Artificial neural networks: an efficient tool for modelling and optimization of biofuel production (a mini review)

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ABSTRACT
In view of the looming energy crisis as a result of depleting fossil fuel resources and environmental concerns from greenhouse gas emissions, the need for sustainable energy sources has secured global attention. Research is currently focused towards renewable sources of energy due to their availability and environmental friendliness. Biofuel production like other bioprocesses is controlled by several process parameters including pH, temperature and substrate concentration; however, the improvement of biofuel production requires a robust process model that accurately relates the effect of input variables to the process output. Artificial neural networks (ANNs) have emerged as a tool for modelling complex, non-linear processes. ANNs are applied in the prediction of various processes; they are useful for virtual experimentations and can potentially enhance bioprocess research and development. In this study, recent findings on the application of ANN for the modelling and optimization of biohydrogen, biogas, biodiesel, microbial fuel cell technology and bioethanol are reviewed. In addition, comparative studies on the modelling efficiency of ANN and other techniques such as the response surface methodology are briefly discussed. The review highlights the efficiency of ANNs as a modelling and optimization tool in biofuel process development.

Abbreviations
AI: Artificial intelligence
ANN: Artificial neural network
BPNN: Back propagation neural network
BWD: Box–Wilson design
COD: Chemical oxygen demand
DOE: Design of experiment
GA: Genetic algorithm
MEC: Microbial electrolysis cell
MFC: Microbial fuel cell
OVAT: One-variable-at-a-time
\( R^2 \): Coefficient of determination
RSM: Response surface methodology

Introduction
Bioprocesses are described as biological systems that are non-linear, complex and unsteady; thus, it is challenging to develop a precise physical-based formula to characterize their physical performance. In addition, the development of accurate bioprocess models continues to baffle experts, as a result of the non-linear nature of the biochemical network interactions that occur during fermentation processes [1]. Bioprocesses are influenced by several parameters which include pH, temperature, hydraulic retention time, substrate concentration, etc.; therefore, the determination of the optimum values of these parameters is crucial for bioprocess development and scale-up [2].

Mathematical and statistical-based models can provide vital information for the understanding, analysis and prediction of biological processes and they are required for the optimization of key parameters in order to improve the process output [3]. These bioprocess models can provide insight on the individual as well as the interactive effect of the various input parameters on the target output. Nevertheless, the non-linearities associated with microbial fermentations have limited the use of these bioprocess models. Non-linear systems as opposed to linear systems are not standardized, which leads to deviations between the results obtained. The implementation of bioprocess models that are able to efficiently encapsulate these non-linearities is of paramount importance for optimization and scale-up of the bioprocess [4].

Biofuel production has emerged as a promising alternative to fossil fuel sources [5]; the development of such alternatives may help overcome the current energy crisis...
and also provides a clean source of energy to combat the phenomenon of global warming [5,6]. Current biofuels include bioethanol, biodiesel, biohydrogen, biogas [7] and fuel cell technologies such as microbial fuel cells (MFC) and microbial electrolysis cells (MEC) [8]. The major limitation of these biofuels may be attributed to the low yields and production rate observed [6].

Modelling and optimization of biofuel production processes will contribute to increased understanding of the process inputs for optimum yield and production rate. The main goal of modelling is to optimize the processes involved in producing these biofuels in order to improve the yields. Various modelling algorithms have been applied in biofuel production processes [6,9–15], and results have shown that modelling and optimization can enhance biofuel yields [11,16].

For instance, Ghosh et al. [16] used the response surface methodology (RSM) to optimize biohydrogen production on inputs of glucose concentration, fixed nitrogen and light intensity in a single-stage photo fermentation with the photosynthetic bacterium *Rhodobacter capsulatus*. Their results showed that these parameters had a significant interactive effect on the biohydrogen yield and nitrogenase activity. The optimized biohydrogen yield (5.5 mol H2/mol glucose) was 85% higher than previously achieved [16].

Traditionally, modelling and optimization of bioprocesses have been carried out using the one-variable-at-a-time approach (OVAT), factorial Design of Experiment (DOE) and RSM [6,17–24]. These approaches have been extensively used and their concepts as well as limitations are well known. For example, OVAT does not consider the interactive effect of parameters on the process and, therefore, the optimum set points may be completely ignored [11,25]. Moreover, it is unfeasible for the search to accomplish an appropriate optimum in a restricted amount of experimental set-ups [26]. The factorial DOE has shown to be unappealing, since it is time-consuming, resource demanding and labour intensive when the numbers of input factors are increased [9]. On the other hand, the RSM disregards the ‘less important’ parameters with a limited understanding of their possible interactive effects on the bioprocess output [11,27].

Artificial intelligence tools have emerged as a promising method for modelling and optimization of bioprocesses. Some of these include artificial neural network (ANN) and genetic algorithm (GA) [12,28,29], fuzzy logic, ant algorithm and particle swarm optimization, all of which are considered suitable in the design of bioprocesses for research and development [11,27]. In the last decade, ANN has been applied in multivariate non-linear bioprocess research and development. They are efficient for the development of bioprocess models devoid of previous information with regard to the kinetics and metabolic fluxes that occur within the cells and cell surroundings [11]. ANN models simulate the linkage that exists in biological neurons with extraordinary capability for learning, analysis, association and adaptation [32].

