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 \cite{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) \cite{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 \cite{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 \cite{4,5}.

BES are complex devices, affected by a number of biological,
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.
models, classifying them into mechanism-based and application-based models. While describing the two types of models, they presented the underlying methodologies and usability of the different approaches based on the required output.

As can be seen, most of the previous review articles are largely focused on MFC models. In the last 2–3 years, several new mathematical approaches have been developed for MFC as well as for other bioelectrochemical systems, such as MEC, MES and MDC [8,21–24]. In addition, novel mathematical strategies using unconventional methodologies such as the artificial intelligence methods or the cellular network models have also been developed [25,26]. These mathematical models have to be comparatively and comprehensively analyzed for applicability and future research thrust that this review aims to meet.

2. Classification of models

The mathematical models developed for BES can be classified using many different factors. For example, on the basis of the mode of extracellular electron transfer (EET) used in the models, which can be either mediated or direct; or on the basis of the microbial population considered in the models, either a pure culture with single species or a mixed culture with multiple species, and so on and so forth. These different factors are described in Table 1.

Other than these factors, the models can also be broadly classified based on their mathematical formulation. For example some models are based on ordinary differential equations (ODEs) considering only time dependence and no spatial dimension or steady state models considering only one spatial dimension. Such a simple formulation based on ODEs helps in solving these models faster at a relatively low computational expense. On the other hand, some models have been formulated using a combination of partial differential equations (PDEs) and ODEs considering both time and spatial dimensions or steady state models with more than one spatial dimension. Such models are typically more comprehensive and provide detailed insights into the system. However the additional complexity also makes them computationally expensive and time consuming.

3. Description of models

Table 2 presents a brief overview of the critical factors considered in some of the important BES models. One of the first mathematical model developed for a BES is the model proposed by Zhang and Halme [27] for an MFC. In this relatively simple model, which is based on ordinary differential equations, the biological processes including the substrate consumption by the bacteria and the redox reaction between the metabolites and mediator HNQ (2-hydroxy-1,4-naphthoquinone) and the electrode redox reaction are modeled using the Monod equation and first order reactions respectively. Citing that H+ ions permeation from anode to cathode and diffusion from air to the surface of cathode electrode are very fast, all mass transport processes are assumed to be non-limiting compared to the biochemical and redox reactions [27].
Nernst equation and Faraday’s law is used to calculate the electro-
motive force and the current respectively. The parameters of the model
are first estimated from experimental results by using the least square
and trial and error methods and the model is then used for predicting
the current output based on the input concentrations of the substrate
and the mediator. A correlation between the total over-voltage and
current output is also obtained [27]. This model creates a simple for-
mulation based on a lot of assumptions but serves as a good starting
point for MFC analysis and acts as a basis for the more advanced models
that were developed later.

Picioreanu et al. [29] developed a more comprehensive multi-
dimensional mathematical model for the anodic chamber of MFCs
considering a mixed culture of bacteria suspended in the anode
chamber and also attached to the anode electrode. Electron transfer
from the microorganisms to the electrode is assumed to occur via a
diffusible redox mediator. Butler-Volmer equation is used to derive
the current density produced in the electrochemical mediator oxidation
and ohm’s law is used to calculate voltage considering activation,
ohmic and concentration over-potentials. A double Monod kinetic equation
is used to calculate the rate of substrate conversion with oxidized med-
iator leading to microbial growth [29]. Rate of microbial growth re-
sulting from substrate conversion with oxidized mediator is expressed
using a double Monod kinetic expression. The bulk of the anode
chamber is considered to be ideally mixed and thus the substrate and
the biomass concentrations in the bulk do not change in space dimen-
sion. However as the substrate is consumed its concentrations changes
as a function time based on rates of exchange with the exterior and the
rates of reactions in the bulk, in the biofilm and on the electrode. Si-
ilarly a mass balance expression is derived for all biomass types de-
pending on the rates of detachment and attachment. Unlike in the bulk,
biofilm and substrate concentrations change both spatially and with
time in the biofilm subdomain depending on the diffusion coefficients
and the respective rates of production and consumption. Migration of
ions in the electric field is however neglected. Picioreanu et al. [29]
used the model to understand the influence of different operational
conditions such as substrate utilization yields, standard potential of the
redox mediator, ratio of suspended to biofilm cells, initial substrate and
mediator concentrations, mediator diffusivity, mass transfer boundary
layer, external load resistance, endogenous metabolism, etc., on evolu-
tion of important parameters such as current, charge, power, sub-
strate concentration and biomass growth rate. They also identified that
current distribution was more uniform in homogeneous biofilms as
compared to more distributed spread-out biofilms [29]. Fig. 3 shows the
prediction of current density and 2D concentration distributions for the
oxidized mediator obtained by Picioreanu et al. [29]. It should also
be noted that while 1D and 2D cases using this model can be solved
quite easily in a short period of time, solving the full 3D model takes
long computational times (14 h for 15 days of MFC operation). Also,
though Picioreanu et al. [29]’s model is more comprehensive than
Zhang and Halme [27]’s initial attempt, it was only applied for the case
of a simple substrate feed (only acetate).

In a later study, Picioreanu et al. [30] extended their previous model
[29] by integrating with the IWA Anaerobic Digestion Model No. 1
(ADM1), which allowed the understanding of the interactions between
coeexisting methanogenic communities and electroactive bacteria
transferring electrons to a microbial fuel cell anode via soluble redox
mediators. Successively, the original model was further extended by
Picioreanu et al. [32] to calculate spatial pH distribution and solutes
speciation by adding the Nernst-Planck fluxes of ions (electromigration
and diffusion) together with an ionic charge balance. This model also
allowed the study of the different two- or three-dimensional geometry
of the electrode/biofilm which was an improvement over previous
model that only allowed the planar electrode system [32]. Three cases
studies were shown to highlight the new features of the model, however
the results were not compared with any experimental data [32].

