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Review

Towards automated design of bioelectrochemical systems: A comprehensive review of mathematical models

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HIGHLIGHTS

- Mathematical models are important for design and optimization of bioelectrochemical systems.
- The mathematical models have been broadly classified based on the type of differential equations.
- Recent developments in BES models and new modeling approaches are described in this review.

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ABSTRACT

This review presents the developments in the mathematical models for various bioelectrochemical systems. A number of modeling approaches starting with the simple description of biological and electrochemical processes in terms of ordinary differential equations to very detailed 2D and 3D models that study the spatial distribution of substrates and biomass, have been developed to study BES performance. Additionally, mathematical models focused on studying a particular process such as ion diffusion through membrane and new modeling approaches such as artificial intelligence methods, cellular network models, etc., have also been described. While most mathematical models are still focused on performance studies and optimization of microbial fuel cells, new models to study other BESs such as microbial electrolysis cell, microbial electrosynthesis and microbial desalination cell have also been reported and discussed in this review.

1. Introduction

Bioelectrochemical systems (BESs) which use microorganisms to facilitate oxidation/reduction processes through the release/capture of electrons from an electrode have drawn increasing attention in recent years as an emerging technology [1]. A BES like any other electrochemical cell (e.g. battery) also includes an anode, cathode and a separating membrane (optional), but the difference lies in how the electrochemical reaction is catalysed. In BES, at least one or both of the electrode reactions are catalysed with the help of microorganisms. By combining living biological systems with electrochemistry, BES can be used for a plethora of applications such as electricity generation (microbial fuel cell, MFC), hydrogen production (microbial electrolysis cells, MEC), synthesis of value-added chemicals (microbial electrosynthesis, MES), desalination (microbial desalination cell, MDC), and removing contaminants (microbial remediation cell, MRC) [2,3]. The type of bacterial population, electrodes and substrates used at the anode and cathode and many other biological and design parameters determine the total cell potential (E_{cell}) of BES, which if positive ($E_{cell} > 0$), the BES can be used to generate electricity and when negative ($E_{cell} < 0$), additional external power may be required to reduce the electron acceptor at the cathode [1,4]. These two scenarios are described in the schematic of BES as shown in Fig. 1. While Fig. 1A represents the schematic for a standard microbial fuel cell (the total cell potential is positive), Fig. 1B represents a more general schematic for other BESs. Depending on the particular application, either anode or cathode or both can be biocatalysed and the electron acceptor and product would vary based on the application. The power required in BES when $E_{cell} < 0$, can also be supplied from renewable energy sources (solar, wind, etc.). At present, renewable electricity from solar photovoltaics and wind-turbines has become readily available, but due to the seasonal nature of sun and winds, these sources do not harmonize well with the market demand and need storage during the off hours. BES offers a perfect technological solution by making it possible to store the electrical energy from renewable sources [4,5].

BES are complex devices, affected by a number of biological,

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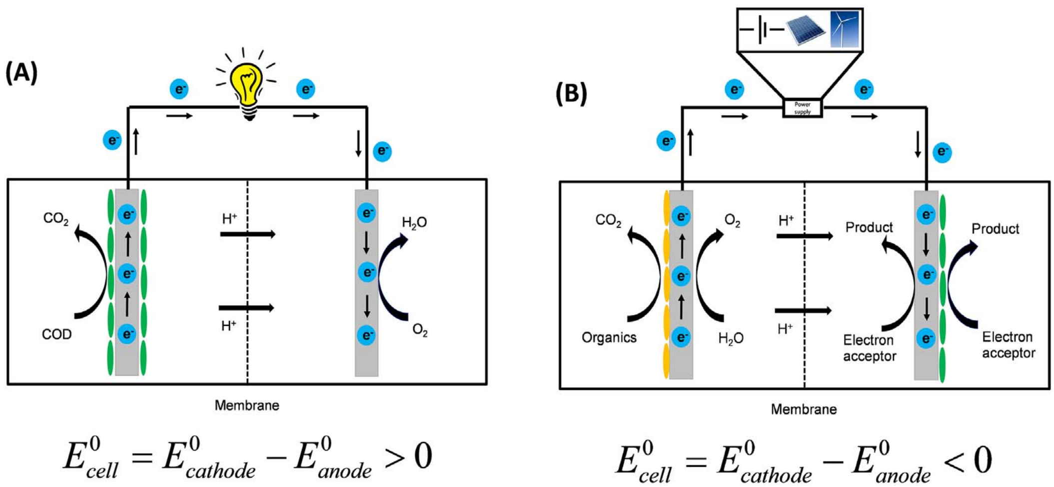

Fig. 1. Schematic of bioelectrochemical systems for two scenarios, (A) Cell potential if positive, typical microbial fuel cell (B) Cell potential is negative (requires additional voltage).