ANNs can be described as a mathematical understanding of the neurological functioning of the human brain. They emulate the brain’s learning process by arithmetically modelling the network structure of interconnected nerve cells [32]. Furthermore, ANNs are entirely data-based with no previous knowledge of the events that govern the process [33]. They consist of an input layer, one or more hidden layers and an output layer (Figure 1). The neurons of the hidden layer assist the network in establishing the complex associations that exist between the input and output parameters [32].

The appeal of ANNs as a modelling tool stems from their extraordinary information-processing features which are attributed primarily to non-linearity, high parallelism, fault and noise acceptance as well as their learning and generalization abilities. In contrast to traditional modelling tools, ANNs offer a model-free, adaptive, parallel-processing and vigorous elucidation with error and failure tolerance. Moreover, their learning capability for processing inaccurate and fuzzy information and their ability to generalize unseen patterns are impeccable [34]. ANN possesses the ability to sketch process input and outputs devoid of causal assumption regarding the division of data. ANNs have gained much attention as significant soft computing tools not limited to data processing and analysis only but can also be applied to solve difficulties in multifaceted and non-linear processes [35].

The rapid development of algorithms and information technology is the major motivation behind the broad application of ANNs in research and development [36]. Currently, ANNs are employed in the prediction of various outcomes including process control, medicine, forensic science, biotechnology, weather forecasting, finance and investment and food science. However, it is noteworthy to state that the use of ANNs in biofuel production is currently in the early phases of its development.

Generally, microbial fermentations exhibit non-linear relationships which could pose several problems during bioprocess modelling and optimization. The application of robust models such as ANN helps to capture this non-linear behaviour, and thus provides a model that links the process inputs to the corresponding output parameters.

This review therefore highlights the efficiency of ANNs as a tool for modelling and optimization of microbial biofuel production and its potential for future application. In this paper, various studies regarding the application of ANN in microbial biofuel production including biohydrogen, biogas, MFC technology and bioethanol were reviewed. The application of ANN for the
optimization of biofuel production technologies such as biodiesel and photo fermentative biohydrogen, to the best of our knowledge, has been scantily reported in literature, and therefore was not included in this review.

In addition, the comparison of ANN to commonly used modelling techniques such as RSM was also highlighted. In the Introduction section, a general description of bioprocess modelling and optimization is discussed. The ‘Principles of ANNs’ section focused on the underlying principle of ANN, while the different types of ANN and training algorithm are reviewed in the ‘ANN types and training algorithms’ section. Furthermore, the application of ANN for the optimization of different biofuel production system is explored in the ‘Application of ANNs in biofuel production’ section; GA coupled with ANN for optimization is discussed in the ‘GA coupled with ANN for optimization’ section. Finally, comparative assessments of ANN with other modelling tools such as RSM and the challenges with the future outlook of ANN application are highlighted in the ‘Comparative assessment of ANN and RSM for modelling and optimization of biofuel production’ section and ‘Challenges and future outlook’ section, respectively.

Principles of ANNs

Mathematical model of a single artificial neuron

The neuron receives inputs $x_1, x_2, \ldots, x_n$ that model the signals coming from dendrites. Usually $x_0$ is assigned a value of $+1$ as the bias input. The inputs are then labelled according to their synaptic weights $w_1, w_2, \ldots, w_n$ that measure their importance. Some of these synaptic weights may be negative to express their inhibitory effect. The weighted sum of input values represents the excitation level of the neuron as follows:

$$\zeta = \sum_{i=1}^{n} w_i x_i$$  \hspace{1cm} (1)

When the threshold $h$ is reached, the value of excitation level induces a neuron output $y$, which models the electric impulse generated by the biological axon. The non-linear output value $y = \sigma(\zeta)$ is determined by the activation function $s$. The mathematical formulation
of neuron function can be expressed according to

\[
y = \sigma(\zeta) = \begin{cases} 
  1 & \text{if } \zeta \geq 0 \\
  0 & \text{if } \zeta < 0
\end{cases} \quad \text{where} \quad \zeta = \sum_{i=0}^{n} w_{i}x_{i} \tag{2}
\]

The output is analogous to the axon of a biological neuron, and its value propagates to the input of the next layer through a synapse.

**ANN modelling**

ANN involves the interconnection of a structure known as artificial neurons similar to biological neurons [34,36]. The principle behind ANNs is to mimic the functioning and learning process of a human brain using an artificial neuron. An artificial neuron is a computational model that is inspired by biological neurons. Biological neurons consist of dendrites, soma, axon and synapses. The dendrites are used for receiving signals from other neurons and can also be referred to as chemical receptors. Additionally, the soma makes up the cell body of a neuron and is involved in processing the input signals. This is followed by the emission of the processed signals to neurons that are in close proximity to the axon. Finally, the neurons are linked via the synapses which also control the transmission of signals among the neurons. The actual structure and functioning of a biological neuron is far more intricate as compared to this simple design of an artificial neuron [34,36].

