Available online at www.sciencedirect.com

ScienceDirect

Current Opinion in Electrochemistry

Review Article

Computational modelling as a design tool for bioelectrochemical systems

Laura Mais[1], Jesus Rodriguez[2], Nicola Melis[1], Annalisa Vacca[1] and Michele Mascia[1]

Abstract

Design of bioelectrochemical systems (BESs) needs to consider complex biological, physicochemical, and electrochemical phenomena, as well as aspects related to mass, charge and momentum transfer. Experimental optimisation of such complex systems will be too expensive in terms of time and cost, so that a model-based approach is a necessary route in BES design. In this work, the relevance of modelling in the literature on BESs is quantitatively assessed, and the main pros and cons of the different models of BES are identified. Among the different models, computational bioelectrochemical models (CBMs) are the most promising, the main potential and drawbacks of CBMs are then discussed, and the issues open for future research are indicated.

Addresses

[1] Università Degli Studi di Cagliari, Dipartimento di Ingegneria Meccanica, Chimica e Dei Materiali, Via Marengo 2, Cagliari 09123, Italy

[2] Centro Nacional Del Hidrógeno, Prolongación Fernando El Santo, S/n, Puertollano Ciudad Real 13500, Spain

Corresponding author: Mascia, Michele (michele.mascia@unica.it)

Current Opinion in Electrochemistry 2024, **44**:101460

This review comes from a themed issue on **Environmental Electrochemistry (2024)**

Edited by **Javier Llanos** and **Ignasi Sirés**

For complete overview about the section, refer Environmental Electrochemistry (2024)

Available online 16 February 2024

https://doi.org/10.1016/j.coelec.2024.101460

Keywords

Computational modelling, Microbial fuel cells, Microbial electrolysis cells, Multiphysics modelling.

Introduction

Bioelectrochemical systems (BESs) are emerging technologies that utilise electrochemically active microorganisms either to transform chemical energy in wastewater to electrical energy, through multiple microbial–electrochemical reactions in microbial fuel cells (MFCs), or to convert organic matter into hydrogen or a wide range of chemicals (such as methane, acetate, hydrogen peroxide, ethanol, and formic acid) with a reduced environmental impact by means of microbial electrolysis cells (MECs).

Phenomena taking place in BES are complex and cover a wide range of biological, physicochemical and electrochemical processes. A large number of factors could then influence the BES [1–4], including the substrate composition and concentration, the electron donors or acceptors availability, the bacteria strains and their electron transfer mechanisms (mediated by natural or artificial mediators or directly by membrane cytochromes) [5], the pH of anolyte and catholyte and the operating temperature. These complex processes result in a nonlinear relationship between the different variables involved, and correctly understanding the mechanisms that govern the performance of BESs with only experimental methods is very difficult [6–9].

The design aspects (anode, cathode, separator materials and geometries) and the operative mode (batch, fed-batch, or continuous) also play a fundamental role. Because of that, a significant number of studies have been conducted to optimise the design and performances of BES [10–12].

To design BES systems, a model-based approach is therefore essential as it allows reducing the expensive and time-consuming steps involved in experimental investigations as well as identifying the technology bottlenecks and improving the process performances [7,13]. Despite the potential, the number of studies on BES modelling is limited compared with the experimental studies, and mostly addressed to MFCs rather than other BES systems [9,14–16]. Moreover, different modelling approaches have been proposed, with different applications and purposes. The analysis of the existing literature may allow one to take stock of the results achieved, and in particular bibliometric and social network analysis may be combined to investigate on the specific topic. Maps based on network data allow the construction of a network based on the relationships among countries, journals, organisations, authors, and keywords related to the investigated topic. The VOSviewer software has been used to perform the

analysis of the data in which specific maps were used to represent the network of the relationships among keywords related to the investigated topic and subtopics.

This work reviews the main characteristics of the different approaches used in BES modelling. The quantitative relevance of modelling in the literature was assessed first with a metadata analysis; the relevant pros and cons of the different models proposed are summarised and then briefly discussed, with focus on the key input parameters and equations, and the potential use of modelling to drive the technology towards plant-scale. The computational modelling as the most promising tool for design, optimisation and scale-up is then critically discussed.

Analysis and discussion of data

Data from bibliographic analysis with SCOPUS have been elaborated with the VOSviewer software (VOSviewer-version 1.6.19 https://www.vosviewer.com/), an effective tool [17] to cluster publications and obtain a comprehensive overview of the results. Records included data of publication year, author, institution, source journal, keywords, title, and abstract.

The first step is to identify the keywords that are relevant to the research question, and should be specific and relevant to the topic of interest. The choice of these terms in the query makes it possible to identify the main research areas in the field.