In addition to the above three comprehensive multi-dimensional
models [29,30,32], Picioreanu et al. [33] also developed a simple
mathematical model based on ODEs that accurately describes the dy-
namics in an MFC anodic chamber with suspended cells and electron
transfer via a diffusible mediator. In this model, all variables are con-
sidered spatially uniform and just a time dependent solution is pre-
vented [33]. This model does not consider any biofilm but includes two
domains in the anode chamber, bulk liquid and the mass transfer
boundary layer adjacent to the anode. The rate of substrate consump-
tion is derived based on the double Monod expression for the substrate
and oxidized mediator concentrations. Current density is expressed
using the Butler-Volmer equation and the voltage is calculated using
Ohm’s law considering the ohmic and activation over-potentials. Mass
balances are formulated for the three soluble components (glucose,
oxidized mediator and reduced mediator) in the bulk liquid and in the
boundary layer [33]. The kinetic and mass transfer parameters in the
model are derived using a parametric estimation study by comparing
with experimental data from Delaney et al. [44]. The model has been
used to investigate the effect of different operational parameters on the
MFC performance [33].

Tables 3A, B, and C present an overview of some of the key equa-
tions used in BES models.

Marcus et al. [28] developed an important mathematical model
describing the biofilm as a conductive solid matrix, which has a specific
conductivity and accepts electrons from the biofilm bacteria and con-
ducts them to the anode electrode without the needs of any electron
shuttles. This approach is based on the experimental findings of certain
type of bacteria that allowed direct (mediatorless) transfer of electrons
to the electrode [46,47]. This dynamic, one-dimensional model con-
siders two microbial species in the biofilm domain [28]. In addition to
the active bacteria which contributed to substrate utilization, this
model also included a diffusive non-conductive layer (made up of in-
active microbes) between the conductive matrix and the bulk anodic
liquid. Ohm’s law is used to calculate the current density and a novel
Nernst-Monod equation is derived to describe the relationship between
the rate of carbon source consumption, its concentration, and the
electrical potential [28]. Here the Nernst model which is typically used
by electrochemists to describe redox potential is combined with the
Monod kinetics used by biologists to describe the dependence of bio-
logical growth on the concentration of electron donor/acceptor to de-
vlop the Nernst-Monod equation that described the relationship between
bacterial kinetics, substrate concentration and the electric potential.
The model includes steady-state mass balance of substrate in the biofilm
based on molecular diffusion and consumption rate and a dynamic mass
balance or the biomass (active and inert) based on the growth, re-
spiration and decay. The conductivity of the matrix has been linked to
the current density and local voltages along the biofilm depth. Marcus
et al. [28]’s model is considered an important milestone in under-
standing electron transfer mechanisms and describes the relations be-
tween concentration of the substrate, local potential values, biofilm
conductivity and the concentration gradient of the species involved in the
process. A representative result from Marcus et al. [28]’s study is
shown in Fig. 4, describing the change in current density and steady
state profiles of the local potential (φ), substrate and active biomass
volume fraction at different detachment rates. This model predicts MFC
performance trends that have been observed before, however it does
not include any direct experimental comparison [28].

Marcus et al. [28] model served as a basis for many advanced direct
conduction based models developed in future. For example, Merkey
and Chopp [36], extended Marcus et al. [28]’s work to develop a two di-
mensional model for studying the influence of anode geometry on the
MFC performance. This model is validated with experimental data and
used for studying the effect of anode numbers, fluid flow speed and
anode density on current production [36]. In a follow-up study Merkey
and Chopp [48] extended their previous model [36], to study the
competitive growth characteristics between two anode-respiring bac-
terial species, one that utilize a diffusive mediator, other that utilizes a
Conductive extracellular polymer (EPS) matrix to transfer electrons to the anode. The competition between the two species for space and nutrients is explored and it is found that the bacteria that conducted electrons using the EPS matrix show optimal growth [48]. Renslow et al. [49] also developed a biofilm model considering dual extracellular electron transfer mechanisms.

Sedaqatvand et al. [50] extended the conduction based approach of Marcus et al. [28] and combined with Genetic Algorithm to estimate the design parameters of a single chamber MFC treating dairy wastewater. They found that in a system with concentration boundary layer and biofilm conductivity as the main resistances, the contributions of ohmic and concentration overpotentials are almost equal in dropping cell voltage [50]. Alavijeh et al. [22] also used Marcus et al. [28]’s model as a basis to develop a general microbial electrochemical cell model that can be used to study both microbial fuel cell as well as microbial electrolysis cell. Though very similar to Marcus et al. [28]’s formulation, this model considers Bernard’s anaerobic digestion kinetics at the anode and in case of MEC it also provides an expression to calculate the net volumetric hydrogen production rate at the cathode based on the cathode efficiency [22]. Kazemi et al. [23] adopted the conductive biofilm approach and developed the first model for MES. Applying Marcus et al. [28]’s approach to model a biocathode, this 1D dynamic model describes microbial based electrosynthesis of organic compounds (acetate) and can provide useful information regarding electron transfer in biofilms and kinetic parameters for bacterial growth [23]. Recently, Teleken et al. [51] also used the conductive biofilm approach to model the bioanode of an MFC inoculated with marine microorganisms.