ANN composed of groups of interconnected processing elements known as neurons and the links between these neurons are known as weights and biases [37]. Furthermore, in contrast to a biological neuron, an artificial neuron receives a sequence of input information \((x_{i})\) linked to a weight factor \((w_{i})\). ANNs are composed of multiple neurons, which imitate the biological neurons of humans. A typical neural network has at least three layers. The first layer is generally referred to as input layer and has input neurons which send data via synapses to the second or hidden layer neurons and then via more synapses to the output layer neurons. More complex systems may have more hidden layers of neurons. The synapses store parameters called ‘weights’ that manipulate the data in the calculations.

Basically, the neuron adds the weighed inputs and forwards the outcome to a transfer function to produce an output. The output information is thereafter transmitted to an alternate neuron as an input or may be employed directly as a network result. The weights are referred to as the attachment strength linking the neurons. As a result of some input signals being more significant compared to others, the utilization of weights as equivalent to the significance of each input signal provides a well-organized process to create an ideal output. The values of weights are adapted during the training phase of the network. There are various algorithms available for the adjustment of weights during network training [38].

The network architecture or topology refers to the pattern of interconnection among the neurons that make up a network [39]. Artificial neurons develop layers with different types of connections between them, i.e. a neuron of one layer can be linked with neurons of at least one other layer. There are different types of connections used between layers and are referred to as inter-layer connections. With regard to inter-layer connections, a neuron in one layer is linked with all the neurons in the subsequent layer, thus resulting in a completely connected network. However, if the neurons are connected to only some of the neurons in the next layer then the network is only partially connected. Usually, neurons in one layer send output information to the next layer, and they may (feedback networks) or may not obtain information back from the next layer. Also, these neurons may or may not be linked with each other in the same layer.

Alternatively, in more complex structures, the neurons communicate among themselves within a layer called intra-layer connections. Regarding the intra-layer connections, once the input information has been obtained from the previous layer, neurons within one layer converse with each other several times prior to transmitting their output to another layer [40]. ANNs are occasionally referred to as machine-learning algorithms, since changing their connection weights (training) causes the network to learn the solution to a problem. The strength of connection among the neurons is stored as a weight-value for the specific connection. The system is able to learn new knowledge by adjusting these connection weights. The learning ability of an ANN is determined by its design and by the algorithmic method selected for training. This algorithm attempts to reduce the error that is computed by various methods depending on the specific technique used to adjust the connections (i.e. the learning algorithm) [34].

The major learning paradigms include (1) supervised learning, (2) unsupervised learning and (3) reinforcement learning. During supervised training, both the inputs and the outputs are provided. The network then processes the inputs and compares its subsequent outputs against the desired outputs. Errors are then computed, causing the system to adjust the weights which control the network. This process is repeated over and over as the weights are constantly adjusted. On the contrary, with unsupervised training, the network is
provided with inputs but without the desired outputs. The neural network system on its own then selects what characteristics it will use to classify the input data [34,41]. Reinforcement learning allows the ANN agents to automatically determine the ideal behaviour within a specific environment. Thus, the ANN learns its behaviour based on the feedback from the environment. A reward feedback or reinforcement signal is required for the network to learn. If the problem is appropriately modelled, the reinforcement learning algorithms can converge to the global optimum [34].

**ANN types and training algorithms**

ANNs are characterized according to their functions. Common ANNs reported in studies include Hopfield [42], Kohonen [36,42], recurrent [36], counter propagation [43], radial basis function (RBF) networks [44] and feed forward back-propagation [24,27,45,46]. The feed forward back-propagation neural network (BPNN) which employs a supervised learning process has been frequently reported in biofuel process modelling as shown in Tables 1–5, and will be discussed in detail.

### Feed forward back-propagation neural networks (BPNN)

This type of network is the most extensively studied which involves the minimization of a performance function [69]. In general, this network is a multilayer perceptron (MLP) architecture, which is the most commonly used one [39]. The MLP includes an input layer with nodes that embody the input variable to the problem, the output layer with nodes that signify the dependent variable (what is modelled) and one or more hidden layers. The back-propagation is usually used for training of feed forward networks and has been extensively studied (Figure 2) [4,39]. By means of supervised learning, this network is able to discover complex patterns in data-sets.

