

Exploring the application of artificial intelligence for bioelectrochemical systems: A review of recent research



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ABSTRACT

Bioelectrochemical systems (BES) offer promising solutions for sustainable energy production and wastewater treatment. However, their complex biological and electrochemical dynamics pose significant challenges for traditional modeling approaches. This review explores the recent advancements in applying artificial intelligence (AI) techniques to enhance the performance and scalability of BES technologies. We detailed the roles of machine learning (ML) algorithms, such as artificial neural networks (ANNs), support vector regression (SVR), and random forest regression (RFR), in predicting critical BES performance metrics. Additionally, we discussed metaheuristic optimization techniques that have improved system design and operational parameters, yielding significant gains in energy recovery and stability. The integration of real-time monitoring and adaptive control systems, powered by AI, is highlighted for its potential to dynamically adjust BES operations in response to fluctuating environmental conditions. Despite these advancements, challenges remain, particularly in data standardization and modeling biological complexity within BES. We outline current limitations and future directions, emphasizing the need for robust datasets, standardized methodologies, and advanced AI frameworks to further unlock the potential of AI-driven BES systems in achieving sustainable bioenergy solutions.

1. Introduction

Bioelectrochemical systems (BES) are innovative technologies that harness microorganisms or enzymatic processes to facilitate electron transfer at electrodes, enabling the conversion of chemical energy from organic materials into electrical energy or other valuable products—including hydrogen, methane, volatile fatty acids, nutrients, and metals, especially from wastewater streams. (Madondo et al., 2023; Singh et al., 2024; Sun et al., 2024). These systems typically consist of an anode, where oxidation occurs, and a cathode, where reduction occurs. Microorganisms involved can either produce electricity through metabolism or metabolize substrates with the help of electricity (Logan et al., 2006; Pant et al., 2012).

BES offers significant advantages and promising potential across various applications, including energy production, wastewater treatment, bioremediation, and biodesalination (Munoz-Cupa and Bassi, 2024; Rabaey and Rozendal, 2010; Wang et al., 2011). This versatility is key to their sustainability.

BES systems have two main domains: microbial fuel cells (MFC) and microbial electrolysis cells (MEC). MFCs generate electricity directly from organic matter through metabolic processes, providing a promising alternative to traditional fossil fuels by utilizing resources such as wastewater and agricultural waste. (Bazina et al., 2023; Logan, 2008; Munoz-Cupa et al., 2021; Verma et al., 2023) (Fig. 1(a)). In contrast, MECs require an external power source to produce hydrogen and other valuable chemicals, facilitating both waste remediation and resource recovery in various sectors (Escapa et al., 2016; Gautam et al., 2023) (Fig. 1(b)). Beyond these primary domains, BES technologies extend to specialized applications, such as microbial desalination cells (MDC), which integrate desalination with bioelectricity generation by removing salt from saline water while producing energy (Odunlami et al., 2023), and microbial electrosynthesis systems (MES), which convert CO₂ or other substrates into valuable organic compounds such as acetate, butyrate, propionate, ethanol, methane, formate, and isobutyrate (Ibrahim et al., 2023; Thatikayala et al., 2021; Zhang et al., 2013). Collectively, these systems highlight the adaptability of BES in addressing multifaceted environmental and energy challenges.

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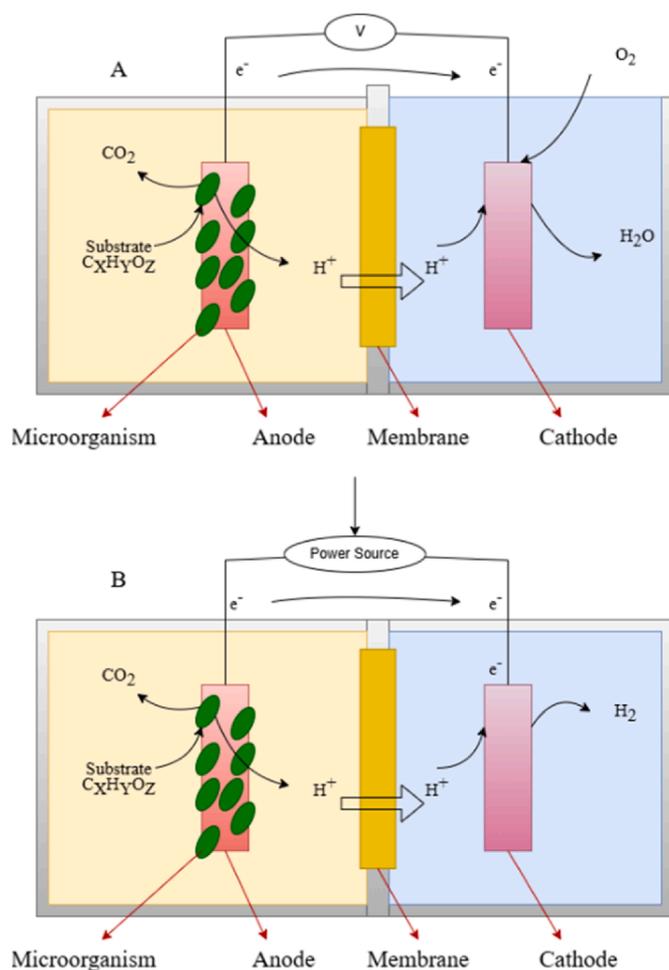


Fig. 1. MFC (a) and MEC (b) mechanisms representations.

BES systems are highly complex, with performance and efficiency heavily impacted by microbial species and operational parameters like pH, temperature, seasonality, and feed composition (Li et al., 2023; Liu et al., 2021; Zou and He, 2018). Traditional first-principle models often fail to capture the complex, nonlinear interactions in BES, as they rely on simplifying assumptions and lack a full mechanistic understanding, resulting in limited predictive accuracy for real-world systems. (Gadkari et al., 2019a, 2019b; Karimi Alavijeh et al., 2015; Koch et al., 2018; Korth and Harnisch, 2019; Shemfe et al., 2018).

Artificial Intelligence (AI) refers to the development of algorithms and systems capable of performing tasks that simulate human intelligence. AI systems can autonomously make decisions based on data, utilizing various methodologies such as rule-based systems, logic, and statistical models (Russel and Norvig, 2009). Recently, AI has been applied in various fields, including disease detection in oncology and cardiology (Esteve et al., 2017), market prediction and risk analysis in finance (Patel et al., 2015), autonomous driving in the automobile industry (Kuutti et al., 2021), intelligent farming practices in agriculture (Kamilaris and Prenafeta-Boldú, 2018), and environmental engineering, such as air monitoring and wastewater treatment (Chang et al., 2024; Lu et al., 2024; Zhang et al., 2024a). Machine Learning (ML), introduced by Samuel (1959) is a subset of AI that involves the use of data-driven algorithms to improve performance over time without explicit programming. ML algorithms demonstrate a remarkable ability to identify complex patterns within biological systems. Mowbray et al. (2021) conducted an exhaustive review of ML applications in biological systems, where nonlinear interactions and inherent variability present significant challenges for traditional modeling methods. The

mathematical modeling of these systems is challenging due to their specificity and the complex dynamics of their components, such as in protein structure prediction due to the vast conformational space and intricate intramolecular interactions (Jumper et al., 2021), or the interpretation of cellular interaction networks (Barabási, 2016). In this context, ML enables the modeling of nonlinear dependencies and the processing of large volumes of biological data, thereby enhancing the ability to analyze and understand complex biological phenomena (Eraslan et al., 2019; Libbrecht and Noble, 2015).

The number of AI-integrated BES studies has steadily increased over the years, with rapid expansion beginning in 2019 (Fig. 2). This trend reflects a growing recognition of AI's potential in modeling, optimizing, and controlling BES. Notably, 2024 alone accounted for 21 publications, representing nearly one-third of all identified studies, which indicates an unprecedented surge of interest in the integration of AI in BES research. The growth is not only quantitative but also typological: while MFCs have consistently dominated the field, MEC-related studies began to emerge more prominently from 2020 onwards and reached a peak in 2024, with 6 out of the 20 publications in that year focusing on MEC systems. In contrast, MDCs appeared only sporadically, with a single study identified in 2018. The cumulative distribution highlights a diversification trend, where AI is increasingly applied to a broader range of BES configurations. This temporal and typological evolution strongly supports the urgency and relevance of conducting a focused and up-to-date review on AI applications in BES, as the field is rapidly expanding in both scope and complexity. The current application of AI in BES primarily focuses on optimizing and predicting performance, with an emphasis on Artificial Neural Networks (ANNs), Fuzzy Logic (FL) systems, and other ML techniques. These learning models are increasingly enhanced by the integration of metaheuristic algorithms, which support parameter tuning and optimization of operational conditions, thereby improving solution robustness and predictive power. These models enable the prediction of key parameters, such as power density (PD) and Chemical Oxygen Demand (COD) removal efficiency for MFC, and hydrogen production for MEC, by adjusting critical variables like membrane type, substrate concentration, and electrolyte characteristics. These parameters are central to evaluating the energy recovery and treatment performance of BES, while the operational variables play a crucial role in determining reaction kinetics, microbial activity, and electrochemical efficiency (Erable et al., 2011; Liu et al., 2020; Mansoorian et al., 2020). AI provides more precise and dynamic control in these technologies, optimizing efficiency for both bioelectricity generation in MFC and chemical production in MEC. The use of advanced algorithms, such as adaptive neuro-fuzzy control systems and optimization methods like Particle Swarm Optimization (PSO), has shown significant potential to improve stability and performance in applications related to wastewater treatment and renewable energy production (Chalak Qazani et al., 2024).

2. Literature review methodology

This review provides an overview of recent advances in the application of AI to BES, with a particular emphasis on its implementation in MFC and MEC, as these two configurations represent the vast majority of AI-integrated BES studies to date. The review examines the objectives pursued through AI integration and evaluates its effectiveness in each context. By adopting this approach, it aims to provide a comprehensive understanding of recent studies, use cases, and emerging perspectives, specifically focusing on performance evaluation, design, operational optimization, adaptive control, and real-time monitoring within BES.