Using the Scopus function "TITLE-ABS-KEY", the query Q1 was performed, with no time limit, and the search was updated on November 6, 2023; of note: the same search would probably yield slightly different results if performed on a different date.

Q1: (TITLE-ABS-KEY (modelling OR modeling OR model) AND (TITLE-ABS-KEY ("microbial fuel cell" OR "microbial fuel cells") OR TITLE-ABS-KEY ("microbial electrolysis cell" OR "microbial electrolysis cells") OR TITLE-ABS-KEY ("bioelectrochemical systems")))

The record was then imported on VOSviewer and subjected to a first analysis: 3462 records have been identified. The map has been created based on bibliographic data obtained from Scopus as data source: the co-occurrence analysis has been performed, in which the relatedness of items is determined based on the number of documents in which they occur together. Moreover, author keywords have been selected as unit of analysis based on the full counting method. Figure 1 shows a visual representation of the results, where the size of the nodes varies with the occurrence (ocr) and then the relevance of the keywords; the links between nodes indicate a relatedness, the thickness of the arcs depends on the number of documents the keywords occurred together in. In particular, only 44 keywords occur together at least 10 times. Colours give an indication of the age of the papers, and a score is attributed to the items, evaluated as the average year of publication (APY) of the papers that report the related keywords. The average publication year of the documents represents custom score attributes in which a keyword or a term occurs, or the average publication year of the documents published by a source, an author, an organisation, or a country.

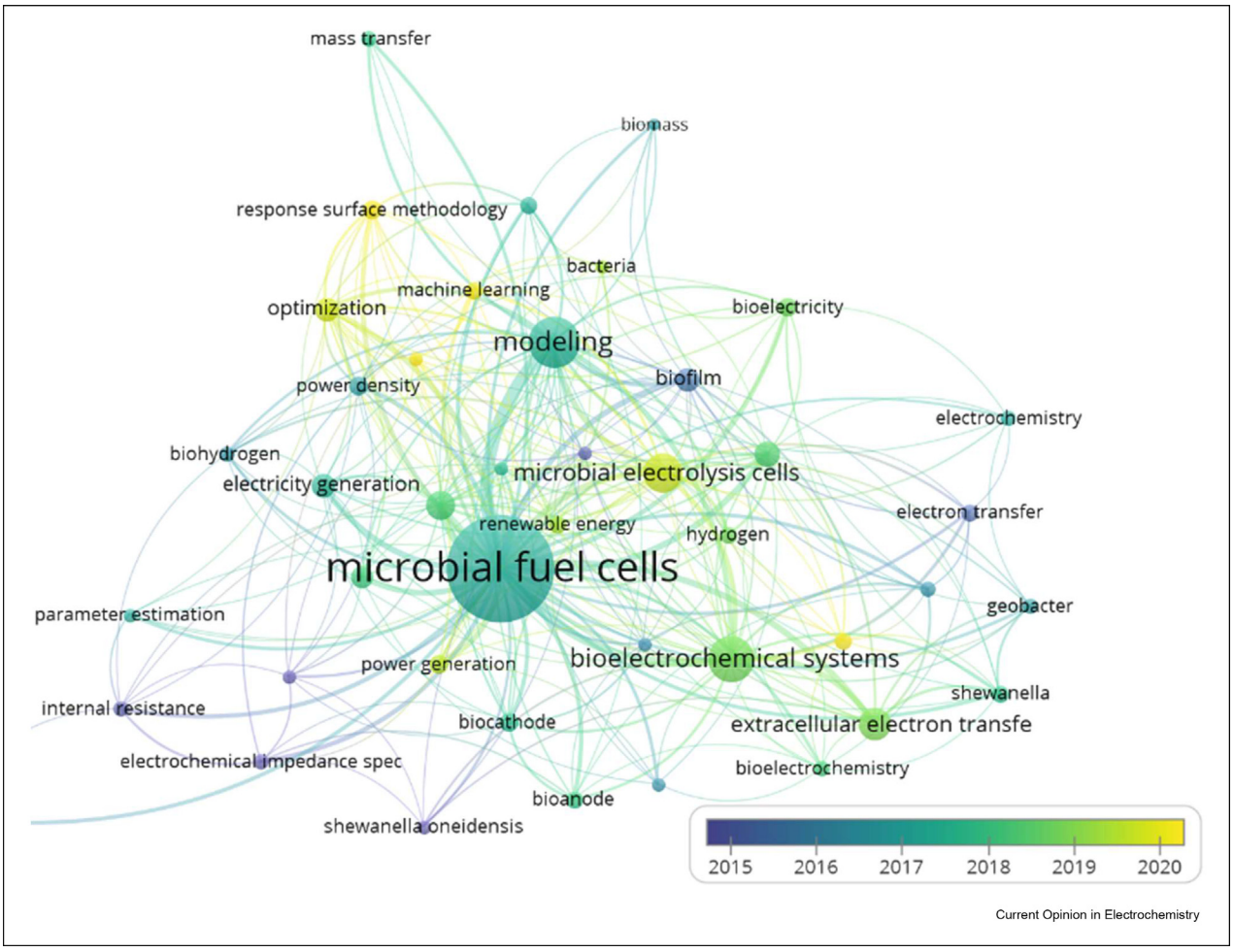
From the node's size, MFCs (ocr = 667) and modelling (ocr = 151) have the highest relevance, with a APY of about 2017; the nodes bioelectrochemical systems (ocr = 128) and MECs (ocr = 90) are representative of articles with a more recent APY, 2018.6 and 2019.5, respectively. These results highlight that the microbial electrochemical technology is of great interest for the scientific community, with growing attention towards microbial electrolysis as a sustainable system for green hydrogen production [18]. The node modelling is strongly related to MFCs, confirming that the number of papers on modelling of MFCs is currently considerably higher than that of MEC.