Other than the seminal model of Marcus et al. [28], which has been...
Table 3

<table>
<thead>
<tr>
<th>Equation</th>
<th>Description</th>
<th>Reference</th>
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<tbody>
<tr>
<td>$\mu = \mu_{max} \frac{S}{K_S + S}$</td>
<td>Monod kinetics</td>
<td>[21,31]</td>
</tr>
<tr>
<td>$q = q_{max} \frac{S}{K_S + S}$</td>
<td>Multiplicative Monod Kinetics</td>
<td></td>
</tr>
<tr>
<td>$q = q_{max} \frac{S}{K_S + S} + \gamma \frac{S}{K_m + \gamma S}$</td>
<td>Nerst-Monod Kinetics</td>
<td></td>
</tr>
<tr>
<td>$q = q_{max} (1 - e^{- \frac{1}{S}})$</td>
<td>Butler-Volmer-Monod equation</td>
<td>[28]</td>
</tr>
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Model to describe microbial growth rate and substrate consumption rate, when growth rate is only limited by the substrate (nutrient) concentration, $\mu = \text{specific growth rate}$, $\mu_{max} = \text{maximum specific growth rate}$, $S = \text{limiting substrate concentration}$, $K_S = \text{half saturation (Monod) constant}$, $q = \text{substrate consumption rate}$, $q_{max} = \text{maximum substrate consumption rate}$. Here microbial growth rate is assumed to be limited by concentrations of substrate and oxidized form of the mediator. $K_m = \text{mediator half saturation coefficient}$, $\gamma = \text{oxidized mediator concentration}$.

Assuming the biofilm as a porous conductive matrix, Marcus et al. [28] derived this equation by combining the Nerst model typically used by electrochemists to describe redox potential with the Monod kinetics. $F = \text{Faraday constant}$, $\eta = \text{local potential}$, $R = \text{ideal gas constant}$, $T = \text{temperature}$.

Substrate and biomass material balance is described assuming biofilm retention with equal influx and effluent rates. This specific model considers that substrate is being consumed by two competing bacterial populations [31]. Subscripts $a$ and $m$ refer to anodophilic and methanogenic bacteria, $X = \text{biomass concentration}$, $S_0 = \text{influx substrate concentration}$, $K_m = \text{decay rate}$, $\alpha = \text{biofilm retention constant}$, $D = \text{dilution rate}$, $t = \text{time}$.

Steady state material balance for substrate based on diffusion and convection. Dynamic mass balance for the active and inactive bacteria based on accumulation, advection, growth and decay of the two microbial communities in the biofilm. $D_{fl} = \text{diffusion coefficient of substrate in the biofilm}$, $\phi_a$ and $\phi_i = \text{volumetric fraction of active and inactive biomass}$, $\chi_{fl} = \text{density of active and inactive biomass}$.

Applicable for both continuous and batch mode ($\phi = 0$), this model provides the biomass and substrate material balances in both biofilm and the bulk liquid. The bulk liquid is assumed to be completely mixed, whereas biofilm is characterized by spatial concentration gradients. Subscript $B$ and $fi$ refer to biofilm and bulk liquid respectively. $D = \text{diffusion coefficient}$, $\phi = \text{volumetric flowrate}$, $K_m$ and $X_m = \text{initial substrate and biomass concentration}$, $r_a$ and $r_B = \text{net substrate reaction rate and net biomass reaction rate in the bulk}$, $r_{fl} = \text{net substrate reaction rate in the biofilm}$, $r_{fl, a} = \text{electrochemical rates of substrate component change on the electrode surface}$, $\eta_{fl}$ and $\eta_{fl, a} = \text{net biomass detachment and attachment rates}$, $v_B = \text{bulk liquid volume}$.

Used to calculate BES cell output voltage and current, accounting for activation, concentration and ohmic polarization losses. $V_{cell} = \text{BES cell voltage}$, $I = \text{current}$, $R_{ext} = \text{external resistance}$, Subscripts $C$ and $A$ represent quantities at cathode and anode respectively. $E^0 = \text{ideal equilibrium cell potential}$, $\eta_{act} = \text{activation overpotential}$, $\eta_{conc} = \text{concentration overpotential}$, $\eta_{ohm} = \text{ohmic overpotential}$.

Expression for current distribution in the conductive biofilm matrix considering electron generation from biomass synthesis and self-oxidation. $j = \text{current density}$, $k_{bio} = \text{biomass conductivity}$, $\eta = \text{local potential}$, $\gamma_1$ and $\gamma_2 = \text{electron equivalence of substrate and active biomass}$, $\tau = \text{time conversion factor}$, $f^0_{e, fl} = \text{fraction of electrons from substrate used for energy generation to support synthesis}$, $\chi_{fl} = \text{density of active biomass}$, $R_{ext} = \text{specified rate of endogenous respiration}$.

Expression for current distribution derived by combining Butler-Volmer kinetics with enzyme kinetics (to represent biochemical conversion). $I_{max} = \text{maximum current density}$, $K_i$ and $K_2$ = lumped parameters, $K_m = \text{substrate affinity constant}$, $f = F(\tau)$.

Adopted and expanded in numerous other studies, another benchmark model was developed by Pinto et al. [31]. In this dynamic model based on ODEs, Pinto et al. [31] describes the anodic chamber of a single chamber MFC considering two microbial populations (anodophilic and methanogenic bacteria). The charge transfer between the substrate and the anode is based on an intracellular mediator, however extracellular electron transfer via nanowires or direct contact with the anode is also considered. The microbial populations are assumed to be both attached (anodophilic and methanogenic) and suspended (methanogenic). Substrate (acetate) is assumed to be uniformly mixed in the anodic chamber and the biofilm formation and retention is simulated using a two-phase growth-washout model. Growth of anodophilic bacteria is described by the multiplicative Monod kinetics and mass balance for substrate and intracellular mediators is also described. The expression for current output is derived using Ohm’s law and the voltage over-potentials [31].