To support this analysis, a structured and iterative literature search was conducted using Google Scholar and Scopus. The search commenced with the most recent publications and was progressively extended to earlier years, revealing that the earliest relevant article applying AI in BES was published in 2013. Therefore, the review covers studies published explicitly within the period from 2013 to 2025. In researching the articles, keyword combinations included carefully

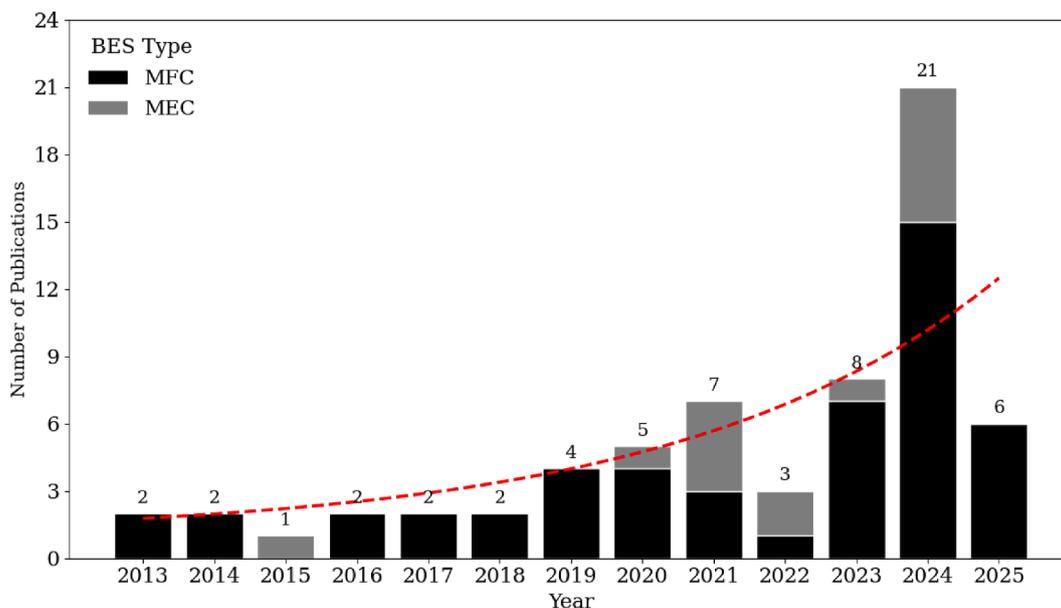


Fig. 2. Trends in AI research for MFC and MEC by year.

selected terms such as “artificial intelligence”, “machine learning”, “AI”, “ML”, “bioelectrochemical”, “bioelectrochemical systems”, “microbial fuel cell”, “microbial electrolysis cell”, and specific algorithm names like “ANN”, “SVR”, and “PSO”. Articles were rigorously selected based on clear criteria: the use of AI-driven prediction, optimization, or control methods applied to BES; clearly defined input and output variables; and reported performance metrics. Furthermore, to avoid selection bias and ensure representativeness, the final selection was cross-validated using a manually curated summary database, aiming to guarantee a diverse coverage across BES types, modeling methodologies, and application scenarios. In addition, references cited within each selected study were thoroughly examined to trace prior publications addressing similar objectives, allowing for a more comprehensive mapping of research progress over time.

In total, 66 publications focusing exclusively on the integration of AI and BES were identified and classified by BES type into MFC, MEC, MES,

and MDC. MFCs dominate the landscape, accounting for 50 out of 66 studies, followed by MECs with 14 and MDCs and MES with a single identified case. These studies were further categorized according to the primary objective of the AI application—namely, performance evaluation, optimization, adaptive control, or real-time monitoring—as this classification allows for a clearer understanding of how AI is being functionally integrated into BES research.

3. AI algorithms applied in BES research

Building on the growing body of research in AI-assisted BES, this section categorizes and examines the most frequently employed algorithms based on their modeling capabilities, adaptation to BES dynamics, and demonstrated application scopes. As shown in Fig. 3, ANNs dominate the landscape, with 32 documented applications, highlighting their adaptability and strong performance in nonlinear environments

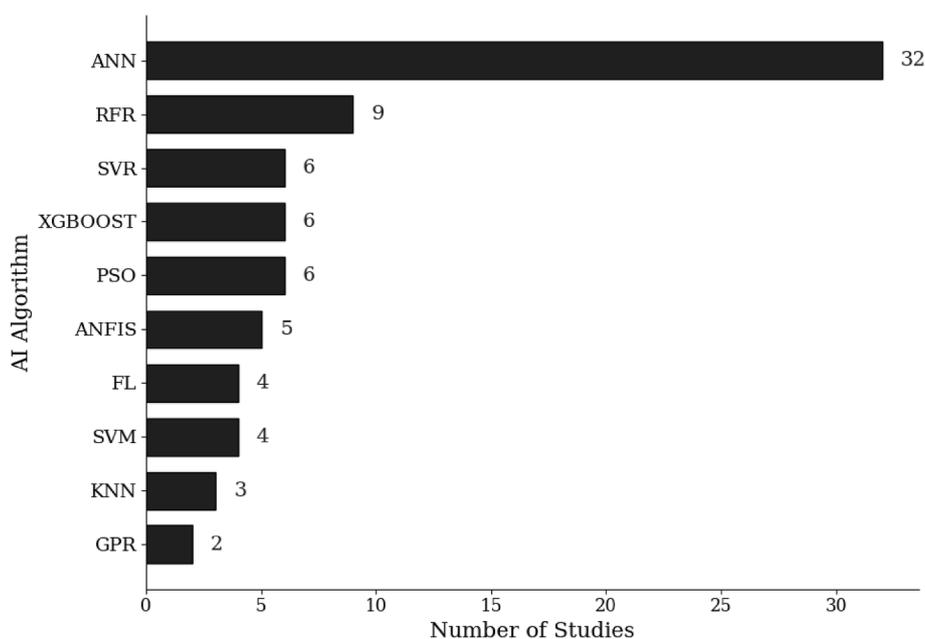


Fig. 3. Number of publications using each AI algorithm in BES research.

typical of BES. SVR, RFR, and Adaptive Neuro-Fuzzy Inference System (ANFIS) follow with fewer but consistent uses, each appearing in 5–9 studies, suggesting a growing interest in algorithmic diversity tailored to different modeling needs. Notably, some studies implemented more than one algorithm, either for benchmarking purposes or to address distinct modeling objectives within the same experimental context (Farahani et al., 2024; Gürbüz et al., 2024; Li et al., 2024). These models have been applied to key performance tasks including PD prediction, COD removal, and biohydrogen production (Abdollahfard et al., 2023; de Ramón-Fernández et al., 2020; Garg et al., 2014; Ghasemi et al., 2021; Wang et al., 2021). Beyond predictive accuracy, the suitability of these algorithms is often determined by robustness to noise, interpretability, and computational efficiency—factors that are crucial in BES characterized by nonlinear interactions and biological variability. Fig. 4 provides schematic overviews that help contextualize their internal mechanisms and implementation logic.

Although ANN-based approaches remain prevalent, their opacity limits mechanistic insight, underscoring the need for interpretable or knowledge-integrated models. The sparse adoption of alternative algorithms reveals methodological niches—uncertainty quantification, fault diagnosis, physics-informed architectures—whose exploration could broaden the analytical repertoire and better align AI tools with the complex, data-scarce nature of BES.

3.1. Artificial neural networks (ANNs)

ANNs are computational models inspired by the structure of the human brain, designed to approximate complex nonlinear relationships (McCulloch and Pitts, 1943). Their layered architecture—comprising an input layer, one or more hidden layers with nonlinear activation functions, and an output layer—enables flexible modeling of BES performance metrics such as PD, COD removal, voltage, biofilm communities, and chemical production, even under sparse or noisy conditions (Garg et al., 2014; Lesnik and Liu, 2017; Lim et al., 2024; Nguyen et al., 2022; Sayed et al., 2024; Tardast et al., 2014; Tsompanas et al., 2019). ANN training involves iterative adjustment of connection weights via algorithms like backpropagation and Levenberg–Marquardt (LM) optimization, minimizing prediction errors (Haykin, 2009). This configuration allows the network to capture underlying patterns without requiring explicit mechanistic equations, an asset in biologically complex systems like BES.

One of the earliest studies demonstrating the predictive capabilities of ANNs in BES was conducted by Garg et al. (2014). In this work, a feedforward ANN was trained to estimate the voltage output of a dual-chamber MFC based on two key operational inputs: temperature and ferrous sulfate concentration. The model achieved a high coefficient of determination (R^2), validating its ability to capture nonlinear interactions in early-stage MFC systems. Despite being outperformed in interpretability by genetic programming in the same study, the ANN's predictive accuracy and data-driven adaptability marked a pivotal moment for AI in BES modeling. This pioneering contribution laid the groundwork for more complex ANN implementations. For instance, Nguyen et al. (2022) proposed a two-hidden-layer ANN optimized via Box–Behnken design to model and forecast methane production and multiple substrate removals in MEC-AD systems. Their model, with an R-value of 0.9870 and mean squared error (MSE) of 0.0579, demonstrated not only precision but also computational efficiency, highlighting ANN's scalability to multi-output, multivariable BES configurations. The consistent use of ANN across different BES types suggests a methodological consensus around its flexibility and suitability for systems characterized by nonlinear dynamics, limited mechanistic information, and multivariate input spaces.

Despite these successes, several recent investigations have highlighted important limitations associated with ANN models in BES applications. Notably, ANNs have been found to require careful hyperparameter tuning to prevent overfitting, especially in cases where

the number of neurons or learning rates are not optimally set. These models can also exhibit limited extrapolation capability and are often sensitive to initial conditions and data partitioning strategies, resulting in reduced generalization when applied to new operating regimes (Esfandiyari et al., 2016; Garg et al., 2014). In some cases, alternative approaches such as genetic programming or ANFIS systems have demonstrated superior robustness and faster convergence, with reduced sensitivity to initial parameter choices (Esfandiyari et al., 2016; Garg et al., 2014; Phan et al., 2024).

Recent studies have further extended ANN use in BES beyond output prediction to include biofilm characterization, system optimization, and microbial community inference. Lim et al. (2024) implemented two ANN models—one to estimate the abundance of seven exoelectrogenic genera, and another to predict MFC power generation (PG) using only sludge physicochemical data. Gurjar and Behera (2023) applied a Bayesian-trained ANN to identify nonlinear drivers of COD removal and PD in an earthen MFC treating leachate, highlighting the model's adaptability in systems with limited mechanistic information. By combining predictive accuracy with sensitivity and regression analyses, their approach successfully revealed the relative influence of variables such as external resistance and cathode area, offering valuable guidance for system optimization even in data-constrained scenarios.

In addition to ANN architecture, some studies have begun exploring advanced ANN variants that are specifically suited to temporal data. Among these, Recurrent Neural Networks (RNNs) and Long Short-Term Memory (LSTM) networks stand out as powerful tools for modeling dynamic processes in BES, particularly where time-dependent behaviors such as voltage variation or substrate consumption are of interest (Hess-Dunlop et al., 2024a).

3.1.1. Recurrent Neural Networks (RNNs)

RNNs are specifically designed to process sequential data, making them highly suitable for time series analysis in BES, such as tracking voltage or substrate concentration changes over time. Unlike ANNs, which process inputs independently, RNNs maintain connections across time steps, enabling them to model temporal sequences and dependencies (Fig. 4(f)) (Elman, 1990). In a recent study, Khoshgoftar Manesh et al. (2024) applied RNN-based deep learning models to predict the performance of MFCs treating textile wastewater. The models were trained using a dataset of 5600 samples derived from over 60 experimental studies, with input variables including initial COD concentration, pH, and time, and output variables including maximum voltage, power density, and COD removal efficiency. This modeling approach is especially important in BES applications, as it enables robust prediction of dynamic behavior across diverse operational scenarios, reduces reliance on extensive experimental trials, and facilitates optimization of system performance under varying wastewater conditions.