Figure 1 also shows smaller nodes related to the application to BES optimisation of the new trends in numerical studies, including machine learning (APY = 2021.5, ocr = 19) and artificial intelligence (APY = 2021.9, ocr = 11): as it could be expected, the APY of the relevant papers is high.

Data in Figure 1 provide a snapshot of the research on modelling BESs: a wider interest can be seen in modelling MFCs than MECs, while in the recent years the interest is shifting towards microbial electrolysis. Hydrogen-related topics including the so-called biohydrogen, are the subject of many recent works, which reflects the general trend of the research on electrochemical technologies. Optimisation and machine learning are subjects that have aroused a lot of interest in the newest research, with less attention paid to fundamental topics of microbial electrochemistry including biofilm growth and internal resistance.

Anyway, different approaches have been used in modelling of BES, based either on physical chemical and biological equations or statistical analysis of data. Statistical models can overcome the need of a complete and exhaustive rationalisation of the involved phenomena, although giving satisfying-to-excellent outcomes in terms of simulation of the results. Despite this, most of the data-driven models might fail in the prediction without a sufficiently large experimental data pool [19]. The design of bioelectrochemical reactors requires the definition of physical features. Consequently, an approach centred on identifying the relevant

Figure 1



Co-occurrence analysis: Visual map of keywords in papers on modelling of bioelectrochemical systems. Colours in the map are based on the average year of publication of the papers; size of the nodes refers to the relevance of the keyword.

phenomena and expressing them through equations might be more indicated. A wide range of models can be identified including equivalent circuits (EC) models [20–22] and complex multidimensional models, with the relevant pros and cons. An in-depth analysis of all these models is out of the scope of this work, and can be found in Refs. [9,23–25]: a summary is shown in Table 1.

Bioelectrochemical and equivalent circuits models use electrochemical impedance spectroscopy [22,26], linear sweep or cyclic voltammetry [24,27] to quantify the internal resistance and the internal capacitance related to anode, cathode, and other components of the cell; however, it lacks predictive capacity as with qualitative descriptions only short-term trends can be predicted. Kinetic and 1-D balance-based models also present the same limits.

Computational bioelectrochemical modelling (CBM) requires the numerical solution of complex, non-linear sets of partial differential equations. The numerical solution of CBM is usually obtained with finite volumes or finite differences methods and requires a considerable number of parameters to be available. However, computational modelling is the state of the art in design for many applications including fluid transfer and chemical reactors, and so it is expected to become for bioelectrochemical systems, where balancing the accuracy of the assumptions and complexity of the solution will be paramount.

Many authors have defined the following steps to build a computational model before solving and validating: i) defining the geometry (domains of integration), ii) choice of the physics (set of equations), and iii) defining and optimising the meshes [14]. The main challenge

Table 1

Breakdown of the main modelling approaches proposed for bioelectrochemical systems.