The model parameters are estimated using the Nelder-Mead simplex algorithm and the model is then used to study the influence of organic load and external resistance on MFC power output and long-term system performance. This ODE based simple model is easy to implement, allows fast numerical simulations and can be used for both process control and optimization [31]. In a follow up study Pinto et al. [35] extended the model to describe MEC operation and predict $H_2$ production rate. In this 1D dynamic model, the two population model described in the previous study was combined with the anaerobic digestion model proposed by Bernard et al. [52] under the assumption that anaerobic degradation of wastewater can be described by a single hydrolysis and fermentation step of complex organic matter conversion to acetate [35]. This is the first model that described $H_2$ production from complex organic matter in an MEC [35].

Ping et al. [31]’s model was also extended further by Ping et al. [24]
to simulate the dynamic behaviour of a microbial desalination cell. This model [24] is also based on ODEs similar to Pinto et al. [31], but in addition to the mass balance for the substrate, microorganisms and the mediators, the mass balance for salt has also been described. After obtaining the model parameters by fitting with experimental data from small lab-scale MDC system, the model is used to predict the effect of different parameters (substrate flow rate, external electrical resistance, salt solution flow rate) on performance of the MDC. The model is also validated with experimental data from a large-scale MDC system [24]. Ping et al. [24]'s model was further extended to study brackish water desalination and wastewater treatment, boron removal using different BESs [53,41]. Recio-Garrido et al. [54] combined the model equations described by Pinto et al. [31] with the equivalent electrical circuit model for of an MFC to understand the effect of charge storage on the fuel cell performance. This combined bioelectrochemical-electrical model allowed for both process optimization (that can be performed offline) as well as online approach that allows real time estimation of electrical parameters such as internal capacitance (C), open circuit voltage (Eoc), and internal resistance of the system, as the simulations are run together with the experiment. This model presents a guiding pathway for development of software sensors for process control and online monitoring of MFCs [54]. Nakasugi et al. [55] also used Pinto et al. [35]'s approach as a basis to model electromethanogenesis (EM) in a BES.

3.1. Anode and cathode combined analysis

All the models discussed so far are limited to the analysis of a single electrode (anode or cathode) of a BES. As has been highlighted in several studies, both the electrodes of BES influence the performance of the process [9,19]. In order to obtain a thorough understanding of the BES, it is important to develop coupled models that include the phenomena occurring at both anode and cathode and should simultaneously simulate both the fast electrical dynamics and mass transfer processes (milliseconds to seconds) along with the relatively slow dynamics of microbial growth dynamics (hours to days) [19].

The first model for BES that considered the phenomena in both anode and cathode chambers was developed by Zeng et al. [34]. This work is based on similar models developed previously for chemical fuel cells such as direct ascorbic acid fuel cells and direct methanol fuel cells [34]. In this two chamber model, both the bio-electrochemical and the electrochemical reactions occurring at anode and cathode respectively are modeled using Butler-Volmer expressions. Protons and cations are neglected in the cathode reaction, however. Both anode and cathode chambers are assumed to be perfectly mixed, and thus the mass balance of components in anode and cathode chambers only varies in time, as a function of the corresponding reaction rates. The charge balance at the anode and cathode is based on the cell current density, the respective capacitances and the reaction rates [34]. The total cell voltage is calculated after accounting for the voltage losses due to activation and concentration over-potentials as well as the membrane and solution resistances. The model parameters are estimated by fitting with experimental data and the model is then used to simulate both steady state and dynamic performance of the MFC as a function of operating parameters such as the acetate feed flow-rate, acetate feed concentration. The model is tested with both simple (acetate) and complex (artificial wastewater) substrate feed. While this is the first model to develop a coupled solution considering both the electrodes, one of the major limitation of this study is that it does not consider the biofilm characteristics at the anode which have been shown to significantly affect the performance of the system. However the model is very easy to implement and can be used as an effective tool for fast optimization studies of MFC and also serves as a good basis for the development of more detailed two-chamber models [34].

Oliveira et al. [37] extended Zeng et al. [34]'s model by including heat balance and biofilm formation and developed a more comprehensive two chamber model for MFC performance analysis. In this 1D steady state model, the bio-electrochemical reaction occurring at the anode is modeled using Tafel and Monod equations and the electrochemical reaction at cathode is described by Tafel equation. Effective Fick model is used to describe the mass transfer in the electrodes and the biofilm, and heat balance is based on Fourier’s law. Interface concentrations of the components are described using partial coefficients assuming local equilibrium [37]. The model predictions are compared with both experimental and previous simulation studies and the model is found to show the correct trends of the influence of current density on the anode and cathode overpotential, on the biofilm thickness, temperature and concentration profiles [37]. With a simple 1D steady state formulation this model is quite easy and computationally less straining.
to solve and can be used for quick optimization studies [37]. Oliveira et al. [37]’s model is an improvement over Zeng et al. [34]’s approach, however it does not include dynamic analysis and thus cannot be used to study and understand how operational parameters influence the MFC performance over time. Also, though this model considers the biofilm and includes the Monod kinetics in the anode electrochemical equation, the biofilm is assumed to remain constant assuming equal microbial growth and biomass losses [37]. This assumption significantly reduces the biofilm functionality in the model [37].