3.1.2. Long Short-Term Memory (LSTM)

LSTM networks, introduced by Hochreiter and Schmidhuber (1997) are a specialized type of RNN designed to overcome the vanishing gradient problem, a common limitation in standard RNNs, and capture long-term dependencies in sequential data. LSTMs achieve this by incorporating a gating mechanism—consisting of input, output, and forget gates—that enables selective retention, updating, or discarding of information over time. Hess-Dunlop et al. (2024a) leveraged LSTM networks to predict energy outputs in Soil Microbial Fuel Cells (Soil MFCs), a type of BES designed to power low-energy devices like agricultural sensors (Gustave et al., 2019). The Soil MFCs, tested in outdoor environments, used carbon-based electrodes, with environmental variables such as soil moisture, temperature, and conductivity monitored alongside energy outputs like voltage, current, and power. The LSTM model, trained on data collected between 2019 and 2022, predicted energy outputs at intervals ranging from 3 min to 1 h. By incorporating quantile regression, the model provided confidence intervals for its predictions, improving reliability and minimizing energy waste. The

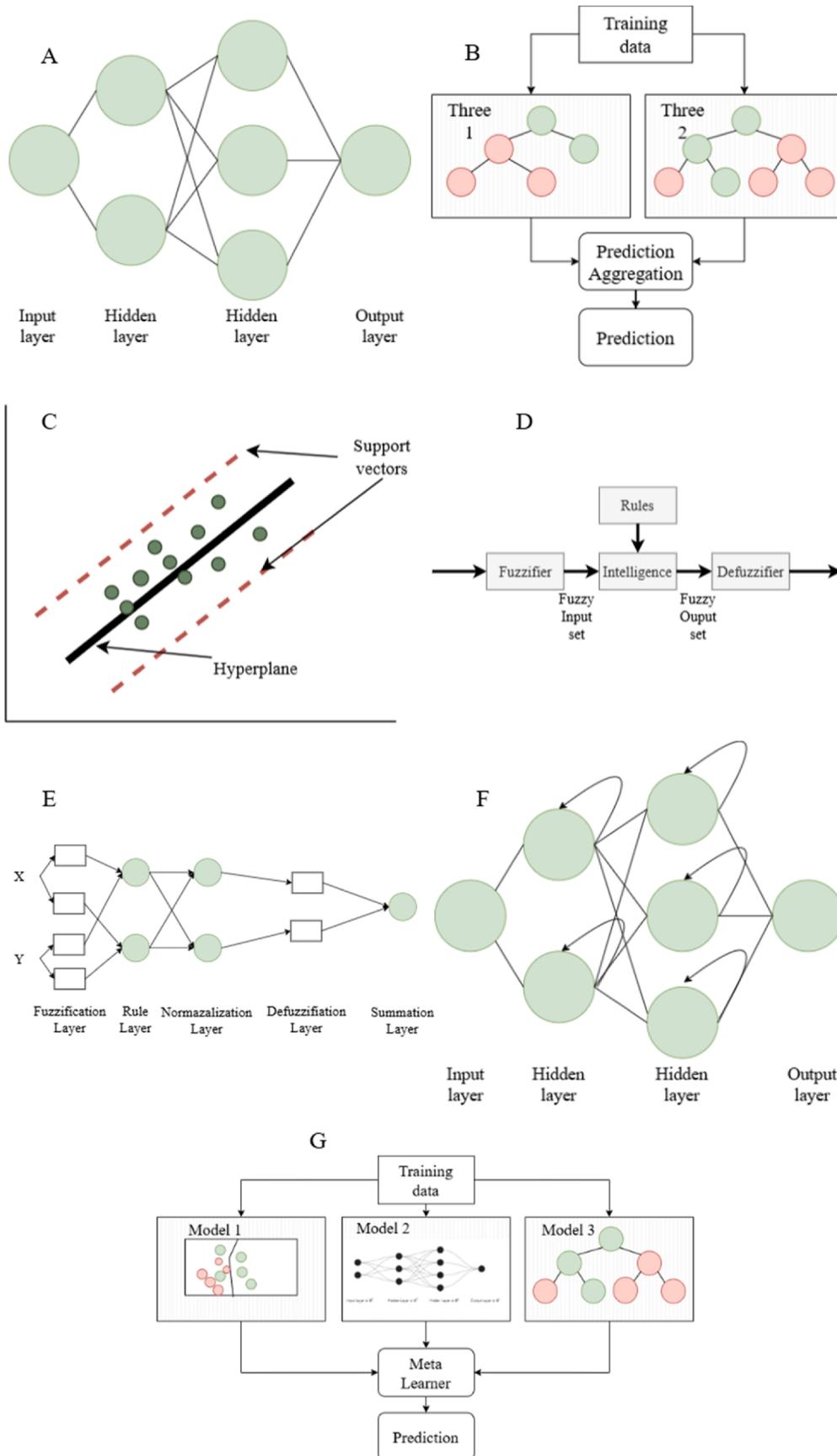


Fig. 4. AI models related to BES illustrations. (a) The architecture of an ANN, showing input, hidden, and output layers. (b) Example of a random forest model with two decision trees and prediction aggregation. (c) Representation of the SVM model with a hyperplane that separates two classes. (d) Scheme of an FL, showing the flow from input, through rules and intelligence, to output. (e) Structure of an ANFIS with fuzzification, normalization, and defuzzification stages. (f) Diagram of an RNN structure, illustrating sequential data processing through cyclical connections. (g) Diagram of an ensemble learning model, combining multiple models through a meta-learner for the final prediction.

results demonstrated high accuracy, showcasing the potential of LSTMs to optimize BES performance for intermittent applications such as agricultural sensing.

3.2. Support Vector Regression (SVR)

SVR is an adaptation of Support Vector Machines (SVM) specifically designed for regression tasks. SVR is highly effective for handling nonlinear data commonly found in BES studies (Garg et al., 2014; Ghasemi et al., 2023; Shabani et al., 2021). It projects data into a higher-dimensional space and identifies a hyperplane that maximizes the margin of tolerance, allowing it to approximate relationships between variables with minimal error (Fig. 4(c)) (Cortes et al., 1995). While SVR is advantageous for modeling efficiency metrics in BES, it requires careful tuning of parameters such as the kernel type and regularization term, which can be computationally demanding (Garg et al., 2014; Malang et al., 2023).

Recent applications of SVR in BES have focused on optimizing performance prediction and tuning key operational variables. For example Wang et al. (2018), employed a quadratic SVR model to model and invert the relationship between five operational variables (Hydraulic Retention Time (HRT), internal reflux ratio, influent COD concentration, influent ammonia nitrogen concentration, and influent nitrate concentration) and output voltage in a MFC. Their model achieved R values of 0.95–0.96 during training and 0.84–0.86 in testing, showing consistently better generalization ability than both ANN and SVR with RBF kernel. This improved generalization is attributed to SVR's suitability for small sample learning and its mathematical foundation, especially under conditions of limited experimental data. ANN models, while effective, were observed to have lower prediction accuracy for both training and testing data in this study, confirming the advantage of SVR for small sample problems. These results underscore SVR's effectiveness in BES, not only for forward regression but also for direct inversion and design of operation spaces with prediction uncertainty.

3.3. Fuzzy Logic (FL)

FL provides a framework for modeling uncertainty and imprecision, which is essential in systems like BES that involve complex, dynamic biological processes. FL uses fuzzy sets and rules based on linguistic variables to capture subtle relationships within the data (Fig. 4(g)) (Zadeh, 1965). FL models require precise membership functions and rules, often defined by domain experts, to ensure reliable outputs. The fuzzy inference process evaluates these rules to generate a fuzzy output, which is then translated into a crisp value through a defuzzification step. For instance, Ghasemi and Rezk (2024) applied FL to predict PD, COD removal, and Coulombic efficiency (CE) in an MFC by transforming experimental inputs—glucose, yeast extract, and aeration rate—into linguistic categories and applying rule-based reasoning to estimate outputs. In another example, Khew Mun Hong et al. (2021) implemented a FL controller in an MEC, where the control inputs (error and its rate of change in hydrogen production) were converted into fuzzy terms and used to determine the voltage adjustment through inference and defuzzification. These studies exemplify how FL supports both interpretive modeling and real-time control in the face of nonlinearity and limited process knowledge.

3.4. Metaheuristic optimization algorithms

Particle Swarm Optimization (PSO), Harris Hawks Optimization (HHO), Equilibrium Optimizer (EO), and Improved Grey Wolf Optimization (IGWO) are AI-based techniques inspired by natural behaviors or social systems. For example, PSO simulates the flocking behavior of birds to reach optimal solutions, where particles update their positions based on personal and global bests, seeking to minimize or maximize an

objective function (Kennedy et al., 1995). Similarly, HHO mimics the hunting strategy of hawks through stages like exploring and attacking, making it highly adaptable to non-linear optimization problems (Heidari et al., 2019). EO draws on the concept of dynamic equilibrium in physics, seeking balance in its search process to refine solutions iteratively (Faramarzi et al., 2020). Finally, IGWO models the hierarchical social structure of grey wolves, incorporating behaviors like hunting and encircling prey, enhancing its ability to navigate complex optimization landscapes (Mirjalili et al., 2014). Their general workflow begins by initializing a population of candidate solutions, which then adjust iteratively based on specific rules and criteria (e.g., attraction to the best-known position). Each candidate evaluates the objective function in each iteration, progressively refining the group toward optimal solutions (Blum and Roli, 2003). These algorithms are particularly effective in tuning parameters and optimizing systems in BES applications, as they can efficiently navigate large, multidimensional solution spaces to enhance model performance (Abdollahfard et al., 2023; Chalak Qazani et al., 2024; Ghasemi and Rezk, 2024; Nguyen et al., 2022).

3.5. Ensemble models

Ensemble models are ML methods that combine the predictions of multiple models to improve overall accuracy and reduce error (Fig. 4(g)) (Abimannan et al., 2023). Techniques such as XGBoost and Gradient Boosting Regression Trees (GBRT) are popular ensemble methods. In BES research, XGBoost has been used effectively to predict the efficacy of biological nutrient removal processes (Emaminejad et al., 2023), while GBRT has shown success in modeling PD and COD removal in MFC by capturing intricate interactions (Abdollahfard et al., 2023). Another widely adopted ensemble method is Random Forest Regression (RFR), which has been applied to various BES tasks due to its robustness and ability to handle noisy, high-dimensional data (Cai et al., 2019; Lesnik et al., 2020).

Within ensemble modeling, one particularly promising approach explored in BES research involves combining theoretical models with ML techniques. In this framework, first-principles models—grounded in established theoretical and mechanistic understanding—are integrated with data-driven methods that extract patterns and insights directly from empirical data. This combination allows for the strengths of both methodologies to be utilized: the interpretability and foundational rigor of mechanistic models, and the adaptability and predictive power of data-driven techniques. As a result, hybrid models are particularly well-suited for complex systems with nonlinear behavior or incomplete theoretical understanding (Asrul et al., 2024; Rudolph et al., 2023).

3.5.1. Random Forest Regression (RFR)

RFR is an ensemble learning technique that enhances predictive accuracy by aggregating multiple decision trees (DTs). A DT is a flowchart-like structure that splits data into branches based on feature values, allowing for straightforward decision-making and predictions. Each tree in the RFR is trained on a random subset of data and employs unique subsets of features to make these splits, which helps reduce overfitting by aggregating their outputs (Fig. 4(b)) (Breiman, 2001). RFR is particularly powerful in BES, where it accurately predicts MEC's CD (Yoon et al., 2024) and MEC hydrogen production rates (Wang et al., 2021). However, a challenge in applying RFR is the exclusion of significant variables that lack sufficient data for numerical representation, such as electrode material properties, such as electrical conductivity and overpotential Yoon et al. (2024) emphasizes that careful feature selection and sufficient data representation are crucial for maximizing prediction accuracy and ensuring interpretability. The robust ensemble structure of RFR makes it particularly well-suited for addressing the variability inherent in BES systems, where biological and chemical conditions fluctuate significantly.

3.5.2. Adaptive Neuro-Fuzzy Inference System (ANFIS)

ANFIS integrates ANNs' adaptability with the interpretive strengths of FL, creating a robust tool for managing nonlinear, uncertain systems (Fig. 4(e)) (Jang, 1993). This dual approach allows ANFIS to balance flexibility and precision, making it suitable for complex BES operations characterized by variability and limited mechanistic understanding. Structurally, ANFIS consists of five layers: fuzzification, rule inference, normalization, output computation, and defuzzification. The system uses a hybrid learning algorithm, typically a combination of gradient descent and least-squares estimation—to iteratively update both the membership function parameters and the rule base, enhancing model adaptability while retaining transparency (Ghasemi and Rezk, 2024; Hosseinzadeh et al., 2020). However, this layered structure can increase computational cost, particularly in large-scale implementations. In the Hosseinzadeh et al. (2020) study, ANFIS was effectively applied to predict hydrogen production and energy recovery from a dual-chamber MFC, demonstrating its accuracy and its potential for deployment in energy-optimizing BES applications.