Type of model	Equations	Output	Parameters	Parametrisation	Pros	Cons
bioelectrochemical models	Current-overpotential equations	Polarisation curves Power curves (MFCs)	Overpotentials (activation and mass transfer) internal resistance	Calculated from polarisation experiments	Simplicity, low time spending for experiments; useful for fast characterisation of existing systems	Oversimplification of phenomena, scarcely useful for design
Equivalent circuits	State-space equations	Phase/frequency plots, including Bode and Nyquist plots; circuit parameters	Circuit parameters	Calculated from electrochemical impedance spectroscopy (EIS)	Simplicity, low time spending for experiments; useful for fast characterisation of existing systems	Oversimplification of phenomena, assumption of linear system as prerequisite scarcely useful for design
Kinetic models	Kinetic equations	Trends with time	Kinetic parameters	Fitting of experimental trends with time; single measures (e.g. conductivity)	Simplicity; useful for lab data interpretation and preliminary design of batch systems	Assumption of fully mixed systems; Scarcely useful for design and scale-up
1D balance-based models	Balance equations (charge, energy, mass); kinetics	1D profiles as a function of length and time	Transport and kinetic parameters; conductivities; flow velocity	Experimental data; single measures (e.g. conductivity)	Low complexity; useful for data interpretation and for preliminary design under ideal flow conditions	Limited to 1D geometries; high number of parameters required; oversimplification of complex geometries and systems under non-ideal flow conditions
Computational bioelectrochemical models	Balance equations (charge, energy, mass); flow equations; kinetics	2D and 3D profiles as a function of length and time	Transport and kinetic parameters; conductivities; flow parameters	Experimental data; single measures (e.g. conductivity)	Useful for design under nonideal conditions; effective in identifying local malfunctions, including starvation zones; monitoring of hard to measure parameters	High number of parameters required, high complexity; high computational spending

facing CBM is finding a compromise between accurate representation of the system and computational cost and time. CMB may be used to solve complex problems, considering spatial and temporal parameters in multi-dimensional systems, and providing numerical description of these hard-to-measure aspects [23,28−30]. CBM numerically simulate several phenomena including biofilm growth, microbial distribution on the electrode, electrode reactions, coexistence of different bacteria, and ion transport through the membrane [27,31−33].

Clearly, this leads to high complexity in building and solving the models, as many parameters, complex geometries, and a variety of phenomena need to be identified, with an increase in computational costs including computational time and memory storage requirements [34]. Several assumptions have been proposed to reduce the computational cost while maintaining acceptable reliability and accuracy discarding phenomena or parameters of low influence:

- Biofilm as a conductive porous solid with a fixed thickness [14].
- Single population of bacteria in the biofilm or neglect bacteria in the bulk [35].
- Simplification of the substrate (single electron donor) [36].
- Substrate evenly distributed in anolyte (equal concentration of reactants in the bulk, the biofilm surface and inside the bacteria) [37,38].

These assumptions facilitate the modelling process, however, some of them may not be adequate; as an example, steady approximation cannot interpret the biofilm growth, where a nucleation-growth mechanism is more effective, single population of bacteria may not represent complex consortia, and concentration gradients cannot be neglected when the anode present porous structures or under flow conditions with low velocities [6].

Parametrisation of CBM would require a complete characterisation of phenomena related to bioelectrochemical processes, many experimental data and/or online analyses to account for variations in time and space, which would ultimately be impractical with BES operations [39]. Strategies to minimise the experimental data have been proposed such as design of experiments (DOE) [40].

Experiments allow determining key parameters of the model, but also its validation. In this case, the error between experimental and simulated values can provide information on phenomena that may be underestimated or inadequately considered. Several parameters were proposed to measure the error of prediction but the most used are the mean square errors (MSE), the root mean square error (RMSE), and the coefficient of determination (R2) [41]. RMSE value below 20% is generally accepted, although a threshold may vary due to diversity of BES systems and cases [37].

Sensitivity analysis can be very useful to determine the parameters that most affect the numerical solution and to assess the validity of the assumptions [42,43]. More sensitive parameters must take priority and should be adjusted to fit the experimental data under specific conditions [37]. Sensitivity analysis can also assist in parameter tuning for accelerated model construction. The sensitivity analysis frequently applied in BES is one-factor-at-a-time method (OFAT); however, this method has intrinsic drawbacks because it cannot evaluate combined effects of different parameters. Setting the parameters out of the appropriate range may result in the hiding of crucial and sensitive values, leading to the underestimation of their significance [44]. More efficient and accurate techniques were also proposed such as the multi-task Lasso adopted to identify the most influent parameters in a serially connected five-module MFC [45]. Sensitivity analysis was anyway used to make suitable assumptions with the minimal impact on accuracy, precision, and computational cost, and to help understand the working mechanisms and interrelations among immeasurable factors in MFCs [46].

The definition of the domains of integration starts from the complex geometries used in BES, with porous structures and irregular shapes. The porous electrodes are present in all BES designs as carbon felt, carbon cloth and carbon brush, which are usually represented as continuous media, with 2D or 3D domains used, depending on the geometry of the cell and on the approximation accepted. Carbon brush was represented with a rectangular domain of integration in 2D modelling [47], while a helix-shaped domain was used in a 3D model [6]. Rectangular domains were also used in modelling filter press-like cells with carbon felt electrodes under steady state or transient conditions [39], where the same material was modelled in 3D where the anode was a packed bed of small rectangular blocks [48]. Continuous media are generally used to represent liquid electrolytes [49] but were also used for soils and ceramic separators in MFCs modelling [50]. Usually, ion exchange membranes used in BESs are modelled considering diffusion and migration according to the Nernst−Planck Equation. The main limitations involve the occurrence of a pH gradient between anode and cathode compartment, and an increase in the ohmic resistance with low electrolyte concentrations [7].