### Table 1. Summary of modelling studies using ANN for biogas production.

| Input parameters                                                                 | Output parameters               | Type of ANN | ANN structure | R² value | References |
|---------------------------------------------------------------------------------|--------------------------------|-------------|---------------|----------|------------|
| pH, glucose, xylose ratio, inorganic size, inorganic age                         | Cumulative H₂                   | FFBPNN      | 4-10-1        | 0.99     | [29]       |
| T°C, pH, Sₒ, (glucose)                                                         | HY                              | FFBPNN      | 3-4-1         | –        | [9]        |
| T°C, pH, Sₒ, (glucose)                                                         | SE(%)                           | FFBPNN      | 3-5-1         | 0.98, 0.99, 0.98 | [10] |
| Sₒ (molasses), inorganic %, T°C                                                | Cumulative H₂                   | FFBPNN      | 4-(6-10)-1    | 0.91     | [24]       |
| ORP, pH, dissolved CO₂                                                          | HPR                             | FFBPNN      | –             | 0.96     | [45]       |
| HRT, Sₒ, (sucrose), ORP, pH, recycle ratio, alkalinity                         | HPR                             | FFBPNN      | 12-20-1       | 0.80     | [46]       |
| OLR, ORP, pH, alkalinity                                                        | HPR                             | FFBPNN      | 4-3-1         | –        | [33]       |
| pH, Sₒ (glucose, sucrose and thin sillage), Xₒ, T °C, time                    | HPR                             | FFBPNN      | 5-6-4-1       | 0.98     | [47]       |
| OLR, pH, VSS yield                                                             | HPR                             | FFBPNN      | 3-8-4-1       | 0.85     | [48]       |
| OLR, HRT, influent alkalinity                                                   | HY, HPR, TOCeff, products conc. | FFBPNN      | –             | –        | [49]       |
| Sₒ (xylose), peptone concentration, pH                                          | HY                              | FFBPNN      | 3-8-1         | 0.99     | [50]       |
| T°C, Sₒ, (glucose), pH                                                         | HY                              | FFBPNN      | 3-6-4-2       | 0.98     | [51]       |
| Acidity, pH, Sₒ, (glucose), HRT                                                | HY                              | FFBPNN      | 4-12-4-1      | 0.99     | [52]       |
| Inoculum type, substrate type, Sₒ (glucose, sucrose, xylose), pH, T °C         | HY                              | FFBPNN      | 5-7-7-1       | 0.90, 0.46 | [53]      |

Note: ORP, oxidation-reduction potential; HPR, hydrogen production; HRT, hydraulic retention time; Sₒ, initial substrate-concentration; SE%, substrate degradation efficiency; Xₒ, initial biomass concentration; T °C, temperature; SE, substrate degradation efficiency; OLR, organic loading rate; TOCeff, effluent total organic carbons; VSS, volatile suspended solids; FFBPNN, feed forward back-propagation neural network; HY, hydrogen yield; R², coefficient of determination.

### Table 2. Summary of modelling studies using ANN for biogas production.

| Input parameters                                                                 | Output parameters               | Type of ANN | ANN structure | R² value | References |
|---------------------------------------------------------------------------------|--------------------------------|-------------|---------------|----------|------------|
| Flow rate, volumetric load, CODᵢₒ, TSSᵢₒ                                      | CODᵢₒ, TSSᵢₒ, biogas production | GRNN RBF    | –             | –        | [54]       |
| OLR, VFA, influent–effluent alkalinity, influent–effluent pH, T °C             | Biogas production              | FFBPNN      | –             | 0.93     | [55]       |
| Sludge concentrations                                                            | Methane production             | FFBPNN      | 5-7-1         | 0.99     | [56]       |
| Co-substrates concentration                                                      | Biogas production              | FFBPNN      | 5-2-1         | –        | [11]       |
| Leachate (pH, alkalinity, COD, sulphate, conductivity, chloride, waste T °C and refuse age) | Methane fraction (%) in biogas | FFBPNN      | –             | 0.96     | [57]       |
| Peak current, pre-peak slope                                                     | COD removal efficiency (%)      | FFBPNN      | 2-3-1         | –        | [58]       |
| T °C, pH, TS, TVS                                                                | Biogas yield                   | FFBPNN      | –             | 0.87     | [12]       |
| H₂S:S LR, H₂S in biogas, total sulphides, pH, OLR                               | H₂S and NH₃ in biogas          | FFBPNN      | 4-3-1         | 0.91, 0.83 | [59]      |

Note: CODᵢₒ, chemical oxygen demand (initial); TSSᵢₒ, total suspended solids (initial); CODᵢₒᵢₒ, chemical oxygen demand (final); TSSᵢₒᵢₒ, total suspended solids (final); OLR, organic loading rate; VFA, volatile fatty acids; T °C, temperature; TS, total solid; TVS, total volatile solid; H₂S:S, hydrogen sulphide-to-sulphur ratio; GRNN, generalized regression neural networks; RBF, radial basis function-based neural network; FFBPNN, feed forward back-propagation neural network; LR, loading rate; R², coefficient of determination.
Feed forward back-propagation describes the manner in which the error computed at the output side is propagated backward from the output layer, to the hidden layer and finally to the input layer. In these networks, the data are fed forward directly into the network with no feedback [34,36] and the neurons can be completely or partially interconnected. During training, the weight and biases are adjusted with the goal of fitting the predicted response closer to the experimental response [69]. BPNNs are versatile and may be employed for data modelling and process control in medicine, forensic science, biotechnology, weather forecasting, finance and investment and food science [27,70–74].