4. Current state of research in AI applications in BES

This section explores current AI applications in BES modeling, focusing on evaluating the performance metrics of both AI models and BES. Studies highlighted here demonstrate the training and assessment of AI models for optimizing operational and design parameters, with comparisons to traditional methods. Additionally, the use of microbial community compositions and specific environmental factors as input variables in advanced models is discussed, enhancing prediction accuracy for stability and energy generation efficiency. Lastly, examples of adaptive control and real-time monitoring illustrate how AI enables dynamic adjustments in BES to maximize performance under variable conditions.

To provide a comprehensive overview of these modeling strategies, Fig. 5 visualizes the variables most frequently used as inputs and outputs in recent AI applications to BES. In both systems, variables such as temperature, voltage, and substrate concentration dominate as inputs, underscoring their central role in governing electrochemical and

biological processes within MFCs and MECs. The repeated emphasis on temperature likely reflects its fundamental influence on microbial activity, metabolic rates, and electron transfer efficiency, making it a critical predictor in both MFC and MEC performance. Similarly, the prominence of voltage and external resistance as input variables can be attributed to their direct impact on electrochemical gradients and current generation, which are essential for evaluating and optimizing device output.

A notable distinction emerges in the output variables: while MFC models frequently target PD, CE, and COD removal, MEC studies are overwhelmingly focused on hydrogen production rate and hydrogen yield. This difference can be ascribed to the divergent technological objectives of each system. MFCs, typically applied in contexts where both energy recovery and wastewater treatment are valued, tend to prioritize efficiency metrics and pollutant removal. In contrast, MECs are engineered primarily for biohydrogen generation, which explains the heavy weighting of hydrogen-related outputs.

The observed patterns likely reflect not only the intrinsic operational differences between MFCs and MECs but also the research community's prioritization of variables that are both measurable and actionable within each application context. It is reasonable to assume that variables like temperature and voltage achieve prominence due to their strong correlation with performance and their relative ease of monitoring and control in experimental setups. Furthermore, the relative scarcity of more complex or system-specific variables in these models may indicate a combination of data availability constraints and a preference for features with established relevance in BES literature.

A more nuanced understanding of these trends emerges from Fig. 6, which quantifies the specific associations between inputs and outputs across the surveyed studies. By providing a matrix view of co-occurrences, the heatmap offers a direct visualization of how experimental and modeling priorities have shaped the field. This heatmap analysis reveals that, within MFC models, inputs such as temperature and pH are not only frequent but are also consistently paired with core performance outputs like PD, voltage, and COD removal, highlighting a targeted approach where fundamental operational variables are leveraged for multiple predictive tasks. Such patterns suggest a deliberate

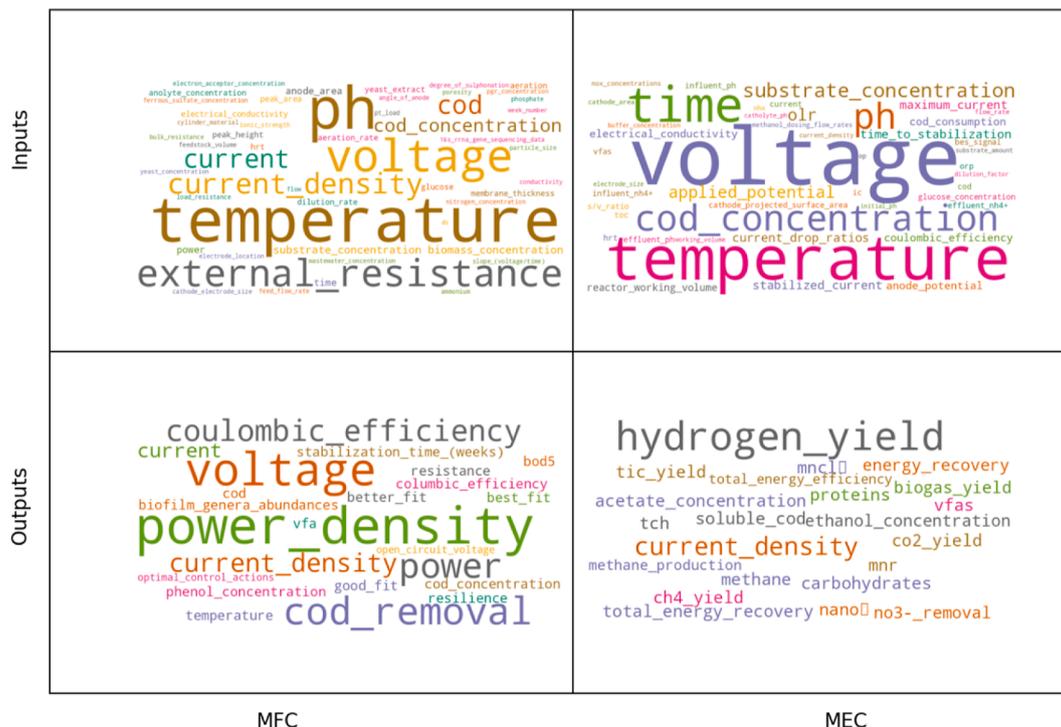


Fig. 5. Most frequent input and output variables used in AI applications for BES.

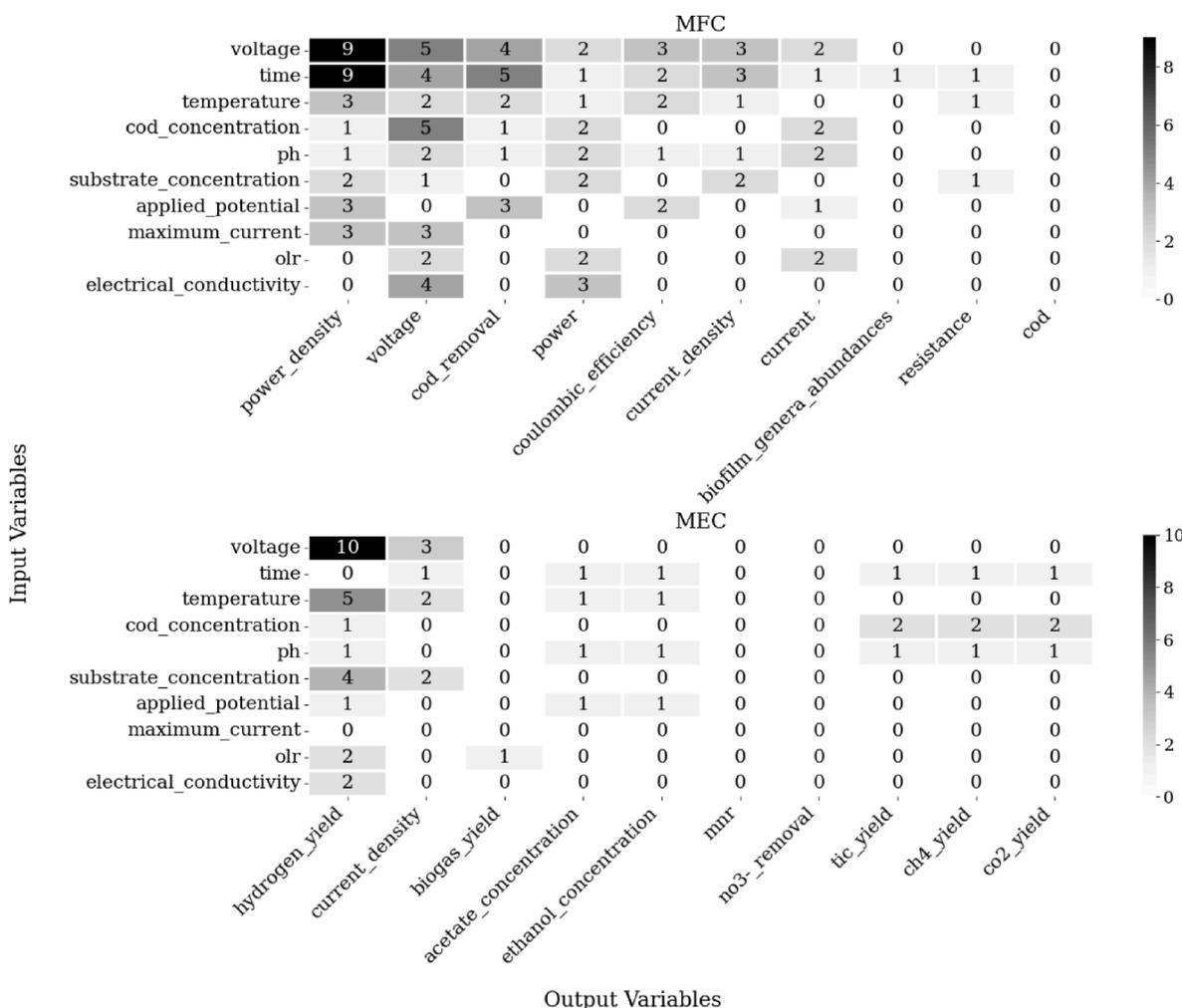


Fig. 6. Input–output variable co-occurrence in AI-based modeling of MFCs and MECs.

emphasis on maximizing predictive accuracy for these core metrics, which are closely tied to the efficiency and stability of MFC operation. In MEC models, the strongest co-occurrence patterns connect voltage and substrate concentration to hydrogen production-related outputs, reflecting a focused modeling strategy aligned with the technological priorities of these systems. This tendency mirrors the technological emphasis in MEC literature on optimizing hydrogen yield, with other input–output pairings receiving comparatively less attention. Interestingly, Fig. 6 also exposes sparsely populated regions in the input–output matrix, pointing to variable combinations that remain underexplored and suggesting potential avenues for methodological innovation in future AI-based BES research. By complementing the global perspective of variable importance from Fig. 6 with detailed insights into input–output pairing, this integrated analysis deepens our understanding of both current practices and latent opportunities in the field. Ultimately, such analyses can inform the design of future studies, encouraging a broader and more holistic exploration of variable interactions within AI-driven BES modeling.

4.1. Evaluation of BES performance

This section presents a systematic analysis of recent AI applications for assessing and improving BES performance, structured around one key scenario: predictive modeling of operational outputs in MFCs and MECs.

The use of ML for predicting MFC and MEC performance has enabled substantial gains in predictive accuracy for outputs such as PD, voltage,

current density (CD), and pollutant removal. However, the true value and limitations of these models become evident when scrutinizing study contexts, variable selection, and system heterogeneity.

For example Oyedele et al. (2023), compared SVR, ANN, Gaussian Process Regression (GPR), and ensemble learners for predicting PD and output voltage in MFCs. Their results showed that GPR achieved the highest overall performance for PD prediction ($R^2 \approx 0.998$), while ANN models outperformed other approaches in output voltage prediction, with R^2 values approaching 0.9999. SVR and ensemble learners performed adequately, but were less effective compared to GPR and ANN, especially in terms of mean absolute deviation and root mean square error (RMSE) for both outputs. The study underscores that model selection should consider the specific output variable of interest, as well as the accuracy requirements for the intended application. Notably, hyperparameter optimization played a critical role in maximizing each model's predictive capabilities.