The use of a mesh analysis strategy, together with suitable assumptions and boundary conditions, can help to realise more complex geometries by defining the node density as a function of the complexity of the phenomena taking place in each node. In porous anode and

cathode finer grids than in the bulk of reactor or channels are used [14,51], solving the model with lower computational cost than using a high number of fine grids all around the geometry. Finer meshes used in the biofilm region reduced the grids from 248,386 to 68,324 with an 8-fold reduction in computational time and an error of only 1.02% [14].

Conclusions and future perspectives

As BES systems are characterised by complexity and multidisciplinary nature, computational modelling has an advantage over other types of models, since CBMs are built with a multiphysics approach that considers electrochemistry, bioelectrochemistry, transport phenomena, fluid dynamics, and mass transfer in space and time. The interaction of different phenomena can be quantified, evaluating the simultaneous effect of several parameters at the same time. The use of CBMs is then paramount in design and scale-up of BESs. The solution of the model with domains of integration that reproduce the geometries of the system under study makes it possible to appropriately analyse the evolution of parameters that are difficult to determine experimentally or even to visualise.

However, these advantages may be balanced by the high computational times and the number of parameters to be available. There are several ways to solve or reduce these problems:

- Simplify the models by physical assumptions, provided that these are accurate to maintain the validity of the model.
- Simplify the geometry as in the classical carbon brush anode.
- Optimise the meshes to reduce the number of grids.
- Use of more advanced computing systems, such as multicore processor [52], as computing is a field with very rapid development and equipment is advancing very significantly with affordable cost reductions.

Moreover, there are still open issues that require more investigation:

- Simulation of the biofilm in its complexity. This is the most critical aspect and the one that tends to be simplified the most in BES models.
- Modelling the cathode reactions. In most BES system models, the focus is on the modelling of the anode; although several consider the cathode phenomena, including biofilm formation, they are still few and far between and require more attention.
- Combining different models (equivalent circuits or statistical models) with CBM models can exploit the advantages of both, while reducing computational time and increasing the accuracy of CBM models [9].

Based on the analysis of the literature and the potentials of the different models, we can conclude that computational modelling is the most promising approach to design and scale-up BESs. Moreover, computational modelling is widely used to design chemical and biological reactors, and it has several strengths when compared to other numerical techniques, including the use of physically based equations. We therefore expect CBMs will become the state of the art in designing BESs within a few years.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

References

Papers of particular interest, published within the period of review, have been highlighted as:

* of special interest

1. Zhang X, Li X, Zhao X, Li Y: **Factors affecting the efficiency of a bioelectrochemical system: a review**. *RSC Adv* 2019, **9**: 19748–19761, https://doi.org/10.1039/C9RA03605A.

2. Maureira D, Romero O, Illanes A, Wilson L, Ottone C: **Industrial bioelectrochemistry for waste valorization: state of the art and challenges**. *Biotechnol Adv* 2023, **64**:108123, https://doi.org/10.1016/J.BIOTECHADV.2023.108123.

3. Jujjavarapu SE, Kumar T, Gupta S: **An overview of computational fluid dynamics in modelling and simulation of microbial fuel cells**. In *Computational fluid dynamics applications in bio and biomedical processes*; 2024:71–99, https://doi.org/10.1007/978-981-99-7129-9_3.

4. Hoang AT, Nižetić S, Ng KH, Papadopoulos AM, Le AT, Kumar S, Hadiyanto H, Pham VV: **Microbial fuel cells for bioelectricity production from waste as sustainable prospect of future energy sector**. *Chemosphere* 2022, **287**:132285, https://doi.org/10.1016/J.CHEMOSPHERE.2021.132285.

5. Kumar P, Kuppam C: **Bioelectrochemical systems: vol. 2 current and emerging applications**. *Bioelectrochem Syst* 2021, **2**: 1–398, https://doi.org/10.1007/978-981-15-6868-8/.

6. * Casula E, Molognoni D, Borràs E, Mascia M: **3D modelling of bioelectrochemical systems with brush anodes under fed-batch and flow conditions**. *J Power Sources* 2021, **487**:229432, https://doi.org/10.1016/J.JPOWSOUR.2020.229432.
The authors model the biofilm growth onto bare surfaces with a nucleation-growth mechanism in 3D geometry; the model can perform with no biofilm at t = 0.