Yao et al. [39] further extended the dual chamber MFC models proposed by Zeng et al. [34] and Oliveira et al. [37], by developing a 2D two phase mass transport model for MFC. This model assumes a steady state mass transport, and does not include diffusion of CO₂, O₂ and acetate into the membrane. An agglomerate model has been used to describe the mass transport process in the cathode catalyst layer. The local over-potential is calculated assuming proton transport in liquid phase and electron transport in the solid phase of the MFC. The model domain included anode chamber (represented by the biofilm and the anode electrode layer), the membrane and the cathode chamber (represented by the cathode catalyst layer and the cathode electrode layer). Everything except the cathode electrode layer is considered as the liquid phase region for electric potential calculations. Reactions at the anode and cathode are represented by the Tafel-Monod expression and the Tafel-like expressions respectively and mass conservations equations were based on the classical two-phase flow theory. To simplify the calculations, the microbial composition is assumed to be uniform over the biofilm and due to steady state assumption the rate of change of biomass over time is also considered zero. The 2D model is solved using the finite volume method and is validated against experimental data which showed good agreement. Subsequently it is used to study the effect of the biofilm and solution conductivity and it is found that while biofilm conductivity had a continuous linear influence on improving the cell performance, the ionic conductivity reaches a plateau after an initial improvement. The mass transfer results show a concentration gradient in the x direction for acetate, while oxygen concentration in the porous cathode show a nearly uniform distribution [39]. Gas-liquid two-phase flow typically occurs in an MFC and this model presents the first formulation to model this two phase flow [39]. However it has a lot of scope for improvement in future by providing a more dynamic analysis with a detailed biofilm growth model and also improving the internal distribution of products and reactants in the model.

Sirinutsomboon [38] developed a 1D dynamic model for a single chamber membraneless MFC considering both anode and cathode. In this study, sucrose (which is a primary sugar of Molasses, a by-product of the sugar industry) is used as a substrate for the anode bacteria and a layer of polytetrafluoroethylene (that is permeable to oxygen) is used to separate the anolyte from the cathode. The rate of substrate consumption at the anode is described using the Nernst-Monod equation, while the oxygen reduction reaction at the cathode is expressed using Monod and Butler-Volmer kinetics. Diffusion of oxygen in the cathode electrode is described by Fick’s second law [38]. The biofilm description in this model is similar to that by Marcus et al. [28]. Biofilm is assumed to be a conductive matrix and the local potential is calculated based on Ohm’s law and the steady-state electron balance [38]. The simulation program for this model is developed in a visual basic interface and is used to study the effect of operational parameters such as the initial substrate concentration, biofilm thickness, cathode thickness, etc. on the system performance. This model does not describe any expressions for change in active biomass concentration and thus the biofilm thickness basically remains the same as the initially selected value [38]. chamber batch MFC model [42] developed a two chamber batch MFC model considering both electrodes based on a lumped formulation. The model consists of three domains, bulk liquid in the anode chamber, biofilm attached to anode and bulk liquid in the cathode chamber. Lactate is assumed to be the substrate at anode, which is reduced by the bacteria to release H⁺ ions and electrons. Electrons are assumed to be transferred to the anode via the direct conduction mechanism proposed by Marcus et al. [28]. Three kinetic models are tested to calculate the bacterial growth rate, namely the Monod equation, Blackman model and the Tessier model. These growth rates are substituted in the Nernst-Monod equation to derive the rate of substrate consumption. Expression for mass balance in the biofilm of the active and inactive biomass, substrate, CO₂ and H⁺ ions are described. Additionally, mass balance for substrate and CO₂ in the anode bulk liquid and O₂ in the cathode bulk liquid are described. The total MFC output voltage is calculated based on the Ohmic, activation and concentration losses. Model parameters are estimated using a parametric estimation study based on experimental data. The model predictions of voltage and current are subsequently compared with experimental results and an excellent agreement is obtained. It is also shown that the Monod model predicts the substrate concentration more accurately as compared to the Backman and Tessier models [42]. This batch MFC model [42] is extended to a continuous two chamber MFC model by Esfandyari et al. [43]. These simple models are quite useful in quick performance testing of MFC voltage and current. However the lumped formulation assumes that all quantities are uniformly distributed and no change occurs spatially, which is a major limitation of this approach [42,43]. Many studies in the past have shown that the substrate and other components have a spatial gradient, particularly in the biofilm which influences the dynamic performance of the BES.

Ismail and Habeeb [56] combined the approaches used in previous models [32,34,37] and developed a two chamber MFC model by integrating the macro-scale dynamic mass balance for solutes and biomass in the bulk liquid with the micro-scale phenomena in the biofilm represented by a 2D model. The fluxes are integrated over the open boundaries of the micro-scale domain to link the two scales in the model [56].

Ou et al. [57–59] published a series of studies focused on developing steady state and transient mathematical models for studying single chamber air cathode MFC systems. It is found that electrical migration did not have a major impact on the power densities of MFC [57]. It is also found that the diffusion and dissolved oxygen content in the cathode are the crucial parameters influencing the performance of the air-cathode MFC [58]. The steady state model showed that PBS buffer solution performed better compared to other buffers (NaHCO₃, NH₄Cl) for pH neutralization [59].

3.2. Life cycle analysis

Along with the steady state and dynamic performance studies of BES, it is also important to conduct a life cycle and economic analysis to determine the environmental and economic implications of the system [4,60–62]. There are some studies that present the environmental costs and benefits based on life cycle assessment (LCA) of microbial electrochemical cells such as MFC and MEC [61,63]. Also, life cycle analysis of BES used for resource recovery from (metal rich) wastewater (e.g. from mining) has been investigated to relate energy flow, charge balance, Coulombic efficiency and rates of treatments of organic waste rich (at anode) and metal rich (at cathode) wastewaters [64,65]. This integrated system thus provides two simultaneous services: reduced metals are deposited on the cathode and organic wastewater is treated at the anode. In a recent study, Shemfe et al. [66] have presented a modeling framework that integrates the dynamic simulation model with life cycle and techno-economic analysis for a BES based on formic acid synthesis. Such integrated models can be used to study the impact of operating parameters of BES based on environmental and economic objectives and need to be explored further.

4. Novel modeling strategies and integrated system models

In addition to the above standard BES models based on ordinary or
partial differential equations, there are several mathematical models that have been developed using other methodologies such as the models based on artificial intelligence or the cellular non-linear network (CNN) model, etc. There are many other models that are based on standard equations but have been developed for studying a specific parameter in a BES (like ion transport, the polarisation curve, control, etc.) or for investigating novel BES applications/designs by integrating with other technologies. A list of several such non-traditional models has been described in the Fig. 5.