**Application of ANNs in biofuel production**

The efficiency of ANNs in bioprocess modelling has been reported in several studies [27,34,75]. More importantly, its use for modelling and optimization of biofuel production has proved valuable [4,11,24,61]. The superiority of

![Figure 2. Feed forward back-propagation training flowchart for artificial neural networks.](image-url)
ANN as a modelling tool essentially lies in its ability to represent the non-linearities in bioprocesses efficiently coupled with the capability of learning from historical data [6]. Other merits include the non-requirement of a prior specification of a suitable fitting function [27].

The development of biofuel production like many other bioprocesses requires the development of an accurate model to achieve process optimization and subsequent scale-up towards industrialization. Several studies have reported the application of ANN for modelling and optimization of the key parameters associated with microbial fermentation in biofuel production [9–11, 24, 76].

**Biohydrogen production**

The production of biohydrogen via the dark fermentation process entails the use of microorganisms under anaerobic conditions to degrade organic matter. Biohydrogen is viewed as an excellent potential replacement for conventional fossil fuels due to its high energy density (122 kJ/g) and its combustion which results in water as the only by-product. However, the commercialization of this process has been limited due to the low yields observed [6]. The use of ANNs for modelling and optimization of biohydrogen production has been largely reported. For instance, Wang and Wan [10] examined the effects of temperature, initial pH and glucose concentration on fermentative hydrogen production using a neural network model based on desirability function. The model successfully interpreted the relationship between the input parameters and their response to substrate degradation efficiency (%), hydrogen yield and the average hydrogen production rate with a coefficient of determination of 0.98, 0.99 and 0.98, respectively.

Process control and a predictive management system could contribute immensely to bioprocess development for hydrogen production. In a study by Nikhil et al. [46], ANN was successfully used to manage the operation of a pilot-scale hydrogen production system for the duration of 450 days. The input parameters included hydraulic retention time, recycle ratio, sucrose concentration and degradation, biomass concentration, pH, alkalinity, oxidation–reduction potential (ORP), acids and alcohol concentration. The ANN model was able to capture the non-linear interactions between the process parameters and the hydrogen production rate as evident from the good agreement between the predicted values and the experimental values [46]. The application of ANN as a soft sensor to predict the performance of hydrogen production system can contribute significantly to the development of an economically viable system.

Similarly, ANN models have been successfully used for real-time monitoring and prediction of biohydrogen production. For example, Rosales-Colunga et al. [45] estimated hydrogen production on inputs of ORP, dissolved CO₂ and pH during hydrogen fermentation. A coefficient of determination (R²) value of 0.95 was observed indicating that the model had good fitness [45]. The authors reported that ANN models successfully estimated the hydrogen production using only on-line parameters, suggesting that this software sensor was a low-cost efficient tool for the monitoring of biohydrogen process. Whiteman and Gueguim Kana [24] comparatively evaluated the modelling efficiency of RSM and ANN by examining the effects of molasses concentration, initial pH, temperature and inoculum concentration on the cumulative volume of hydrogen. RSM and ANN models gave R² values of 0.75 and 0.91, respectively.

Alalayah et al. [51] comparatively assessed ANN and Box–Wilson design (BWD) for biohydrogen yield prediction on the inputs of temperature, pH and glucose concentration. Findings from the above-mentioned study illustrated that the ANN model provided a higher level of prediction accuracy compared to the BWD model. This was due to ANN’s ability to overcome several limitations observed with the use of BWD [51]. In a study by Nasr et al. [47], an ANN model was developed on inputs of initial pH, initial substrate concentration and biomass concentration, temperature and time on hydrogen production using available knowledge in the public domain. Virtual experimentation was carried out using 313 data points from 26 published experiments. An R² value of 0.99 was obtained. The authors suggested that the use of existing knowledge for ANN model development on the influence of key parameters will assist in determining the optimal set points for biohydrogen production and contributes to the reduction in the process development time [47].

In our recent study, the application of ANN for virtual experimentation was assessed using published data from 64 selected studies. Two intelligent models were developed on the inputs of temperature, pH, inoculum type, substrate type and substrate concentration with the hydrogen yield as the output parameter. Hydrogen yield expressed as mole of hydrogen per mole of substrate (Mol_Model) or as cumulative volume of hydrogen per gram of substrate (Vol_Model). The results indicated that the Vol_Model (mL H₂/g substrate) was more efficient for prediction on the considered inputs with an R² value of 0.90 compared to 0.46 by the Mol_Model (mol H₂/mol substrate) [53]. The implementation of such models based on findings from several studies can significantly reduce the process development time and cost.

Other studies reported on optimization of biohydrogen production using ANN are summarized in Table 1.
Important aspects of the developed neural network models such as the type of ANN used, ANN structure and coefficient of determination ($R^2$) are presented.

**Biogas production**

The production of biogas involves the anaerobic digestion of organic materials. Biogas mainly comprises methane (55%–70%), carbon dioxide (30%–45%) and hydrogen (less than 10%) [77]. The methane upgraded from biogas may be used for heat and electricity generation or as a fuel for vehicles [78]. Optimization of this process may improve the production and application of biogas as an alternative fuel to conventional fossil fuel sources. The use of ANNs for biogas production has been widely studied. For instance, Levstek and Lakota [34] reviewed the use of ANNs for compounds prediction in biogas from anaerobic digestion. These authors summarized some of the most significant studies on the assessment and prediction of biogas constituents during biogas production using ANNs.