7. Jadhav DA, Carmona-Martínez AA, Chendake AD, Pandit S, Pant D: **Modeling and optimization strategies towards performance enhancement of microbial fuel cells**. *Bioresour Technol* 2021, **320**:124256, https://doi.org/10.1016/J.BIORTECH.2020.124256.

8. Long F, Wang L, Cai W, Lesnik K, Liu H: **Predicting the performance of anaerobic digestion using machine learning algorithms and genomic data**. *Water Res* 2021, **199**:117182, https://doi.org/10.1016/J.WATRES.2021.117182.

9. Li Z, Fu Q, Su H, Yang W, Chen H, Zhang B, Hua L, Xu Q: **Model development of bioelectrochemical systems: a critical review from the perspective of physiochemical principles and**

mathematical methods. *Water Res* 2022, **226**:119311, https://doi.org/10.1016/J.WATRES.2022.119311.

10. Debnath K, Dutta S: **Bio-electrochemical system analysis and improvement: a technical review**. *Clean Circ Bioecon* 2023, **6**: 100052, https://doi.org/10.1016/J.CLCB.2023.100052.

11. Zheng T, Li J, Ji Y, Zhang W, Fang Y, Xin F, Dong W, Wei P, Ma J, Jiang M: **Progress and prospects of bioelectrochemical systems: electron transfer and its applications in the microbial metabolism**. *Front Bioeng Biotechnol* 2020, **8**:495918, https://doi.org/10.3389/FBIOE.2020.00010/BIBTEX.

12. Addagada L, Goel M, Shahid MK, Prabhu SV, Chand S, Sahoo NK, Rout PR: **Tricks and tracks in resource recovery from wastewater using bio-electrochemical systems (BES): a systematic review on recent advancements and future directions**. *J Water Process Eng* 2023, **56**:104580, https://doi.org/10.1016/J.JWPE.2023.104580.

13. Jadhav DA, Chendake AD, Vinayak V, Atabani A, Ali Abdelkareem M, Chae KJ: **Scale-up of the bioelectrochemical system: strategic perspectives and normalization of performance indices**. *Bioresour Technol* 2022, **363**:127935, https://doi.org/10.1016/J.BIORTECH.2022.127935.

14. * Ouyang T, Hu X, Liu W, Shi X, Lu J: **An innovative model for biofilm-based microfluidic microbial fuel cells**. *J Power Sources* 2022, **521**:230940, https://doi.org/10.1016/J.JPOWSOUR.2021.230940.
The authors model the effect of both temperature and substrate concentration in microfluidic MFCs; space–time profiles could help identifying malfunctions.

15. Sayed ET, Rezk H, Abdelkareem MA, Olabi AG: **Artificial neural network based modelling and optimization of microalgae microbial fuel cell**. *Int J Hydrog Energy* 2024, **52**:1015–1025, https://doi.org/10.1016/J.IJHYDENE.2022.12.081.

16. Oyedeji MO, Alharbi A, Aldhaifallah M, Rezk H: **Optimal data-driven modelling of a microbial fuel cell**. *Energies* 2023, **16**: 4740, https://doi.org/10.3390/EN16124740.

17. McAllister JT, Lennertz L, Atencio Mojica Z: **Mapping a discipline: a guide to using VOSviewer for bibliometric and visual analysis**. *Sci Technol Libr* 2022, **41**:319–348, https://doi.org/10.1080/0194262X.2021.1991547.

18. Gautam R, Nayak JK, Ress NV, Steinberger-Wilckens R, Ghosh UK: **Bio-hydrogen production through microbial electrolysis cell: structural components and influencing factors**. *Chem Eng J* 2023, **455**:140535, https://doi.org/10.1016/J.CEJ.2022.140535.

19. Cheng Z, Yao S, Yuan H: **Linking population dynamics to microbial kinetics for hybrid modeling of bioelectrochemical systems**. *Water Res* 2021, **202**:117418, https://doi.org/10.1016/J.WATRES.2021.117418.

20. Littfinski T, Nettmann E, Gehring T, Krimmler S, Heinrichmeier J, Murnleitner E, Lübken M, Pant D, Wichern M: **A comparative study of different electrochemical methods to determine cell internal parameters of microbial fuel cells**. *J Power Sources* 2021, **494**:229707, https://doi.org/10.1016/J.JPOWSOUR.2021.229707.

21. Rossi R, Logan BE: **Impact of external resistance acclimation on charge transfer and diffusion resistance in bench-scale microbial fuel cells**. *Bioresour Technol* 2020, **318**:123921, https://doi.org/10.1016/J.BIORTECH.2020.123921.

22. Timmerman LR, Raghavan S, Borole AP: **Advancing microbial electrolysis technology via impedance spectroscopy and multi-variate analysis**. *Front Energy Res* 2022, **10**:756900, https://doi.org/10.3389/FENRG.2022.756900.

