CI&CEQ
Chemical Industry & Chemical Engineering Quarterly

Available online at
Association of the Chemical Engineers of Serbia AChE
www.ache.org.rs/CICEQ

Chem. Ind. Chem. Eng. Q. 29 (1) 61–74 (2023) CI&CEQ

SAHRA HAMDOLLAHI
LUO JUN

School of Mechatronic Engineering and Automation, Shanghai University, Shanghai, China

A REVIEW ON MODELING OF PROTON EXCHANGE MEMBRANE FUEL CELL

Article Highlights

- Simplicity is one of the specifications of empirical/semi-empirical models
- The analytical models are helpful for one-dimensional designs with short-time computing processes
- Mechanistic models explain the basic actions of a fuel cell, like the distribution of current density
- The present study enlightens the importance of combining different modeling strategies
- Optimization algorithms like genetic algorithms are used to increase the precision of the model

Abstract

Fuel cells are electrochemical devices that convert chemical energy into electrical energy. Among various fuel cells proton exchange membrane fuel cell (PEMFC) is considered one of the most promising candidates for the next generation power sources because of its high-power densities, zero-emission, and low operation temperature. In recent years, modeling has received enormous attention and interest in understanding and studying the PEMFC phenomena. This article reviews recent progress in PEMFC modeling. Empirical/semi-empirical, analytical, and mechanistic models, zero-to-three dimensional models, and multiphase flow models, such as multiphase mixture, multi-fluid, and VOF models, are different types of PEMFC modeling approaches, respectively, in terms of parametric, dimensional and two or three-phase flow. The present study enlightens the importance of combining different modeling strategies and parameter identification in PEMFC modeling to achieve precise models to reduce the time and cost of experiments.

Keywords: proton exchange membrane fuel cell, PEMFC, modeling, fuel cell performance, empirical/semi-empirical, multiphase flow model.

REVIEW PAPER

UDC 544.6:621

The serious condition of climate change and global warming in the 21st century is mainly because of the drastically increasing amount of carbon dioxide in the earth's atmosphere. The reason for this incident is the growth in fossil fuel-based energy consumption through inefficient converters and conventional energy. Therefore, detecting a new energy converter, which is low pollution emission and high energy conversion efficiency, becomes a significant matter. Among numerous possibilities, fuel cells that convert chemical energy directly into electrical energy through electrochemical reactions without including any moving part are one of the most encouraging energy converters in the coming years [1].

Full cells have 40–50 % higher energy conversion efficiency and less noise than internal combustion engines because fuel cells do not have moving parts [2]. Proton exchange membrane fuel cells (PEMFCs), alkaline fuel cells (AFCs), direct methanol fuel cells (DMFCs), molten carbonate fuel cells (MCFCs), phosphoric acid fuel cells (PAFCs), and solid oxide fuel cells (SOFCs) are various kinds of fuel cells [3]. PEMFCs have attracted the most attention and investment among the six fuel cell types. PEMFCs, working at low temperatures (60–80 °C), are more appropriate for portable and automotive power

Correspondence: S. Hamdollahi, Building 9, No. 333, Nanchen Road, School of Mechatronic Engineering and Automation, Shanghai University, Shanghai 200444, China.
E-mail: S_hamdollahi@yahoo.com
Paper received: 26 January, 2022
Paper revised: 17 June, 2022
Paper accepted: 12 July, 2022

https://doi.org/10.2298/CICEQ220126014H

applications. PEMFCs are featured by zero emissions, low noise, easy scale-up, rapid startup, and high-energy conversion efficiencies. The schematic view of a PEMFC is shown in Figure 1.

Fundamentals of PEMFCs

A PEMFC is an appealing choice for various fuel cell types as a strong contender for an alternative clean energy generation for stationary and automotive applications. It is mainly because of PEMFC's rapid startup, low operating temperature, low pressure, high efficiency in energy conversion with zero greenhouse gas emission, and high power density [4,5]. However, for a PEMFC's wide-range commercialization, several technological obstacles must be overcome, including cell durability and degradation triggered by water and heat management problems [5,6]. Therefore, the cell performance of PEMFCs is mainly determined by numerous factors, including the manufacturing process, the mechanical design, the electrochemical reaction kinetics, the transport phenomena in the cells, and the operating conditions [7].

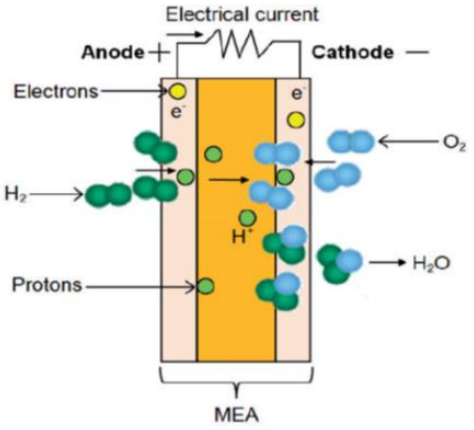

Figure 1. A schematic view of operation in PEMFC [8].