The reference list cited against each category in Fig. 5 is not exhaustive. The aim here is to highlight some notable work and guide the readers towards the relevant literature.

4.1. Polarisation curve

Wen et al. [67] developed an MFC model based on polarisation curve and found that reaction kinetics and mass transfer losses contributed the most towards the MFC performance. Hamelers et al. [45] derived the Butler-Volmer-Monod kinetic model to represent the biochemical and electron transfer reactions at the bio-anode of an MFC and applied this model to a set of polarisation curves obtained under different growth conditions and anode materials. When compared to the polarisation curves obtained using the Nernst-Monod model, the Butler-Volmer-Monod model is shown to provide a better agreement with experimental data [45].

4.2. Ion transport

Harnisch et al. [68] developed an explicit model to describe ion transport across ion exchange membranes. Diffusion and migration of ions is described using the Nernst-Planck equation. They showed that the presence of membrane causes a pH gradient and a significant voltage drop (due to increase in ohmic membrane resistance) [68]. Some other BES Models developed by Dykstra et al. [69], Liu et al. [70] and Qin et al. [71], are focussed on studying ion transport through membranes and ammonia recovery at the cathode.

4.3. Control models

Yan and Fan [72] combined the two chamber dynamic model proposed by Zeng et al. [34] with a fuzzy logic based PID (proportional-integral-derivative) controller to achieve a constant voltage output in an MFC. In a later study Fan et al. [73], designed a model predictive controller that is based on Laguerre function and exponential data weighting and found that this improved controller provides good steady-state behaviour as well as satisfactory dynamic property. Abul et al. [74] also developed a control-oriented dynamic model for MFC with state-space representation. The model is validated against experimental data from a membrane-less single-chamber MFC system. The model predictions of open circuit anode potential, cathode potential and substrate concentration showed good agreement with the experimental results.
4.4. Artificial intelligence (AI) methods

Garg et al. [25] used artificial intelligence (AI) methods namely, the multi-genre genetic programming (MGGP), artificial neural network (ANN) and support vector regression (SVR) to model the voltage parameter (based on temperature and ferrous sulfate concentrations) of MFC system during, before and after start-up operating conditions. In terms of generalization ability and the computational time, MGGP model showed the best performance followed by ANN and SVR. Lesnik and Liu [75] used ANN based machine-learning, data-mining approach to develop a stochastic model for predicting the microbial assemblages and reactor characteristics in a study involving 33 MFCs using a number of substrates and three different wastewater compositions. The ANN-based models successfully predicted changes in both biofilm communities and reactor performance at a given taxon level within 2–16% error incorporating both biotic and abiotic parameters. The models that used biotic interactions show more accurate predictions than those that did not use them [75]. These AI based models show great potential in predicting the performance of BES systems.

4.5. Proton condition in biofilm

Marcus et al. [76] developed a novel modeling platform, Proton Condition in Biofilm (PCBIOFILM) describing the release of protons from anode-respiring bacteria (ARB) that are common in biofilm anodes of different microbial electrochemical cells [76]. This model helps in linking the proton condition to the diffusion and reactions at the biofilm anode. PCBIOFILM model explains how changes of pH in the biofilms are controlled via proton transport by the diffusion of phosphates and carbonates (alkalinity carriers) and why carbonates provide higher current density, faring as a better source of alkalinity than phosphates. In a following study, Marcus et al. [77] further expanded the PCBIOFILM model by including electrical neutrality and an electrical field to study the impact of migration on ion-transport.

4.6. Equivalent electrical circuit model

Coronado et al. [78] developed a simple equivalent electrical circuit (EEC) model to represent the fast process dynamics linked to the electrical properties of a MFC operated with pulse-width modulated connection of the electrical load. This simple EEC model described the slow and fast output voltage responses using two resistors and a capacitor. All the electrical elements are assumed constant and the model parameters are obtained by data fitting using experimental results. Though this model has a limited predictive capacity it may be useful for performance optimization and real time MFC control. The on-line parameter identification strategy employed in another study by Coronado et al. [79], highlighted its usability for real time MFC monitoring. Fig. 6 shows the MFC Equivalent Circuit Model described by Coronado et al. [79]. Park et al. [80] developed a more advanced EEC model by representing equivalent capacitance in parallel and series resistances that allowed dynamic characterisation of both output voltage and current and helped in explaining the anodic electron flow and electrical charge storage in an MFC system. In addition to the above more specific EEC models are described in Xia et al. [20].

4.7. BES integrated with membrane filtration

Membrane bioelectrochemical reactors (MBERs) obtained by integrating membrane filtration with bioelectrochemical systems can produce high-quality effluents (free from volatile suspended solid (VSS) and pathogens) and are thus being proposed as a useful approach for sustainable wastewater treatment. Li and He [81] developed a mathematical model for MBERs by combining microbial fuel cell and membrane bioreactor models that are linked by organic loading rates (OLR), aeration intensity, and reactor configuration. This model is used to predict the substrate consumption, membrane fouling, current generation and nitrogen removal within MBERs. Furthermore, Li et al. [82] developed a mathematical model for MBERs with an external membrane module.

4.8. Integrated photo-bioelectrochemical system

Luo et al. [83] adopted the approaches developed in previous studies [31, 24] to develop a mathematical model for integrated photo-bioelectrochemical (IPB) system for simultaneous wastewater treatment and bioenergy recovery. While most of the basic equations are adopted from Pinto et al. [31], this model also considered the mass balance in the cathodic chamber for the substrate (COD), suspended algal biomass, dissolved oxygen, \( \text{NH}_4^+ \)-N, \( \text{NO}_3^- \)-N, and total phosphorus in the cathode. Additionally the current generation terms included the overpotential introduced by oxygen concentration in the cathode. Total 53 model parameters are estimated using data fitting against results from experiments. The IPB reactor performance is studied at different operational conditions (influent COD concentration and the anolyte flow rate) [83]. This is the first model developed for an IPB system and more advanced models can be developed by including the pH calculations, spatial concentration gradient in the cathode and including more diverse mechanisms of algal-bacterial consortium in the cathode.