23. Ahmadi S, Rezae A, Ghosh S, Malloum A, Banach A: **A review on bioelectrochemical systems for emerging pollutants remediation: a computational approaches**. *J Environ Chem Eng* 2023, **11**:110021, https://doi.org/10.1016/J.JECE.2023.110021.

24. Kumar T, Jujjavarapu SE: **Advances in anode configurations for a microbial fuel cell via a computational fluid dynamics electrochemistry and its experimental validation**. *J Chem Technol Biotechnol* 2023, **98**:3016–3030, https://doi.org/10.1002/JCTB.7397.

25. Jadhav GS, Jagtap YD, Bhowmick GD, Ghangrekar MM. *Modelling of bioelectrochemical systems: biophysicochemical processes and mathematical methods, microbial electrochemical technologies: fundamentals and applications*, vols. 1–2; 2024: 529–554, https://doi.org/10.1002/9783527839001.CH21.

26. Nguyen CL, Adekunle A, Gomez Vidales A, Moreau A, Tartakovsky B, Woodward L: **Evaluation of the constant phase element and capacitance equivalent circuit models for microbial fuel cell monitoring**. *J Electroanal Chem* 2022, **922**: 116784, https://doi.org/10.1016/J.JELECHEM.2022.116784.

27. Geetanjali, Rawat S, Rani R, Kumar S: **Kinetic modeling for miniaturize single-chambered microbial fuel cell: effects of biochemical reaction on its performance**. *Environ Sci Pollut Contr Ser* 2023, **1**:1–10, https://doi.org/10.1007/S11356-023-28798-X/FIGURES/5.

28. Day JR, Heidrich ES, Wood TS: **A scalable model of fluid flow, substrate removal and current production in microbial fuel cells**. *Chemosphere* 2022, **291**:132686, https://doi.org/10.1016/J.CHEMOSPHERE.2021.132686.

29. * Kamperidis T, Tremouli A, Peppas A, Lyberatos G: **A 2D modelling approach for predicting the response of a two-chamber microbial fuel cell to substrate concentration and electrolyte conductivity changes**. *Energies* 2022, **15**:1412, https://doi.org/10.3390/EN15041412.
The authors numerically evaluate the effect of composition and conductivity.

30. Wang X, Zhang Y, Zhang C, Li J, Xue M, Xia W: **Influence of electrodes configuration on hydraulic characteristics of constructed wetland–microbial fuel cell systems using graphite rods and plates as electrodes**. *Sustainability* 2023, **15**: 6397, https://doi.org/10.3390/SU15086397.

31. Yang Z, Yang A: **Modelling the impact of operating mode and electron transfer mechanism in microbial fuel cells with two-species anodic biofilm**. *Biochem Eng J* 2020, **158**:107560, https://doi.org/10.1016/J.BEJ.2020.107560.

32. Ouyang T, Hu X, Shi X, Liu W, Lu J, Li W: **Mathematical modeling and performance evaluation of a cathodic bi-population microfluidic microbial fuel cell**. *Energy Convers Manag* 2022, **267**:115900, https://doi.org/10.1016/J.ENCONMAN.2022.115900.

33. Ghasemi M, Rezk H: **Performance improvement of microbial fuel cell using experimental investigation and fuzzy modelling**. *Energy* 2024, **286**:129486, https://doi.org/10.1016/J.ENERGY.2023.129486.

34. Rabaey K, Angenent L, Schröder U, Keller J: **Bioelectrochemical systems: from extracellular electron transfer to biotechnological application**. *Water Intell Online* 2009, **8**, https://doi.org/10.2166/9781780401621.

35. * Gadkari S, Fontmorin JM, Yu E, Sadhukhan J: **Influence of temperature and other system parameters on microbial fuel cell performance: numerical and experimental investigation**. *Chem Eng J* 2020, **388**:124176, https://doi.org/10.1016/J.CEJ.2020.124176.
The authors model the effect of temperature on the performance of MFCs in 2D geometry; profiles of temperature could help identifying local malfunctions.

36. Cai WF, Geng JF, Pu KB, Ma Q, Jing DW, Wang YH, Chen QY, Liu H: **Investigation of a two-dimensional model on microbial fuel cell with different biofilm porosities and external resistances**. *Chem Eng J* 2018, **333**:572–582, https://doi.org/10.1016/J.CEJ.2017.09.189.

37. Luo S, Sun H, Ping Q, Jin R, He Z: **A review of modeling bioelectrochemical systems: engineering and statistical aspects**. *Energies* 2016, **9**:111, https://doi.org/10.3390/EN9020111.

