe BES dynamics involves single population modeling. Also, to further simplify material balances the mass transport processes are assumed to be fast compared with the biochemical and redox reactions, such that the concentration of reactants in the bulk solution, inside the bacteria and on the anode surface are considered to be equal. In essence, such models consider the anodophilic microorganisms to be suspended in the anodic liquid.

The first such model was proposed by Zhang and Halme [22] to describe an MFC. This model was developed before the recent concept of mediator-less MFCs was introduced [19]. Accordingly, the model described an MFC with an external mediator (2-hydroxy-1,4 naphthoquinone or HNQ), which was used in the experiment to facilitate electron transfer (Fig. 1A). Model dynamics was based on the electrochemical and mass balances of a batch reactor. Carbon source consumption was modeled by Monod-type kinetics, while first order redox reactions at the anode and between the metabolites and the mediator were assumed. The electrochemical balance used the Nernst's equation to describe the open-circuit voltage, the Tafel approximation to calculate the activation overpotential, and Ohm's law to describe the ohmic overpotential. The concentration overpotential was assumed to be negligible. Finally, the output current of the cell was given by Faraday's law of electrolysis. The model assumed constant biomass density thus lacking dynamics of microbial growth. In spite of this and other limitations, this model presented the main principles of bioelectrochemical modeling, which were utilized in a number of subsequent models.

The development of modern mediator-less MFCs [3,19] necessitated an updated version of the ideal-mixing model, which was developed by Zeng et al. [23]. This is the only work that considers both the anode and cathode compartments. Mass balances were obtained assuming an ideally stirred tank reactor (STR) with Butler–Volmer expressions incorporated into the reaction kinetics to simulate the electrochemical balance. A sensitivity analysis of the parameters with respect to the power output of the MFC revealed the electron transfer coefficient of the cathode as the most significant factor limiting the performance of the MFCs. The model was used to describe MFC operation on acetate and synthetic wastewater. While the model adequately described MFC operation on acetate, the discrepancies observed when operating the MFC on synthetic wastewater might be related to the limitations of the single-species model.