4.9. Integration with activated sludge model

Wastewater treatment typically involves more diverse substrate feed and bacterial population, however this is seldom reported in the mathematical models for BES. Capodaglio et al. [84] attempted to address this issue by integrating the 1D dynamic model of Capodaglio et al. [31] with the Activated Sludge Model No. 2d (ASM2d) and a more complex substrate feed represented in particulate (X) and soluble (S) forms. This model is used to predict the growth rate of microorganisms, COD degradation, methane production, and current generation in a MFC system. The results from the model also showed reasonable comparison with experimental data [84]. In a recent study, Krieg et al. [85] developed a correlation between parameters from the activated sludge model number 1 (active heterotrophic and autotrophic biomass) and the measured current output of a MFC in a laboratory wastewater treatment plant.

4.10. Cellular non-linear network model

Tsompanas et al. [26] used a novel approach to study MFC performance. They used a cellular non-linear network (CNN), which is a uniform regular array of locally connected continuous-state machines, or nodes that update their states simultaneously in discrete time. Tsompanas et al. [26] used this network to simulate the reactions in a two chamber MFC assuming electron transfer via diffusible mediators. The double Monod limitation equation is used to calculate the substrate

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![MFC Equivalent Circuit Model](image_url)

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Fig. 6. MFC Equivalent Circuit Model described by Coronado et al. [79], consisting of two internal resistances R1 and R2 and internal capacitance C. [Figure has been reprinted from J. Process Control 35, 59-64; Copyright (2015) with permission from Elsevier.]

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consumption rate, Fick’s second law to represent diffusion and the Butler-Volmer equation to calculate anode current density and these are reflected in the local rule of the CNN structure. This model is designed in 2D and is used to study a cross sectional area near anode. The model is used to predict the spatial gradients of substrate and biomass as well as to investigate the effect of operating parameters on the current generation [26]. This new approach of using an array of analog dynamic processors or cells to represent a complex physical system has great potential and should be explored further to understand the coupled mechanisms governing BESs.

4.11. Microfluidic BES models

Mardanpour et al. [86] and Mardanpour and Yaghmaei [87] developed dynamic mathematical models to study microfluidic MFC and MEC systems. Mardanpour et al. [86]’s model for microfluidic MFC describes the substrate consumption and the bacterial distribution of both suspended and the bacteria attached to the anode electrode based on the transport parameters obtained from chemotaxis. The model is validated with experimental results from a glucose fed microfluidic MFC and is used to study the evolution of spatial distribution of the biomass and substrate, and effect of external resistance, substrate flow rate, and hydraulic diameter on the microfluidic MFC performance. It is found that the power generated in the system is inversely proportional to the hydraulic diameter of the microchannel. A similar model is used by Mardanpour and Yaghmaei [87] to study microfluidic MEC performance. The net hydrogen production rate is calculated based on the generated current and the cathode efficiency, and is also validated against experimental results from a glucose fed MEC.

CFD model is developed for two different types of helical anodes of a tubular MFC reactor. The fluid dynamics model helped in studying the influence of the flow channel geometry on the flow regime. Michie et al. [89] also studied three different helical anode geometries using computational fluid dynamics methodology and showed that fluid flow profiles have a major influence on the COS consumption and current generation. Kim et al. [90] studied the influence of fluid flow on the MFC performance using CFD models to simulate 12 MFC configurations obtained by varying the shape type (triangular or rectangular), length, angle and number of internal structures. Vilá-Rovira et al. [91] also developed a CFD model to study the hydrodynamics in BES anode comparing different electrode materials such as graphite rod, granular graphite, and stainless steel mesh or graphite plate. The results showed that anodes made of granular graphite or stainless steel mesh provided better water flow distribution and also favored higher attachment of biomass which would help in improving the BES performance. Zhao et al. [92] coupled the CFD with multi-order Butler-Volmer reactions to develop an integrated model for the anode of a tubular microbial fluid cell. While the multi-order Butler-Volmer reaction model described the substrate consumption and energy recovery, the CFD model analyzed the fluid flow behaviour and species transport. It is shown that the multi-order kinetic models provided a simpler methodology to study MFC performance as compared to the Monod-limitation equation used in many of the previous studies. The current generated using the model is compared with experimental results and showed good agreement. In a later study Zhao et al. [93] also used this coupled model to compare the performance of tubular reactor using three different anode geometries, two with granular activated carbon (GAC) as a reactive or as a non-reactive porous medium and one with no GAC. The results from this model showed that presence of GAC led to better flow distribution that helped in increasing current generation by at least 17%. Sobieszuk et al. [94] developed a CFD model for the anode chamber of a dual-chamber MFC working in continuous mode. The model is used to determine the exit age distribution or the residence time distribution (RTD) of the fluid flow, that are used to obtain the hold-back value and the mixing quality in the reactor and subsequently the optimal hydraulic retention.

4.12. Hydrodynamic analysis

In addition to the reaction kinetics, fluid flow patterns in the BES have been shown to have a significant impact on the performance of the system [88]. Some mathematical models have been developed specifically to focus on understanding the influence of hydrodynamics on the BES performance. In one of the first such studies by Kim et al. [88], a
time [95] used CFD modeling to study the fluid flow distributions of air-cathode single chamber microbial fuel cells with two different geometries, one in the shape of square and other shaped like a drop. The results are used to determine the optimum shape based on the percentage of exposed area between the two geometries.