38. Ouyang T, Liu W, Shi X, Li Y, Hu X: **Multi-criteria assessment and triple-objective optimization of a bio-anode microfluidic microbial fuel cell**. *Bioresour Technol* 2023, **382**:129193, https://doi.org/10.1016/J.BIORTECH.2023.129193.

39. * Dziegielowski J, Mascia M, Metcalfe B, Di Lorenzo M: **Voltage evolution and electrochemical behaviour of soil microbial fuel cells operated in different quality soils**. *Sustain Energy Technol Assess* 2023, **56**:103071, https://doi.org/10.1016/J.SETA.2023.103071.
The authors model the formation of cathodic and anodic biofilms in the same cell, either cathode or anode limitations can be identified.

40. Raychaudhuri A, Behera M: **Review of the process optimization in microbial fuel cell using design of experiment methodology**. *J Hazard Toxic Radioact Waste* 2020, **24**, https://doi.org/10.1061/(ASCE)HZ.2153-5515.0000503.

41. Ur Rahman MZ, Rizwan M, Liaquat R, Leiva V, Muddasar M: **Model-based optimal and robust control of renewable hydrogen gas production in a fed-batch microbial electrolysis cell**. *Int J Hydrog Energy* 2023, **48**:30685–30701, https://doi.org/10.1016/J.IJHYDENE.2023.04.184.

42. Ashraf HM, Abu-Reesh IM: **Variance-based global sensitivity analysis of a multi-population, single-chamber microbial fuel cell operating in continuous flow mode at steady state**. *Biomass Convers Biorefin* 2022, **1**:1–15, https://doi.org/10.1007/S13399-022-03429-6/FIGURES/10.

43. Naseer MN, Zaidi AA, Dutta K, Jaafar J, Wahab YA, Cai Y: **A Novel Computational Platform for Steady-State and Dynamic Simulation of Dual-Chambered Microbial Fuel Cell**. *J Electrochem Soc* 2023, **170**, 094504, https://doi.org/10.1149/1945-7111/ACF882.

44. Lin CW, Chung YP, Liu SH, Chen WT, Zhu TJ: **Optimizing the parameters of microbial fuel cells using response surface methodology to increase Cr(VI) removal efficiency and power production**. *Process Saf Environ Protect* 2023, **172**:369–378, https://doi.org/10.1016/J.PSEP.2023.02.028.

45. Das I, Jadhav GS, Jagtap YD, Bhaskar N, Ghangrekar MM: **Statistical methods for modelling and performance analysis of bioelectrochemical systems**. *Microb Electrochem Technol Fundament Appl* 2024, **1–2**:583–604, https://doi.org/10.1002/9783527839001.CH23.

46. Lim CE, Chew CL, Pan GT, Chong S, Arumugasamy SK, Lim JW, Al-Kahtani AA, Ng HS, Abdurrahman M: **Predicting microbial fuel cell biofilm communities and power generation from wastewaters with artificial neural network**. *Int J Hydrog Energy* 2024, **52**:1052–1064, https://doi.org/10.1016/J.IJHYDENE.2023.08.290.

47. Gadkari S, Gu S, Sadhukhan J: **Two-dimensional mathematical model of an air-cathode microbial fuel cell with graphite fiber brush anode**. *J Power Sources* 2019, **441**:227145, https://doi.org/10.1016/j.jpowsour.2019.227145.

48. * Hernández-García KM, Cercado B, Rodríguez FA, Rivera FF, Rivero EP: **Modeling 3D current and potential distribution in a microbial electrolysis cell with augmented anode surface and non-ideal flow pattern**. *Biochem Eng J* 2020, **162**:107714, https://doi.org/10.1016/j.bej.2020.107714.
First 3D model of a microbial electrolysis cell.

49. Gadkari S, Gu S, Sadhukhan J: **Towards automated design of bioelectrochemical systems: a comprehensive review of mathematical models**. *Chem Eng J* 2018, **343**:303–316, https://doi.org/10.1016/J.CEJ.2018.03.005.

50. Casula E, Kim B, Chesson H, Di Lorenzo M, Mascia M: **Modelling the influence of soil properties on performance and bioremediation ability of a pile of soil microbial fuel cells**. *Electrochim Acta* 2021, **368**:137568, https://doi.org/10.1016/j.electacta.2020.137568.

51. Hu X, Tan X, Shi X, Liu W, Ouyang T: **An integrated assessment of microfluidic microbial fuel cell subjected to vibration excitation**. *Appl Energy* 2023, **336**:120852, https://doi.org/10.1016/J.APENERGY.2023.120852.

52. Xia C, Zhang D, Pedrycz W, Zhu Y, Guo Y: **Models for microbial fuel cells: a critical review**. *J Power Sources* 2018, **373**:119–131, https://doi.org/10.1016/J.JPOWSOUR.2017.11.001.