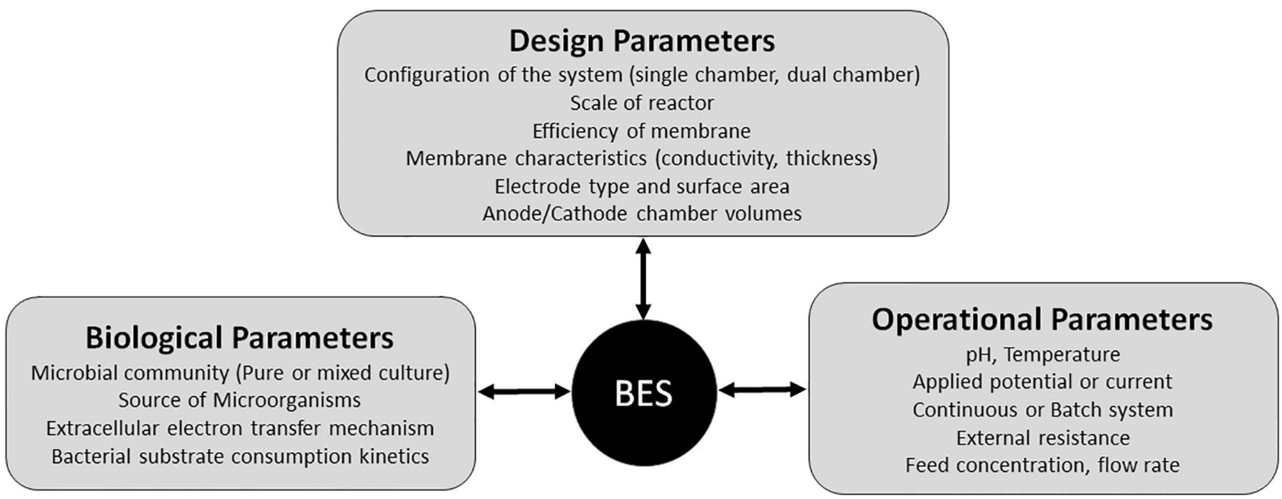

Fig. 2. List of some important parameters that influence the BES performance.

physical-chemical and electrochemical factors that are dynamically related to each other [6–8]. The performance of any type of BES depends on a number of parameters such as the type of microorganisms and feed (wastewater), membrane or separator characteristics, voltage or current supplied, mixing and diffusion phenomena, surface area of electrodes, etc. Fig. 2 shows some of most important operational, design and biological parameters that determine BES characteristics. Performance improvement of BES is still challenging and thorough understanding of the relationships among the various parameters and their dynamic processes is important to make this technology more efficient [9].

A number of experimental studies have been conducted to investigate the effect of operational parameters on BES performance [10–15]. These have helped in improving the BES performance in terms of net electricity/ product generation and scalability, but it is still much lower than that obtained from conventional technologies for similar applications [16–18,7]. Furthermore, the detailed understanding of the mechanisms governing the different processes in a BES device from a physical, chemical and biological perspective is still very patchy. Working of BES involves complex interplay between biological and electrochemical processes and thus the development of mathematical models is critical to the design and optimization of these systems in future [18,6,9,19]. However compared to the experimental studies, the number of mathematical models of BES is very limited. Also, within the relatively small number of numerical studies, most research is dedicated to microbial fuel cell (MFC) modeling and very limited work on other BES systems [9,19,20]. Some of the previous review articles have outlined the developments in the BES models. For example, Oliveira et al. [6] presented a very comprehensive review of all the developments in mathematical models of MFC. They highlighted the influence of several important parameters on the MFC performance and outlined the progress made on scaling up of BES cells. They also identified the various limitations that result in the suboptimal power output levels obtained from MFCs. Similarly Ortiz-Martínez et al. [9] reviewed and classified the prominent mathematical models describing MFC. They also outlined the advantages and shortcomings of the different modelling approaches including those based on optimization techniques. [18] presented a much broader review of BES modelling efforts including models developed on both engineering and statistical approaches. They also presented the strengths and weaknesses of using the two approaches and how these may influence BES optimization. Recio-Garrido et al. [19] presented an extensive review of the dynamic models of MFC and MEC, along with the studies on BES optimization and control. They point out that mathematical models that account for the biofilm growth dynamics of mixed population of microbes can be most useful in BES system optimization. They also suggest on-line monitoring and development of software sensors can provide better control and real-time performance update of important parameters which would be crucial in obtaining a stable system performance. Recently Xia et al. [20] presented a detailed review on different MFC