5. Perspectives and recommendations

The last decade has witnessed an exceptional growth in the number of numerical studies of BES, particularly MFC. As we have seen, an array of different options in regards to the time and spatial dependence, biofilm and electrodes can be used while developing the mathematical models for BES. Fig. 7 shows a schematic of these various options and the corresponding sub-options that need to be considered in BES models.

These mathematical studies, together with a large number of experimental investigations have to a large extent proved the feasibility of MFC towards commercialization and have led to the emergence of several new start-ups focusing on bringing MFC to the market. However other BESs such as microbial electrolysis cell, microbial electroosynthesis and microbial desalination cell are still in the early development stages and need to overcome significant challenges in terms of overall efficiency and scalability before they can be ready for commercialization.

Researcher working on theoretical investigation of BES can choose any of the above mathematical models or develop their own mathematical models based on their final goal. If one is only looking for a quick performance test of a BES (to get an approximate estimate of the power output of an MFC or hydrogen production rate in an MEC), spatial variation of biomass and substrates in the electrode chambers may be neglected and simple models based on ODEs such as Pinto et al. [31,35,34,33], etc., can be used to obtain the required information. On the other hand if someone wants to closely study the biomass growth/decay, decomposition of complex substrate in pure/mixed bacterial culture, competition between bacterial communities, or other important phenomena in chemical/bio electrodes that influence the system performance, it would be useful to consider the detailed biofilm and substrate characteristics including the respective mass, charge and heat balances. However one can start with a simple 1D model and then successively more complex multi-dimensional analysis can be performed as described in Piccioreanu et al. [29,30,32,36,37,39], etc. It is also important to specify the electron transfer from or to the bacterial population. For bacteria that are known to act as a conductive matrix and transfer electrons via direct conduction, the Nernst-Monod model proposed by Marcus et al. [28] is a useful tool to describe the relation between substrate consumption rate and the voltage over-potential. Similarly mediated electron transfer can be modeled via different mediators (intracellular, redox, etc.) depending on the bacterial culture as has been described in previous studies such as Piccioreanu et al. [29,31], etc.

For researchers working on upgrading the existing models or development of new mathematical modeling approaches for BES, it is important to understand and address the shortcomings in the existing approaches. The 1D and 2D models based on the conductive biofilm approach [28,36], very closely capture the biomass growth/decay rates and use the Nernst-Monod equation to describe the electrochemical kinetics. However these models have neglected the electrolyte phase potential and the cathode kinetics in their calculations. These factors influence cell voltage and current profiles and ultimately the system performance. Also the conduction based models do not include ion transport and changes in pH in the electrode chambers, which is one of the major limiting factors in the two chamber BES configuration. Additionally, as the biofilm is being considered a porous solid conductor, the treatment of transport in such porous media should include diffusion theory applied at the pore scale, which is missing in the current approach.

In regards to the ODE based mathematical models (space independent models or 1D steady state models) one of the major issues is the gross oversimplification or non-consideration of the biofilm [31,33,34]. In order to understand the working of BES and depending on the type of BES, either improving its power generation capacity or COD removal efficiency or production formation rates, it is crucial to account for the electron exchange mechanisms between biofilms and electrodes. Different bacteria types exhibit different extracellular electron transfer mechanisms and determine the polarisation potential, making it one of the major current-limiting factor in any BES setup. Additionally, biofilm growth/decay rates also significantly influence the system performance and thus need to be accurately described in the mathematical models to predict realistic performance.

The multidimensional mathematical models such as those proposed by Piccioreanu et al. [29,30,32] provide a comprehensive description of the mass transfer, electrochemistry and biofilm kinetics, however the major drawback of such models are the long solution times and the required computational resources. The intricacies of the model also add additional resource time and complexity to the already onerous parameter estimation algorithms, vastly limiting their usability. Improvements in multiprocessing capabilities and programming may help to reduce the computational expense of these complex models and make them more useful for system optimization but their current use is still very limited. It is best recommended to simplify the 3D model than solving it in its full entirety. These multidimensional models are also focussed on the anode chamber and do not include the cathode kinetics or the electrolyte potential. Adding the additional physics can help to make these models more robust and reliable.

Also, most of the current BES mathematical models consider simple ‘representative’ wastewater as substrate. To predict the effective performance of real systems it is important to develop models with more complex biomass and substrate populations as would be potentially used in large scale practical applications. Also existing models of MEC typically consider a non-limiting cathode and predict the hydrogen production rate without including the dynamics of the cathode chamber. It is important to develop more detailed cathode models accounting for the different voltage losses that occur in both anode and cathode chambers for better predictions of MEC performance. Similarly for MES, where the existing mathematical models have only considered the cathode chamber, it is essential to account for the concentration gradients and the voltage losses of the complete cell (including both electrodes) to obtain more credible predictions.

Securing the relevant experimental parameters that are used in the mathematical models and the final experimental results for model validation, is quite challenging for all types of BES. However this information is crucial in developing a legitimate model that can be used to accurately describe the BES performance. It would be pragmatic to conduct complementary experimental studies together with mathematical models development, to obtain the relevant parameters and results for model validation. Use of novel modeling approaches such as artificial intelligence methods and cellular networks also show great potential in evaluating the influence of process parameters on BES systems and need to be explored further. Additionally, it is pivotal to link these parameters with their life cycle environmental and techno-economic performances for commercialization on a large scale.

The development of comprehensive mathematical models for the BES is essential to obtain a deeper insight into the physico-chemical and biological mechanisms governing the processes. The numerical models could compliment experiments and help to further develop BES at a reduced cost and time. Such model based design and optimization approaches which are common in chemical and bio-process engineering will be very important in advancing bioelectrochemical systems towards commercialization.

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