Also, Ozkaya et al. [57] investigated the effect of leachate, pH, alkalinity, chemical oxygen demand (COD), sulphate, conductivity, chloride, temperature (°C) and refuse age on the methane fraction (%) in biogas. The ANN model was developed to capture the effect of the inputs on methane fraction using field-scale bioreactors. These models were shown to be versatile and potentially suitable for large-scale production [78]. In another study, a multilayer BPNN with two hidden layers and sigmoid function was trained to simulate the digestion process during biogas production. The ANN model successfully captured the underlying patterns in the training data-set with input parameters of temperature, total solids, total volatile solids and pH. The performance of the ANN model demonstrated its efficiency with an $R^2$ value of 0.87 [12].

In a study by Elnekave et al. [54], three different ANNs, namely BPNN, RBF and generalized regression neural networks (GRNN), were used to model the effect of flow rate, volumetric load, initial chemical oxygen demand (COD$_m$) and initial total suspended solids (TSS$_m$) on final chemical oxygen demand (COD$_f$) and final total suspended solids (TSS$_f$) for biogas production. The results indicated that the BPNN gave the best predictions with an average deviation in the range of 6.4%–15.6% from the experimental values. The optimized model was able to achieve a relatively high COD removal efficiency (77%–79%) with simultaneous biogas production of 880–11,000 m$^3$/day.

Gueguim Kana et al. [11] developed a recipe for optimum biogas production using combined substrates of saw dust, cow dung, banana stem, rice bran and paper waste. A BPNN with a topology of (5-2-1) coupled with GA was used to generate the optimum substrate profile. The assessment of the optimal profile for biogas production led to an 8.64% increase in biogas production and significant reduction in the lag phase of three days compared with eight days in the non-optimized production system [11].

Biogas production through the MFC technology can contribute considerably to the development and the utilization of renewable energy systems. In an attempt to unravel the challenges faced in the development of this technology, Strik et al. [59] investigated the effects of different concentrations of trace compounds on biogas production during anaerobic digestion. Coefficients of determination of 0.91 and 0.83 were reported for hydrogen sulphide concentration and ammonia, respectively. Based on the prediction of the neural network model, the report indicated that the performance of the biogas production could tolerate up to 93 ppm.

Co-digestion of organic wastes can bring about improvement in the nutrient balance, the processing capacity and the overall biogas yield [79]. An insight into the co-digestion of different organic waste matter for biogas production pointed out the optimum combination ratios for the different wastes. Mahanty et al. [56] investigated the co-digestion of industrial waste from different sources, including paper, chemical, petrochemical, automobile and food, using ANN. The model was based on BPNN with a topology of (5-7-1). According to the model, chemical industrial waste had the highest significance on the specific methane yield with the least impact achieved from the automobile waste. The authors concluded that the ANN model offered a better performance with regards to prediction ability and the significance analysis compared to the regression model [56]. In another study, the ANN was used to monitor an anaerobic bioreactor treating high strength wastewater. The input parameters were peak current and pre-peak slope with COD removal efficiency (%) and methane production as the output parameters. In the above-mentioned study, the neural network model estimated accurately the COD removal efficiency and methane production [58]. Other studies on the use of ANN for optimization of biogas production are presented in Table 2. Moreover, noteworthy characteristics pertaining to the developed neural network models such as the type of ANN used, input and output parameters ANN structure and $R^2$ values obtained are presented.

**MFC technology**

MFC and MEC make up the microbial fuel technology. While MFCs generate an electric current from the
microbial decomposition of organic compounds, MECs partially reverse the process by using bacterial metabolism to generate hydrogen from organic material with an electric current \[80\]. MFC technology has been shown to be efficient for energy generation with simultaneous wastewater treatment \[81\]. Although these systems prove useful, they are still limited by the low yields and lack of information pertaining to the influence of the interactive effects of key parameters on the process output. Thus, there is a need to optimize the process parameters to enhance hydrogen and electricity production as well as to improve its efficiency for wastewater treatment.

Mathematical models have been employed in bioprocess development \[82–84\]; however, their application in MEC and MFC technologies has been scarcely reported. These models may assist in testing the hypotheses regarding the microbial community composition, microbial activity and mode of electron transfer in these systems.

Tardast et al. \[60\] considered the influence of pH, biochemical oxygen demand (BOD), COD and total suspended solids (TSS) on current generation in MFC using sugar, beer, municipal, dairy and wastewater industry as substrates. The mean square errors (MSE) for sugar, beer, municipal, dairy and paper industry wastewater were 1.54, 1.28, 0.64, 1.34 and 0.30, respectively.

In another study by the same authors, an ANN model was applied for the prediction of power density on inputs of pH, temperature and electron acceptor concentration. The ANN model had a low MSE and \(R^2\) value of 0.0023 and 0.99, respectively, suggesting high prediction accuracy. The low MSE and high \(R^2\) value showed that the ANN was able to accurately model the considered inputs with the corresponding output \[61\].