In an innovative application of super learners, Zakir Hossain et al. (2023) trained two models—BA-SVR (Bayesian Algorithm Support Vector Regression) and BA-BRT (Bayesian Algorithm Boosted Regression Trees)—using data from a single-chamber MFC fed with human urine, equipped with a ceramic (terracotta) membrane and a carbon veil anode. The feedstock flow rate was maintained at 0.1 mL/min, with continuous operation and stainless steel as the cathode. These models, using membrane thickness, external resistance, and anode area as inputs to predict PG, benefit from Bayesian methods for hyperparameter optimization, which are computationally more efficient than grid search (Alibrahim and Ludwig, 2021). They also outperformed the traditional

surface methodology (RSM) model, with BA-SVR achieving a mean absolute error (MAE) of 2.94 μW and BA-BRT at 7.53 μW , while the RSM method had significantly higher errors (MAE = 48.67 μW). The study highlights that the superior accuracy and robustness of BA-SVR and BA-BRT models rely on careful hyperparameter optimization, as inadequate tuning can still result in underfitting or overfitting, and the development process remains computationally demanding. The authors further note that some intrinsic limitations, such as undisclosed structural characteristics in SVR that may affect robustness, persist as open research questions. They underscore the need to rigorously validate and generalize these super learner approaches for more complex, multivariable BES systems beyond the scope of their present study.

Gurjar and Behera (2023) adopted a Bayesian-trained ANN to identify drivers of COD removal and PD in leachate-fed MFCs, revealing that feature selection and probabilistic interpretation are crucial for improving reliability when input variables are uncertain. Lim et al. (2024), applying ANN models to power prediction and exoelectrogenic community analysis in MFCs, emphasized the need for operational variables such as water content and biofilm electrical conductivity to achieve meaningful predictive results ($R^2 = 0.9147$ for power output). In a study focused on MECs, Hosseinzadeh et al. (2020) developed and compared ANN and ANFIS models to forecast hydrogen production rate, cathodic hydrogen recovery, CE, and total energy recovery using inputs such as anode potential, cathode potential, electrolyte conductivity, and solution pH. While both models achieved high predictive accuracy, ANFIS outperformed ANN in terms of RMSE and MAE, particularly for hydrogen recovery ($R^2 = 0.99$). Moreover, the study showed that ANFIS required fewer epochs to converge, was more stable during training, and provided better generalization when the dataset was limited in size, highlighting its suitability for complex, nonlinear BES datasets where interpretability and robustness are critical for energy optimization.

Despite these advances, persistent gaps are evident: model transferability to full-scale or field-operated BES remains largely untested, and only a minority of studies rigorously address external sources of error, such as environmental noise or sensor drift. While ML can reveal the relative importance of input variables, as seen in feature importance analyses by (Lim et al., 2024; Yoon et al., 2024) most models are still highly context-dependent and lack integration with mechanistic system understanding.

A notable development is the use of microbial community composition as a predictive input variable. Lesnik et al. (2020) investigated this approach by exposing 17 MFCs to a controlled low pH shock and analyzing the ability of several ML algorithms (Partial Least Squares (PLS), KNN, RF, and ANNs) to predict two measures of functional stability—resistance (drop in current) and resilience (recovery time)—using genomic profiles. Models based on the abundance of specific genera achieved good accuracy for resistance classification (70.5%, $\kappa = 0.54$), while prediction of resilience was less accurate (up to 65.3%, $\kappa = 0.36$ –0.42), particularly when using only selected genera as input. The authors attribute this difference not only to the inherently higher ecological complexity of resilience—which depends on broad community structure rather than a few taxa—but also to factors such as small sample size, limited diversity of perturbations, and the challenge of capturing all relevant biological interactions in the dataset. Notably, using whole-community amplicon sequence variants (ASV) profiles or compressed data improved resilience prediction, highlighting the importance of data richness and structure. Thus, the results indicate that both the complexity of the process and data limitations—sample size, input type, and choice of algorithm—jointly impact model performance, and that further progress will require larger, more diverse datasets and refined modeling strategies.

4.2. Optimization of BES design and operation

In recent literature on AI applications in BES, optimization methodologies are implemented following predictive modeling to identify

parameter sets that yield maximum system performance. After developing ML-based models to describe system behavior, subsequent optimization—frequently using metaheuristic or hybrid algorithms—enables the determination of operational and design conditions associated with optimal output metrics (Abdollahfard et al., 2023; Ghasemi et al., 2021; Rezk et al., 2023; Rezk and Sayed, 2024; Zou et al., 2024). This section reviews approaches to parameter optimization, distinguishing between operational strategies, system design, and wastewater treatment, and addresses current methodological advances and practical limitations.

4.2.1. Optimization of BES operational parameters

Recent studies have demonstrated that the integration of AI-based optimization algorithms with predictive models can substantially improve the operational performance of BES. One of the earliest examples of this approach was presented by Fang et al. (2013), who combined Uniform Design (UD), Relevance Vector Machine (RVM), and Accelerated Genetic Algorithm (AGA) to optimize a single-chamber MFC. This combined framework successfully modeled the nonlinear effects of ionic strength, initial pH, nitrogen concentration, and temperature on system performance, ultimately predicting a PD of 1097 mW/m^3 and a CE of 73.0%. The close agreement between predicted and experimental results demonstrated the reliability of probabilistic regression models and evolutionary optimization in early MFC development. This work also highlighted how data-efficient strategies can reduce experimental workload while capturing complex interactions between operational variables.

Building on this foundation, Ghasemi et al. (2021) optimized PD and COD removal in a dual-chamber MFC using an ANFIS model in conjunction with PSO. Their study identified optimal input conditions—including the degree of sulfonation in the proton exchange membrane (PEM), specifically a sulfonated polyether ether ketone membrane, platinum (Pt) loading at the cathode, and aeration rate—that maximized power output to 62.8 mW/m^2 and achieved nearly complete COD removal (99.999%). Sensitivity analysis revealed that Pt loading and membrane sulfonation had the greatest influence on system behavior.

A related approach was taken by Abdollahfard et al. (2023), who employed RFR and Gradient Boosted Regression Trees (GBRT) to model and optimize the same set of parameters. Their models not only reproduced the experimental results but, in some cases, outperformed them, further reinforcing the robustness of AI-driven optimization strategies for reactor design and configuration.

In the context of MECs aimed at biohydrogen production, Rezk and Sayed (2024) applied a hybrid ANFIS-AGTO (Artificial Gorilla Troops Optimizer) framework to simultaneously enhance hydrogen yield and energy recovery. With optimized conditions including 41.25 mM buffer concentration, a dilution factor of 3.9, and 1.0 V applied voltage, the system achieved a hydrogen yield of 843.3 $\text{mL}/\text{g-VS}$ and an energy recovery rate of 155.2%, representing a 34.7% improvement over prior optimization strategies. Their framework demonstrated a success rate of 96.7% in identifying high-performance operational configurations.

Collectively, these studies confirm that coupling AI-driven predictive models with optimization algorithms can effectively identify operational settings that maximize BES performance. Notably, Rezk and Sayed (2024) demonstrated significant improvements over conventional response surface methodologies, while other studies validated AI-derived conditions through close agreement with experimental measurements (Abdollahfard et al., 2023; Asrul et al., 2024; Ghasemi et al., 2021). These findings underscore the growing potential of hybrid AI approaches for BES optimization, although further research is needed to confirm their scalability under real-world operating conditions.

4.2.2. Optimization of BES design

AI-driven optimization has also been applied to BES design variables, enabling the systematic identification of configurations that enhance

system performance [Rezk et al. \(2023\)](#). developed a strategy combining fuzzy modeling with the EO to optimize membrane thickness, external resistance, and anode area in a ceramic-based MFC fed with urine. The fuzzy model, built on Gaussian membership functions and nine IF–THEN rules, accurately captured nonlinear input–output relationships and outperformed RSM, which failed to model complex variable interactions. EO, inspired by mass balance in dynamic systems, was employed to identify optimal parameter combinations, and its results were benchmarked against other metaheuristics (PSO, HHO, Jellyfish optimizer, and Slime mould algorithm) over 30 runs. EO consistently achieved the highest power output (492.85 μW) with the lowest standard deviation (0.82), indicating high robustness and convergence reliability. ANOVA and Tukey Honestly Significant Difference tests confirmed the statistical significance of the improvements. Nonetheless, the authors noted that the model's performance was sensitive to data quality and input range normalization, highlighting the importance of well-designed datasets and appropriate scaling in AI-based BES design optimization.

[Zou et al. \(2024\)](#) addressed BES design optimization in a MEC anaerobic digestion system targeting both methane production and total energy efficiency. Using a combination of Box–Behnken experimental design, ANN, and Non-dominated Sorting Genetic Algorithm II (NSGA-II) for multi-objective optimization, they evaluated four critical variables: electrode side length, substrate amount, applied voltage, and initial pH. The ANN model outperformed RSM, capturing nonlinear interactions more effectively. Multi-objective optimization via NSGA-II generated a Pareto front with <3% deviation from experimental results, highlighting the utility of evolutionary algorithms in resolving trade-offs between energy output and efficiency. Notably, the study identified larger electrode sizes as especially influential in enhancing methane yield. However, the authors also reported practical limitations: the RSM model failed to capture complex variable interactions, and the ANN, while more accurate, required careful parameter tuning and normalization to avoid model bias. Furthermore, optimal conditions for methane production and energy efficiency were not identical, emphasizing the inherent conflict between objectives in BES and the need for compromise solutions when scaling up. In both cases, the integration of advanced modeling and optimization algorithms led to more accurate prediction of system behavior and the identification of design parameters that directly translated to experimentally validated performance gains.

4.2.3. Wastewater treatment optimization

The implementation of ML has brought notable advances to the optimization of wastewater treatment in BES, both in contaminant removal and resource recovery. Nevertheless, the literature reveals persistent challenges regarding data quality, variable selection, and the robustness of models under realistic conditions ([Emaminejad et al., 2023](#); [Ghasemi et al., 2021](#); [Gurjar and Behera, 2023](#); [Mohammad and Ishaq, 2024](#); [Zakir Hossain et al., 2023](#)).

One line of progress comes from industrial applications, which have also seen gains through hybrid modeling. For example, [Asrul et al. \(2024\)](#) integrated ANN and convex optimization to simultaneously enhance COD removal and hydrogen production in MECs treating sago wastewater. Their work demonstrated the potential for simultaneous improvement in treatment and resource recovery, but also made clear that these approaches require representative, diverse datasets to avoid overfitting and to generalize reliably.

Interpretability remains a major concern, particularly in FL-based systems. [Khew Mun Hong et al. \(2021\)](#) applied FL to predict bio-hydrogen production and contaminant removal in MFCs using real wastewater, finding that success was contingent on iterative refinement of membership functions and the continual incorporation of expert knowledge into the rule base.

Additional works by [Luo et al. \(2025\)](#) and [Ghasemi et al. \(2023\)](#) has highlighted the value of combining deep learning and ensemble

methods with systematic input selection. Both studies reported that including substrate composition, operational factors, and system design variables enhanced predictive power for both treatment efficiency and power output when processing complex wastewaters.

Despite these advancements, much of the reported success remains confined to laboratory and pilot scales. Most models still require broader, more heterogeneous datasets, and rigorous external validation under fluctuating wastewater compositions. Moving forward, achieving robust, scalable optimization in BES will demand a tighter integration of data-driven modeling with process-level understanding and adaptive input strategies.

4.3. Adaptive control and real-time monitoring

The integration of AI into BES has extended beyond static modeling to encompass real-time process adaptation and continuous monitoring under dynamic conditions. Adaptive control strategies, often grounded in ANNs, FL, or combined learning systems, enable real-time regulation of voltage, current, or biogas output in the face of process uncertainties and delays ([Demir and Eren, 2022](#); [Fu, 2025](#); [Ma et al., 2025](#)). In parallel, real-time monitoring frameworks—especially those based on time-series models, ANNs, and ensemble algorithms—have enhanced the interpretation of biosensor data for water quality surveillance and system diagnostics ([Emaminejad et al., 2023](#); [Feng et al., 2013](#); [Naik and Eswari, 2021](#)). Together, these AI-driven approaches form the foundation for dynamic BES operation, facilitating both responsive control and intelligent decision-making. The following subsections explore recent advances in adaptive control architectures and real-time monitoring systems, with a focus on the models, algorithms, and deployment contexts.