The concept of the MEC technology for hydrogen production is a relatively new research area \[80\]. Hence, the use of conventional modelling approaches for the optimization of hydrogen production in MECs has been scantily reported \[85–87\]. In our previous study, we developed a committee of ANN models with the topology (6-(6, 8, 11, 12, 14)-1) on hydrogen production using MECs with inputs of substrate type, substrate concentration, pH, temperature, applied voltage and reactor configuration \[15\]. The coefficients of determination for the five models were 0.90, 0.81, 0.85, 0.70 and 0.80, respectively. According to the sensitivity analysis results, substrate type, applied voltage, substrate concentration and pH had a high impact on the performance of the MEC system \[15\]. The use of accurate and reliable models such as ANNs will help broaden the knowledge on both MFC and MEC systems together with the improvement in the yield and wastewater treatment efficiency. As shown in Table 3, few reported studies have modelled and optimized the electricity and biohydrogen production from MFC technologies using ANN.

### Microalgae biodiesel production

Biodiesel will play a major role in providing an alternative fuel for automobiles in the near future. The use of microalgae for biodiesel production represents a renewable and sustainable energy source due to their high biomass productivity and ability to treat both air and wastewater sources \[88\]. The advantages of using microalgae as opposed to oil crops (e.g. soybeans) are not limited to the simple structures and high photosynthetic efficiency but also include the ease of cultivation with moderate requirements and capability for wastewater treatment \[89\]. Additionally, microalgae can be produced throughout the year, since the growth conditions can be controlled compared to plant sources that only grow seasonally \[90\].

Nonetheless, the commercialization of microalgae biomass for biofuel production is still facing significant difficulties. These include high production costs and low yields \[88\]. In light of these challenges, the optimization of biomass production and lipid profile during biodiesel production could play a vital role in the development of microalgae biodiesel. The utilization of ANNs for the prediction of chemical compositions of lipids for biodiesel production has been reported \[91–93\]. However, its use in microalgae biodiesel production has been scarcely reported. Mohamed et al. \[14\] comparatively examined ANN and RSM models for the determination of the effect of glucose concentration, yeast extract and sodium nitrate on the lipid productivity of Tetraselmis sp. FTC 209. The optimized parameters were reported to enhance the lipid productivity for up to 173.11 mg/L per day. Their findings also revealed that even though both ANN and RSM efficiently modelled the effects of the interactions between the input and the output parameters, the ANN model was more robust for prediction in non-linear systems \[14\].

Similarly, Wu and Shi \[65\] investigated the effect of glucose concentration on biomass concentration (Chlorella pyrenoidosa 15-2070) with the use of a hybrid ANN model and a deterministic kinetic model. The optimized biomass concentrations and maximum productivity for the hybrid ANN were 10% and 40%, respectively, higher than those predicted by the deterministic kinetic model \[65\]. Likewise, Galvão et al. \[94\] investigated the influence of pH on biomass concentration using ANN and indicated that the neural network model was able to efficiently predict the process output. The aforementioned reports and other studies on the use of ANNs for...
optimization of biomass concentration for microalgae biodiesel production are summarized in Table 4.

**Bioethanol production**

Another renewable and sustainable fuel alternative to the depleting petroleum sources is bioethanol. The production of this fuel occurs via the microbial fermentation of organic matter [64]. The most commonly used substrates for bioethanol production are corn, sugar cane and wheat [64]. However, its uncompetitiveness with fossil fuels due to high production cost has limited its implementation. The main goal of bioethanol optimization is to increase yields, while reducing costs.

As shown in Table 5, the application of ANNs for modelling and optimization of bioethanol production is still limited. Ahmadian-Moghadam et al. [4] investigated the effect of initial substrate (molasses) concentration, live yeast cells and dead yeast cells as input process parameters on bioethanol production using *Saccharomyces cerevisae*. An $R^2$ value of 0.93 was obtained, which shows that the model was suitable for recognizing patterns in the data and accurately predicted the ethanol yield [4]. In a recent study by Betiku and Taiwo [66], the effect of breadfruit hydrolysate concentration, hydraulic retention time and pH on bioethanol production was evaluated using ANN and RSM. The ANN model had an absolute average deviation between the predicted and observed value of 0.09% compared to 1.67% by RSM [66]. These results further confirm the ANN modelling accuracies compared to other techniques such as RSM. A summary of research studies on bioethanol process modelling and optimization using ANN is presented in Table 5. In this table, the ANN type and topology used as well as the obtained coefficient of determination are presented.

**GA coupled with ANN for optimization**

GA is an artificial intelligence-based stochastic non-linear optimization technique [95]. This class of algorithm was devised based on the evolutionary process of natural selection and genetics in nature [96,97]. While ANNs are typically used for modelling non-linear associations between the process input variables and the target output, GA is an optimization algorithm that determines the optimum input set points for the maximum process output [98]. GA has proved to be effective in solving various optimization problems in bioprocess development [99]. Once the ANN model is developed and validated, it is deemed as an objective function for optimization by the GA module. In its operational principle, a population potential optimal solution called chromosome is created.

These chromosomes bear the genes, which are individual parameters to be optimized and may be binary coded. Individuals within this generation (G0) are assessed for their suitability to enhance the process using an objective function. The best fitted individuals are then selected to form the parent for the next generation [24,27,100].

The selected parents are combined arbitrarily using ‘crossing over’, thereby imitating the biological phenomenon of natural selection. In order to improve this process, mutations are added and genes on specific chromosomes are arbitrarily substituted with values that occur within the search range. This creates the next generation of potential solutions. This process is repeated several times till an optimum threshold is met, therefore, generating a potential global optimal solution [24,100]. The application of ANN–GA for biofuel production has been reported [4,9,11,12,24,76,66,100,101]. Application of ANN would provide more insight into the optimum conditions required for maximum biofuel production.

Prakasham et al. [29] reported a 16% increase for the optimization of biohydrogen production using a neural network coupled with GA. The authors reported a coefficient of determination of 0.99 and a high correlation between the predicted and the experimental values. Based on their results, the authors suggested that the pH of the medium, carbon source, inoculum age and concentration all played a significant role in the metabolic activity of the hydrogen-producing bacteria and the overall hydrogen yield. A maximum hydrogen yield of 378.29 mL/g substrate was achieved with the optimum conditions of pH 5.8, glucose-to-xylose ratio of 2:3, inoculum size of 84 mg and 13 h inoculum age. The authors suggested the use of ANN–GA for bioprocess optimization [29].

**Comparative assessment of ANN and RSM for modelling and optimization of biofuel production**

Several studies have comparatively examined the use of ANN and RSM for bioprocess modelling and optimization [27,76,102] and, specifically, for biofuel production [9,14,24,50,66,67]. In a study by Wang and Wan [9], the influence of temperature, initial pH and glucose concentration on hydrogen production from mixed cultures was established using BPNN. The prediction accuracy and optimization abilities of the RSM and ANN models were compared. The results showed that the root mean square error and the prediction error for the neural network model (17.80% and 7.70%) were much lower than that of the RSM model (38.40% and 16.60%) indicating the efficiency of ANN over RSM for predicting non-linear
systems [9]. Whiteman and Gueguim Kana [24] compared the ability of RSM and ANN to model and optimize biohydrogen production. Prediction errors of 15.12% and 119.08% were obtained for ANN and RSM, respectively. The authors concluded that the neural network model was more efficient to navigate the optimization space. This result was also in accordance with Betiku and Taiwo [66]. Similarly, Mohamed et al. [14] comparatively used ANN and RSM models for modelling and optimizing biodiesel production. These authors reported that, although RSM was able to relate the considered process inputs to the output, the ANN model was more robust for predicting the non-linear systems. Many studies have reported better prediction accuracy using ANN in comparison with RSM. The lower efficiency observed with the RSM models may be attributed to the limitations of quadratic equations to represent complex non-linearities observed in biological systems [27].

In a study by Karthic et al. [50], RSM and ANN models were developed for the prediction of hydrogen yield on inputs of xylose concentration, pH and peptone concentration. An $R^2$ value and prediction error of 0.99% and 3% compared to 0.96% and 13% was obtained for ANN and RSM, respectively. Esfahanian et al. [67] reported the use of RSM and ANN to model biomass yield and bioethanol concentration on the inputs of pH, temperature and glucose concentration. Their results indicated that both model types were able to encapsulate the non-linear associations; however, ANN showed a higher level of accuracy with a prediction error of 1.90% compared to RSM (2.57%) [67]. The summary of these comparative studies is presented in Table 6. Although both ANN and RSM have been reported to be suitable in modelling and optimization of bioprocesses, ANN has proved to be more efficient for non-linear processes such as microbial fermentations.

### Challenges and future outlook

Despite the highlighted efficiency of ANN, several limitations are still needed to be addressed in order to enhance its application in future studies. For instance, ANN modelling of bioprocesses with very small data sizes may be problematic in several instances and unlikely to provide sufficient information for network training. In addition, its application for real-time monitoring and control of bioreactors used for biofuel production has been scantily reported. Other challenges include the determination of optimum factors that influence the model development phase such as, data division and pre-processing, suitability of network architecture and model validation.

The implementation of systematic approaches for model development such as data division and networking, network architecture and the development of valid models on smaller data size ($<20$) will enhance the development of bioprocesses, including biofuel production. Moreover, the mining of existing bioprocess data using artificially intelligent systems such as ANN could unravel hidden useful knowledge on these bioprocesses. The use of ANN model for real-time monitoring and control of bioreactors can also contribute immensely to the development of a viable biofuel production system.

### Conclusions

Recent bioprocess modelling and optimization studies have employed ANN as a tool. These algorithms are very powerful in modelling biofuel production due to its flexible learning algorithm, diverse network topology, fast learning algorithm and high error tolerance for non-linear processes such as those associated with microbial fermentations. As highlighted in this review, ANNs have shown a higher prediction accuracy compared to other modelling strategies such as RSM. This trend has been reported in various studies. The implementation of these models for future studies on biofuel bioprocesses will help curb costs and time during process development.

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