4.3.1. Adaptive control

The application of adaptive control frameworks in BES has advanced significantly with the integration of ML and hybrid intelligent systems, addressing the inherent nonlinearities and environmental fluctuations characteristic of these processes. Recent literature demonstrates that adaptive control strategies, particularly those utilizing data-driven or combined models, can dynamically adjust operational setpoints to maintain optimal performance in the face of disturbances or changing system conditions.

A notable illustration is the work by [Yewale et al. \(2020\)](#), who introduced a multiple model-based (MMB) control for continuous MFCs. In the study, a dynamic bank of local models was paired with a weighted k-nearest neighbors (WkNN) algorithm for real-time model selection. By partitioning the operational range into linear regimes and switching between pre-trained models based on live measurements, this framework demonstrated a dramatic 65% reduction in settling time versus conventional single-model control. The WkNN approach proved especially robust during large substrate concentration shocks (up to 50%), achieving rapid recovery of power and temperature, and outperformed other switching algorithms in both speed and accuracy. These results not only highlight the effectiveness of ML-based model switching in adaptive control, but also its practical benefit in real, dynamically operated MFCs.

Hybrid neural models have also been proposed for adaptive regulation in MECs. [Xiao et al. \(2021\)](#) introduced a two-stage architecture combining a NARX model for time-series prediction of intermediate variables and an ANN for final output estimation. This structure enabled the controller to assimilate sequential operational data and forecast methane yield with higher accuracy ($R^2 = 0.918$) than conventional single-stage neural models. The adaptive control strategy further benefited from dimensionality reduction techniques for input selection and regularization, reducing the risk of overfitting and improving interpretability for real-time applications. The demonstrated improvement in prediction and control precision is particularly relevant for

biogas upgrading scenarios, where system dynamics and process targets may shift over time.

Neuro-fuzzy controllers, and particularly ANFIS, have also shown strong performance for adaptive regulation. Demir and Eren (2022) compared ANFIS controllers optimized using PSO and improved IGWO for voltage control in double-chamber MFCs. The IGWO-ANFIS controller achieved the lowest settling times (47.8 h) and minimal overshoot, maintaining robust voltage tracking and stability even in the presence of substantial nonlinearity and parameter uncertainty, and outperformed both PSO-ANFIS Proportional–Integral–Derivative (PID) control strategies.

Additional approaches introduced in recent literature include the finite-time Pade-based adaptive fuzzy neural network (PAFNN) controller for MFCs described by Fu et al. (2025). The authors developed a PAFNN controller for MFCs to address the challenges of input delay and multi-disturbance—two critical issues affecting voltage regulation and power output stability. The proposed controller integrates Pade approximation to model and compensate for start-up phase delays caused by microbial adaptation, while a fuzzy neural network (FNN) with nine fuzzy rules and radial basis functions is employed to approximate unknown nonlinearities and external disturbances in real time. The adaptive mechanism updates network weights online, ensuring the convergence of tracking errors through Lyapunov stability theory. Simulation results under three scenarios—no disturbance, noise disturbance, and multi-disturbance—demonstrated that the PAFNN outperformed traditional adaptive fuzzy and backstepping controllers in both convergence speed and disturbance rejection. Moreover, the controller achieved smoother voltage profiles and reduced fluctuation during early operation. Nonetheless, the authors note that under high disturbance intensities, long-term output power still declined slightly after extended operation, suggesting the need for further robustness improvements for deployment under complex real-world conditions.

Ma et al. (2025) conducted a systematic comparative analysis of a fractional-order PID (FOPID) controller with five tuning parameters optimized using a chaos-enhanced particle swarm optimization algorithm (SLRGE-IPSO). Their study benchmarked the proposed SLRGE-IPSO-FOPID controller against several established control strategies, including classical PSO-tuned FOPID (PSO-FOPID), PSO-PID, Backstepping, Sliding Mode Control (SMC), Fuzzy Sliding Mode Control (FSMC), Adaptive Sliding Mode Control (ASMC), and Adaptive Fast Terminal Sliding Mode Control (AFTSMC). Performance evaluation focused on key metrics such as settling time, steady-state error, overshoot, and robustness under sensor noise and nonlinear system dynamics. The results demonstrated that SLRGE-IPSO-FOPID achieved the lowest settling time (8.30 s), the smallest steady-state error (0.0387), and minimal overshoot (3.88%) among all methods tested. Additionally, the controller maintained stability and exhibited minimal oscillations in both the control input and output voltage, even in the presence of sensor noise. The authors report that, in all evaluated scenarios, SLRGE-IPSO-FOPID outperformed the benchmark controllers in terms of convergence speed, accuracy, and disturbance rejection, supporting its potential.

Fu (2025) proposed a robust control strategy for MFCs based on a Chebyshev neural network-enhanced adaptive sliding mode controller, designed to handle four major operational challenges: hard nonlinearities, parametric uncertainty, external disturbances (matched and unmatched), and sensor noise. The controller integrates output feedback with a Chebyshev neural network to approximate unknown nonlinear dynamics and uncertainty terms in real time, while sliding mode control ensures robustness against noise and estimation error. Adaptive laws are used to update neural network weights and upper bounds of disturbance and noise effects, guaranteeing closed-loop stability via Lyapunov theory. Simulation results under a severe scenario—including parametric shifts, sinusoidal disturbances, and Gaussian noise—demonstrated that the proposed controller achieved smoother voltage profiles, faster transient response, and better steady-state accuracy compared to

adaptive fuzzy and backstepping controllers. Additionally, the control signal remained stable and bounded due to the use of hyperbolic tangent functions instead of discontinuous sign functions. These findings highlight the potential of Chebyshev-based adaptive control for real-world BES implementations under uncertain and noisy conditions. al applicability in real-time MFC voltage control.

4.3.2. Real-time monitoring

The deployment of AI-enhanced real-time monitoring in BES has enabled continuous system tracking, early warning of operational disturbances, and data-driven process optimization. One prominent application is the use of ANN models to interpret output features from MFC biosensors. For example, ANN models trained with response metrics such as peak area and acceleration rate have achieved R^2 values of 0.99 in predicting COD concentration, outperforming manual and traditional correlations. This approach also allows the identification of temporal patterns indicative of sensor failure, providing a robust basis for online water quality monitoring (Feng et al., 2013). Similar methods have been used for detecting phenol in wastewater: both ANN and time-series models based on voltage and current output can track phenol degradation and microbial activity in real time, supporting their use for in situ monitoring and early intervention (Naik and Eswari, 2021).

The integration of ML models with bioelectrochemical sensor data in wastewater treatment plants has improved the monitoring of biological nutrient removal (BNR) processes. XGBoost models, using real-time BES voltage signals as predictors, have achieved R^2 values of 0.872 for nitrate removal. Notably, these models identified the BES signal as the most important feature for detecting variations in biodegradable carbon, allowing 86.9% of shock loading events to be correctly detected and enabling timely process interventions (Emaminejad et al., 2023).

AI-powered real-time monitoring is also being adopted in Internet of Things (IoT)-based environmental sensing. Panja and Meharia (2024) developed a system where voltage, temperature, and water level from an MFC are wirelessly transmitted to the cloud, and energy output is forecast using an ARIMA model. The model achieved low RMSE values (0.0119 and 0.0113) in two independent trials, demonstrating its utility for dynamic energy management in off-grid sensor networks. Here, coupling MFCs with a solar power bank allowed for long-term autonomous operation, while AI-driven predictions guided adaptive scheduling of IoT devices.

In agricultural applications, LSTM models have proven effective for predicting the energy output of soil-based MFCs. These deep learning models support more accurate scheduling of low-power sensor networks, reducing failed and missed activation rates compared to naive baselines. Quantile regression further enables confidence intervals on predictions, optimizing energy use for remote autonomous monitoring (Oyediji et al., 2023).

The utility of AI is not limited to single-analyte monitoring. Du et al. (2022) demonstrated that multiple algorithms—including SVM, ANN, RF, GLMNET, KNN, and PLS—can be applied in MEC biosensors for simultaneous real-time quantification of heavy metals (MnCl_2), nitrates (NaNO_2), and antibiotics (tetracycline HCl). Their comparative analysis showed that SVM achieved the lowest RMSE for MnCl_2 (0.21), ANN performed best for NaNO_2 (RMSE = 0.23), and GLMNET provided optimal prediction for tetracycline HCl (RMSE = 0.27). These findings illustrate how the selection of an appropriate algorithm can enhance the accuracy of high-throughput, multi-toxicant monitoring in complex wastewater environments.

Collectively, these studies demonstrate that combining ML, time-series modeling, and IoT data infrastructure enables not just continuous monitoring but also actionable insights for operational intervention and predictive maintenance in BES. The consistent use of AI across diverse BES platforms—from lab-scale biosensors to full-scale nutrient removal processes and distributed IoT systems—has improved both the precision and responsiveness of real-time monitoring strategies in the field.

4.4. Additional studies on AI applications in BES: complementing the main review

Beyond the core studies discussed in detail above, a broader spectrum of recent literature continues to expand the landscape of AI applications in BES. Table 1 presents a curated selection of works that, while not individually analyzed in previous sections, collectively illustrate the increasing methodological diversity and creative exploration taking place across the field. These studies highlight the versatility of AI, ranging from supervised learning algorithms and ensemble models to semi-supervised approaches (Farahani et al., 2024; Mehta et al., 2024; Mohammad and Ishaq, 2024), each adapted to address specific application objectives and BES types.

Notably, the reviewed works reveal an emerging trend toward integrating ensemble models and dimensionality reduction methods with traditional BES configurations to achieve more nuanced optimization and system monitoring (Farahani et al., 2024; Gürbüz et al., 2024; Mohammad and Ishaq, 2024). Semi-supervised learning, as applied to microbial consortium selection Mehta et al. (2024), exemplifies how innovative strategies are opening new avenues for addressing complex, multi-dimensional challenges in system design and operation. The cumulative evidence also suggests a move toward data-informed modeling, where variable selection, feature importance, and sensitivity analysis are increasingly leveraged to guide experimental focus and operational decision-making (Gürbüz et al., 2024; Li et al., 2024; Lim et al., 2024).

Analysis of the distribution of research objectives across the compiled literature reveals a distinct emphasis on optimization tasks, with adaptive control and real-time monitoring also receiving substantial attention in recent years (Demir and Eren, 2022; Esfandyari et al., 2016; Wang and Wang, 2019). As illustrated in Fig. 7, this trend signals a notable shift in the community's focus: from foundational performance evaluation toward the development and deployment of AI-driven strategies capable of dynamically enhancing system operation and resilience. Such a progression highlights not only the maturation of AI applications within the field, but also the growing ambition to implement more robust, responsive, and intelligent BES management approaches.

5. Challenges and future opportunities

The application of AI has demonstrated immense potential to optimize BES and evaluate system performance, enhance efficiency, and enable novel functionalities. However, these advancements are accompanied by significant challenges that hinder broader adoption and scalability. Overcoming key obstacles, including data inconsistency, the inherent complexity of biological interactions, and the absence of standardized modeling frameworks, is critical to advancing the development and implementation of AI-driven BES.

5.1. Data acquisition and model implementation

The accuracy and reliability of predictive models are strongly influenced by the quality of the input data. One of the main challenges in applying AI to BES includes the difficulty of obtaining consistent data due to operational variability. This limits the size and quality of datasets needed to train AI models effectively. Moreover, the complex and non-linear characteristics of BES systems pose significant challenges for model tuning, increasing the risk of overfitting and limiting their capacity to generalize effectively.

Beyond data consistency and model tuning, creating a robust foundation for AI in BES requires standardization across studies. The lack of uniformity in experimental designs and data collection protocols complicates the development of comprehensive and comparable datasets, essential for building generalizable AI models. Without standardized frameworks, models trained on specific datasets may struggle to perform

reliably when applied to different BES configurations, limiting scalability and adaptability across diverse operational settings.

Looking ahead, future opportunities involve not only expanding the range of physical and operational variables considered during BES modeling, but also improving the strategies used to train and optimize ML models. In addition to optimizing system-level parameters—such as electrode configuration, substrate concentration, and applied voltage—recent studies have employed metaheuristic algorithms to fine-tune internal parameters of ML models, including structural hyperparameters. These approaches have proven effective in addressing complex, multi-objective optimization problems, particularly where traditional methods like genetic algorithms exhibit limitations in efficiency.

For instance, Chalak Qazani et al. (2024) applied multi-objective PSO to optimize a T2FNN for simultaneous prediction of PD and COD removal in MFCs, achieving R^2 values close to 0.99 and identifying optimal trade-offs between objectives. Nasrabadi and Moghimi (2022) used PSO to optimize the weights of an ANN surrogate model for a microfluidic MFC, reducing computation time by approximately 50 times compared to GAs while maintaining prediction errors below 5%. In another study, Rezk and Sayed (2024) implemented AGTO to fine-tune an ANFIS model for MECs, obtaining over 90% RMSE reduction and a 30% increase in hydrogen production compared to traditional modeling approaches. Similarly, Chou et al. (2022) used metaheuristics to optimize the internal parameters of an LSTM model for power prediction in plant-based MFCs, reporting improvements of over 20% in accuracy compared to manually tuned configurations.

5.2. Modeling biological complexity

Another major barrier to the effective application of AI in BES is the limited understanding of microbial interactions and dynamics within these systems. Biological factors can be unpredictable and highly variable (Badrick, 2021), significantly increasing the uncertainty inherent in AI models. Understanding this complexity is crucial for improving their accuracy and reliability. One promising approach involves integrating multi-omics data—such as metagenomics and metatranscriptomics into AI frameworks to capture the functional and structural dynamics of microbial communities. For instance, Yu et al. (2019) demonstrated that combining metagenomic and metatranscriptomic analyses with targeted metabolite profiling can elucidate interspecies interactions and metabolic pathways in microbial consortia, enhancing the predictive capabilities of computational models. Similarly, recent studies have highlighted the potential of AI-driven models to process and interpret large-scale transcriptomic data, enabling the discernment of gene expression changes in microbial communities and improving the modeling of complex biological systems (Yan et al., 2025). Effectively adapting AI to account for these complex microbial behaviors remains a critical challenge, as these behaviors influence system performance in ways that are difficult to capture and model accurately.

5.3. Real-time processing

Despite recent progress in real-time monitoring of BES enabled by AI, significant challenges remain before such systems can be robustly implemented in real-world, long-term scenarios. As highlighted in studies using ANN and time-series models for biosensing (Feng et al., 2013; Naik and Eswari, 2021), issues such as sensor signal drift, fouling, and fluctuating environmental backgrounds continue to impact data reliability. In practical deployments, maintaining stable and interpretable sensor output over time remains problematic, particularly when dealing with complex wastewater matrices or variable influent composition.

Most AI models developed for BES applications have been trained and validated using datasets collected under controlled laboratory or pilot-scale conditions. While such settings often yield high predictive

Table 1
Overview of BES studies using AI.

BES Type	AI Application Objective	AI Algorithm	Performance Metrics	Notable Contribution or Innovation	Reference
MFC	BES Performance Prediction	ANN, ANFIS	R^2 : 0.998 (ANN), 0.999 (ANFIS) for PD; R^2 : 1.000 (both) for CE	<ul style="list-style-type: none"> First comparative modeling of MFC PD and CE using both ANN and ANFIS. Identified a simpler structure and tuning procedure for ANN with comparable accuracy. 	Esfandiyari et al. (2016)
		GP, MARS	RMSE: as low as 4.12 (PD), 1.57 (Voltage); MAPE: 3.8%–5.9%; R^2 : not explicitly stated	<ul style="list-style-type: none"> Developed explicit models for predicting PD and voltage in microfluidic MFCs using GP and Multivariate Adaptive Regression Splines (MARS). GP showed superior robustness and accuracy under dynamic conditions and enabled parametric and sensitivity analysis. 	Garg and Lam (2017)
		ANN	R^2 : 0.9993, MSE: 6.0616	<ul style="list-style-type: none"> First application of ANN to predict PG in an MFC fueled by untreated giant reed cellulose. Demonstrated the influence of particle size and optimized GR concentration for bioelectricity production. 	Ismail et al. (2019)
		RNN	R^2 : 0.95 (PD), 0.928 (COD), 0.701 (Voltage); Corr. Coef.: up to 0.975	<ul style="list-style-type: none"> Trained RNN models on 5600 data points aggregated from over 60 MFC studies to predict voltage, PD, and COD removal in textile wastewater treatment; demonstrated robust cross-study generalizability and validated model accuracy using experimental data from a novel dual-chamber MFC setup. 	Khoshgoftar Manesh et al.
		CatBoost, XGBoost, RF, GB, DT, AdaBoost	R^2 : 0.9969 (CatBoost); RMSE: 6.9888 (CatBoost); MSE: 48.8430 (CatBoost)	<ul style="list-style-type: none"> First to model MFC performance using landfill leachate as substrate with ensemble ML algorithms; integrated feature selection and sensitivity analysis to identify key environmental drivers, with CatBoost achieving superior predictive accuracy and robustness. 	Mohammad and Ishaq (2024)
		FL	$R^2 = 0.86$ (PD); RMSE = 0.0512;	<ul style="list-style-type: none"> Combined FL modeling with central composite design to simulate and quantify the influence of reactor volume, anode area, and external resistance on current and PD in MFCs. Developed statistically significant predictive equations with strong agreement to laboratory results, offering a simplified yet robust framework for understanding and optimizing MFC behavior across broad operational ranges. 	de Lima Cardozo et al. (2024)
		ANN, SVM	R^2 : 0.9898 (ANN), 0.98 (SVM); RMSE: 7.65 (ANN), 9.81 (SVM); MAE: 5.09 (ANN), 6.38 (SVM)	<ul style="list-style-type: none"> Developed predictive models for OCV in MFCs using ANN and SVM. Incorporated dynamic input parameters including pH, temperature, and total dissolved solids (TDS). Identified TDS as the most influential factor on voltage output through sensitivity analysis. 	Murugesu et al. (2025)
		ANN	R^2 : 0.99889, MSE: 6.4203	<ul style="list-style-type: none"> First study analyzing anode inclination impact on MFC performance; used ANN to predict optimal inclination and flow rate for maximal PG from dairy wastewater. Identified optimal angle (100°) and flow rate (1.8 mL/min) for maximum PG via ANN simulation. 	Jaheel et al. (2016)
		ANFIS, PSO	R^2 : 0.989 (PD), 0.982 (COD); MSE: 0.909 (PD), 6.791 (COD)	<ul style="list-style-type: none"> ANFIS-PSO significantly outperformed ANOVA in optimizing MFC for both PD and COD removal. Multi-objective optimization yielded PD of 61.787 mW/m² and COD removal of 96.21%. 	Ghasemi et al. (2021)
		ANN	R : up to 0.95, MSE: 7.90, Convergence time: 7.8 s	<ul style="list-style-type: none"> Compared three second-order ANN training algorithms—Quasi-Newton (QN), LM, and Conjugate Gradient (CG)—to predict ceramic MFC PG under varying urine flow rates; LM achieved highest accuracy and fastest convergence Demonstrated the feasibility of low-cost urine-fed MFCs for energy generation and model generalizability across experimental configurations 	de Ramón-Fernández et al. (2020)
		ANN, FBI	R^2 : 0.9783 (Power), 0.9914 (COD); RMSE: 0.512 (Power), 0.178 (COD)	<ul style="list-style-type: none"> Developed highly accurate ANN models to simulate voltage, current, and PG in dual-chamber MFCs using food industry wastewater. Validated model predictions with experimental results under varying operational conditions. Demonstrated ANN's potential for simulating and forecasting MFC behavior in complex, real-world wastewater scenarios. 	Sayed et al. (2024)
		DT	R^2 : 0.98; Experimental validation accuracy: 77%–99%	<ul style="list-style-type: none"> First use of DT regression to optimize banana peel waste-based MFCs with <i>S. cerevisiae</i>; identified optimal operating conditions (temperature, resistance, pretreatment) for high PD; validated with experimental and computational results 	Verma et al. (2023b)

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Table 1 (continued)

BES Type	AI Application Objective	AI Algorithm	Performance Metrics	Notable Contribution or Innovation	Reference
BES Adaptive Control & Real-Time Monitoring		PCA, Classification Tree, SHAP	F1 Score: 0.83 (low), 0.71 (high); Accuracy: 76% (train), 71.8% (test)	<ul style="list-style-type: none"> First comprehensive modeling of plant MFCs using a meta-dataset of 229 observations and 159 variables Combined dimensionality reduction (PCA), explainability (SHAP), and DTs to identify optimal material and operating conditions for maximum PG 	Gürbüz et al. (2024)
		ANN	R^2 : 0.9954 (PD), 0.9932 (COD); RMSE: 0.0512 (PD), 0.0272 (COD); MPE: 33.82%, 8.24%	<ul style="list-style-type: none"> First study to model and predict MFC performance using greywater-syrup substrate and a novel Ekowe clay-carrageenan PEM ANN outperformed RSM in predicting both PD and COD removal across 30 experimental runs 	Obasi and Nevo (2024)
		XGBoost, CatBoost, AdaBoost, SVR, NSGA-II	R^2 : 0.894 (XGBoost); RMSE: 40.997 (XGBoost); Errors: CD 0.79%, PD 0.5%, COD 1.89%, CE 1.27%	<ul style="list-style-type: none"> Enhanced MFC performance by modeling and optimizing Wolf vitamin solution concentration using a suite of predictive algorithms combined with NSGA-II. Achieved 395.6 mW/m² PD and 78% COD removal at 5.8 mL dosage, offering a robust nutrient optimization strategy 	Farahani et al. (2024)
		SS-kNN	Accuracy: 100% (training), 85.71% (testing); AUC: 1.0 (Best class)	<ul style="list-style-type: none"> Pioneered the use of semi-supervised kNN to predict optimal microbial consortia in MFCs using performance indicators (voltage, COD removal, exopolysaccharide production, voltage stability); demonstrated superior performance (0.703 V, 49.88% COD removal) and eliminated the need for combinatorial microbial testing through data-driven strain selection. 	Mehta et al. (2024)
		ANN	R^2 : 0.996 (Voltage), 0.988 (Power); RMSE: 0.014 (Voltage), 0.219 (Power)	<ul style="list-style-type: none"> First to model MFCs fed with dried waste activated sludge using ANN Identified temperature as the most influential factor on voltage and PG; validated model with close alignment between predicted and experimental values under optimal conditions (55°C, pH 9, 16 g/L WAS) 	Wei et al. (2024)
		ANN, ELM, RVM, GPR, SVM	R^2 : up to 0.9998 (ELM); MSE: 1.97E-6 (ELM); MAPE: 0.0004 (ELM); DS: up to 0.9950 (RVM)	<ul style="list-style-type: none"> Introduced a novel intelligent explicit model predictive control (EMPC) using ML for real-time control of MDCs, enabling efficient and stable tracking without online optimization 	Wang and Wang (2019)
		ANN, SVM, RFR, k-NN, LDA, QDA	Accuracy: up to 93% ± 6%, Kappa: up to 0.87	<ul style="list-style-type: none"> Novel integration of microbial community data with ML to predict feed substrates in MFC. Comparative evaluation of six classification algorithms to identify the most robust and accurate model. RFR identified as the best performer (96.2% accuracy), highlighting its suitability for bioinformatics applications in BES. 	Cai et al. (2019)
		ANS	Visual slope convergence between weeks 12–16	<ul style="list-style-type: none"> For the first time, implemented an artificial neural search (ANS) model to predict the power stabilization period in MFCs. 	Singh et al. (2019)
		SVR	R^2 : 0.94 (test), 0.98 (train); MAPE: not reported	<ul style="list-style-type: none"> First energy-autonomous MFC-based sensor using SVR to estimate COD with embedded ML on a microcontroller Integrates sensing and power in a single unit for field deployment 	Shabani et al. (2021)
		NARX	$R = 0.99978$ (train), 0.99988 (validation), 0.99994 (test), 0.9998 (overall); MSE = 1.049×10^{-5} (cross-MFC test)	<ul style="list-style-type: none"> First implementation of NARX for time-series prediction of MFC voltage to support autonomous feeding schedules in soft robotics Validated on an independent MFC system with near-perfect accuracy 	Tsompanas et al. (2021)
		ANN	R^2 : up to 0.976; MAPE: as low as 7.5%; MAX error: 3.39–25.36 mg	<ul style="list-style-type: none"> Developed an AI-enhanced MFC biosensor to predict BOD₅ values significantly faster than conventional methods. Trained ANN using experimental MFC voltage data to estimate BOD₅ with high accuracy and low error margins. Demonstrated a prediction time reduction from 5 days to under 1 h while maintaining reliable performance. 	Medvedev et al. (2023)
		GSCPSO	ISE:0.001245, IAE: 0.09031, ITAE: 0.02743	<ul style="list-style-type: none"> Developed an improved PSO algorithm to optimize PID controller parameters in MFCs. Achieved significantly better performance (ISE, IAE, ITAE) than standard PSO and Ziegler–Nichols methods. Validated improved system stability and control efficiency in dynamic MFC response. 	Wang et al. (2024)
	LSTM	Voltage MAPE: 2.33%–5.71%; Total Energy Error: 43.31% to +29.30%; Failed Activations: 0%	<ul style="list-style-type: none"> Developed a forecasting framework for energy generation in soil MFCs using LSTM networks with 	Hess-Dunlop et al. (2024b)	

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Table 1 (continued)

BES Type	AI Application Objective	AI Algorithm	Performance Metrics	Notable Contribution or Innovation	Reference
MEC	BES Performance	ANN	$R^2 = 0.70\text{--}0.90$ (individual models), 0.85 (committee average); Sensitivity = 0.68 (substrate), 0.37 (voltage).	<ul style="list-style-type: none"> quantile regression, tailored for intermittent computing applications. Introduced new evaluation metrics (missed and failed activations) and demonstrated that predictive scheduling doubled activation success rates compared to baseline methods, enhancing energy-aware computing in low-power biosensor systems. 	Sewsynker et al. (2015)
		RFR	R^2 : Not explicitly stated; Feature importance via Mean Decrease Gini	<ul style="list-style-type: none"> First use of a committee of ANNs to model biohydrogen yield in MECs Enabled accurate simulation of non-linear interactions between six key input parameters, identifying substrate type and applied voltage as the most influential 	Wang et al. (2021)
		ANN	R^2 : 89.02% (CSMEC), 94.14% (CSTR); MSE: 0.408 (CSMEC), 0.519 (CSTR)	<ul style="list-style-type: none"> Achieved record hydrogen yield from lignocellulosic hydrolysate in a 10-L MEC with biocathodes Used RFR to correlate microbial community data with current density, revealing <i>Enterococcus</i> spp. as key electroactive taxa and quantifying the impact of fermentative bacteria on performance 	Quashie et al. (2023)
		RFR, GBDT, XGBoost, 2S-XGBoost	R^2 : 0.877 (XGBoost-acetate), 0.647 (XGBoost-ethanol); 0.727 (2S-XGBoost ethanol); MSE: as low as 0.00013	<ul style="list-style-type: none"> First predictive ANN model of biogas production from food waste in a CSMEC demonstrated higher performance of CSMEC over CSTR and validated ANN model accuracy across multiple training algorithms, with LM achieving best fit Applied multiple ML models to predict acetate and ethanol production from microbial electrosynthesis using electricity and CO₂. Employed Bayesian optimization to fine-tune hyperparameters, enhancing model accuracy. Identified XGBoost as the most effective model, offering high predictive performance and generalizability. 	Li et al. (2024)
	BES Optimization	ANN, PSO	R^2 : 0.87–0.99; PCC: 0.93–0.99; NRMSE: 0.078–0.221; Error vs Experimental	<ul style="list-style-type: none"> Developed the first dynamic model for a single-chamber anode brush MEC using acetic acid, then simulated and optimized it via ANN and PSO Identified co-optimal conditions yielding 1172.2 mL/g H₂, 191.8 mL/L/h HPR, and 16.8% TER, demonstrating significant gains in computational speed and predictive accuracy 	Phan et al. (2024)

Abbreviations: GB: Gradient boosting; MARS: Multivariate Adaptive Regression Splines; 2S-XGBoost: 2-Stage XGBoost; CSTR: Continuous Stirred Tank Reactor; CSMEC: Continuous Stirred Microbial Electrolysis Cell; MAPE: Mean Absolute Percentage Error; ISE: Integral of Squared Error; IAE: Integral of Absolute Error; ITAE: Integral of Time-weighted Absolute Error; ELM: Extreme Machine Learning; FBI: forensic-based investigation algorithm; NRMSE: normalized root mean squared error; PCC: Pearson correlation coefficient.



Fig. 7. Distribution of AI application studies in BES by research objective and system type.

accuracy, numerous studies caution that performance tends to degrade in full-scale or real wastewater environments, where fluctuating background matrices and unanticipated disturbances prevail. For example, Du et al. (2022) highlight the challenges associated with differentiating toxicants in complex wastewater streams, noting that variations in the physicochemical environment can impact the reliability of ML-based biosensors and necessitate further validation and model adaptation when transitioning beyond well-controlled experiments. To improve generalizability, a promising strategy involves combining real-time sensing with adaptive learning mechanisms that dynamically recalibrate model parameters as environmental conditions evolve, thereby enhancing robustness in operational deployments.

The integration of IoT architectures and cloud-based data management platforms introduces significant opportunities for remote and distributed monitoring in BES, as demonstrated in recent developments (Panja and Meharia, 2024). However, these advances are accompanied by challenges such as data security, communication latency, and the computational constraints of deploying real-time inference on resource-limited hardware. Achieving reliable, autonomous, and scalable real-time AI-driven monitoring will thus depend not only on advances in model robustness, but also on the standardization of sensor platforms, validation across multiple operational environments, and the development of resilient hardware and communication protocols capable of supporting long-term, autonomous system operation.

Looking forward, future opportunities involve the deployment of edge computing and federated learning approaches to enable decentralized model updates, and the use of digital twins to test model resilience under synthetic disturbances before field application. Ultimately, progress in real-time processing will depend on the convergence of AI innovation, sensor engineering, and scalable system integration, alongside ongoing efforts to standardize protocols and establish best practices for industrial and environmental BES applications.

6. Future perspectives

Incorporating advanced models such as Large Language Models (LLMs) into BES design holds significant promise. LLMs, renowned for their capacity to process and interpret complex, high-dimensional data, can identify intricate relationships between operational parameters and microbial dynamics, leading to optimized BES configurations. For instance Jin et al. (2024), in the field of protein research proposed a framework to predict protein-protein interactions with high accuracy. This approach leverages a structured reasoning pathway that simulates biological signaling cascades, enabling the model to better understand complex, sequential relationships between proteins. Such a framework demonstrates the potential of LLMs to process intricate biological data and uncover insights into molecular interactions. Applying similar methodologies to BES could enhance our understanding of the multifaceted interactions within these systems, facilitating the development of more efficient and resilient designs. Furthermore, recent advances in scientific LLMs, as surveyed by Zhang et al. (2024b), underscore the model's expanding capability to interpret biological and chemical data specifically. These tailored LLMs could unlock new insights in BES by generating more precise models of microbial and chemical interactions, which are crucial for optimizing reactor configurations and operational conditions.

However, the integration of LLMs into BES applications requires adaptations beyond generic language modeling. As their default training prioritizes contextual relevance over numerical precision, domain-specific fine-tuning and hybrid approaches are essential. Coupling LLMs with mechanistic models or constraining their outputs with physical and biological knowledge can enhance their scientific validity. These strategies are necessary to ensure that LLM-generated insights meet the accuracy standards required for bioelectrochemical modeling.

To fully leverage the capabilities of AI in BES research, the establishment of comprehensive, publicly accessible data repositories is essential. Such repositories would provide standardized, high-quality datasets necessary for training robust AI models. In the realm of genomics, the creation of extensive databases has been instrumental in advancing AI-driven insights, enabling cross-study analyses and improving predictive performance (Clayton et al., 2020; Herrmann et al., 2020). Implementing similar data-sharing initiatives in BES research could foster collaborative research efforts and enhance model performance by ensuring consistent and diverse data sources. These data-sharing frameworks would not only accelerate model development but also support the scalability and adaptability of BES technologies, leading to more versatile applications in environmental monitoring and bioenergy production.

7. Conclusions

This review demonstrates the application of AI in advancing BES through improved modeling, system optimization, and control strategies. AI techniques have enhanced predictive accuracy and surpassed traditional modeling approaches, enabling more effective forecasting of PG, microbial dynamics, and energy recovery. The exploration of ML algorithms and optimization methods reveals both their strengths and the current limitations in addressing the inherent complexity of BES environments.

Despite these advances, significant challenges remain. The high variability of BES configurations and the complex interactions between microbial and electrochemical components hinder model generalization and scalability. Moreover, inconsistencies in experimental protocols and data collection restrict reproducibility and limit the development of transferable AI solutions. Addressing these barriers requires the creation of standardized, accessible datasets to support robust models applicable across diverse BES systems.

Emerging approaches such as hybrid modeling and transfer learning offer promising avenues to enhance model adaptability and reduce dependence on large datasets. Integrating richer microbial and electrochemical data into AI frameworks can deepen mechanistic insights and further improve energy efficiency and product recovery.

Throughout this review, emphasis was placed on elucidating how specific AI methods—ranging from regression models to metaheuristic optimizers—have been applied to solve core BES challenges, including PD prediction, contaminant removal, and operational tuning. This structured narrative unifies the technical content and highlights the ongoing convergence of AI innovation and bioelectrochemical system development.

CRedit authorship contribution statement

Miguel Esteban Pardo Gómez: Writing – review & editing, Writing – original draft, Visualization, Methodology, Investigation. **Evan Park:** Writing – review & editing. **Ying Zheng:** Writing – review & editing. **Amarjeet Bassi:** Writing – review & editing. **Tianlong Liu:** Writing – review & editing, Writing – original draft, Validation, Supervision, Resources, Project administration, Methodology, Investigation, Funding acquisition, Conceptualization.

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.

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