Governing equations for PEMFC modeling

The electrochemical reaction that occurs in the PEMFC [7]:

On the anode side: $2H_2 \rightarrow 4H^+ + 4e^-$

On the cathode side: $O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$

Reaction in the cell: $2H_2 + O_2 \rightarrow 2H_2O$

Mass, momentum, chemical species, ionic and electrical current, and thermal energy are the physical quantities transported in a PEMFC. For example, three-dimensional PEMFC transport equations are given as follows [8]:

Continuity equation:

$$\frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho \omega)}{\partial z} = -\frac{\partial \rho}{\partial t}$$

where velocity in the x, y, and z directions present respectively by u, v, and ω, ρ is the density of reactant gases. The continuity equation concerns membrane and electrode porosity (ε).

$$\frac{\partial(\rho\varepsilon u)}{\partial x} + \frac{\partial(\rho\varepsilon v)}{\partial y} + \frac{\partial(\rho\varepsilon \omega)}{\partial z} = S_m$$

Mass conservation:

In the gas diffusion layers and gas channels, there is not happening any reaction therefore S_m (kg m^{-3} s^{-1}) that presents mass source term is considered as zero. The next equations calculate the mass source term in the catalyst layer because there is a reaction of reactants; therefore, the mass source term is not zero. Mass source terms for hydrogen, oxygen, and the dissolved water content (λ) in the catalyst layer are:

For gas channels and GDLs: $S_m = 0$

For the anode catalyst layer: $S_{H_2} = -\frac{M_{H_2}}{2F} R_{an}$

For the cathode catalyst layer: $S_{O_2} = \frac{M_{H_2O}}{2F} R_{cat} - \frac{M_{O_2}}{4F} R_{cat}$

where M is the molecular weight (kg/mol) of the species and F is the Faraday constant.

Momentum Conservation:

$$\frac{\partial\left(\varepsilon\rho\vec{V}\right)}{\partial t} + \nabla\left(\varepsilon\rho\vec{V}\vec{V}\right) = -\varepsilon\nabla P + \varepsilon\mu\nabla^2\vec{V} + S_m$$

where μ is the dynamic viscosity, S_m is the source term of momentum conservation, and P is the pressure. For porous media, the momentum conservation equation can be written as follows:

$$S_m = -\frac{\mu}{K}\vec{V}$$

where K is the permeability.

Species conservation:

$$\frac{\partial(\varepsilon\rho\omega_k)}{\partial t} + \nabla\left(\varepsilon\rho\omega_k\vec{V}\right) = -\nabla\left[\left(D_k\nabla(\rho\omega_k)\right)\right] + S_k$$

where ρ is density, S_k is the species source term, ω_k is the species concentration, and D_k is the species diffusion coefficient.

The species source term for the liquid water is:

For gas channels and GDLs: $S_k = 0$

For the catalyst layers: $S_{H_2} = -\frac{1}{2F} R_{an}$, $S_{O_2} = -\frac{1}{4F} R_{cat}$, $S_{H_2O} = \frac{1}{2F} R_{cat}$.

Energy conservation:

$$\frac{\partial\left(\varepsilon\rho c_p T\right)}{\partial t} + \nabla\left(\varepsilon\rho c_p T\vec{V}\right) = \nabla\left(k\nabla T\right) + S_E$$

where k is the thermal conductivity, T is the temperature, c_p is the specific heat at constant pressure and S_E is the energy source term.

Electrical current:

$$-\nabla\left(\sigma_e \nabla \phi_e\right) = S_e$$

Ionic current:

$$-\nabla\left(\sigma_i \nabla \phi_i\right) = S_i$$

where S_E and S_i are respectively the electron and proton flow source term, Φ_E and Φ_i are the solid phase potential and membrane phase potential and σ_E and σ_i represent the electrical conductivity.

Butler-Volumer equation can calculate the transfer current. In the anode $S_m = R_{an}$ and $S_e = -R_{an}$; however, on the cathode side $S_m = -R_{cat}$ and $S_m = -R_{cat}$.

Current density in anode and cathode are as followings:

$$R_{an} = R_{an}^{ref}\left(\frac{c_{H_2}}{c_{H_2}^{ref}}\right)^{\gamma_{an}}\left[\exp\left(\frac{\alpha_{an,an}F\eta_{an}}{RT}\right) - \exp\left(\frac{\alpha_{cat,an}F\eta_{an}}{RT}\right)\right]$$

$$R_{cat} = R_{cat}^{ref}\left(\frac{c_{O_2}}{c_{O_2}^{ref}}\right)^{\gamma_{cat}}\left[\exp\left(-\frac{\alpha_{cat,cat}F\eta_{cat}}{RT}\right) - \exp\left(\frac{\alpha_{an,cat}F\eta_{cat}}{RT}\right)\right]$$

where, η is the local surface overpotential, γ_{an} and γ_{cat} are concentration dependence, α is the transfer coefficient and R_{an}^{ref} and R_{cat}^{ref}, respectively, are the reference current density of anode and cathode.

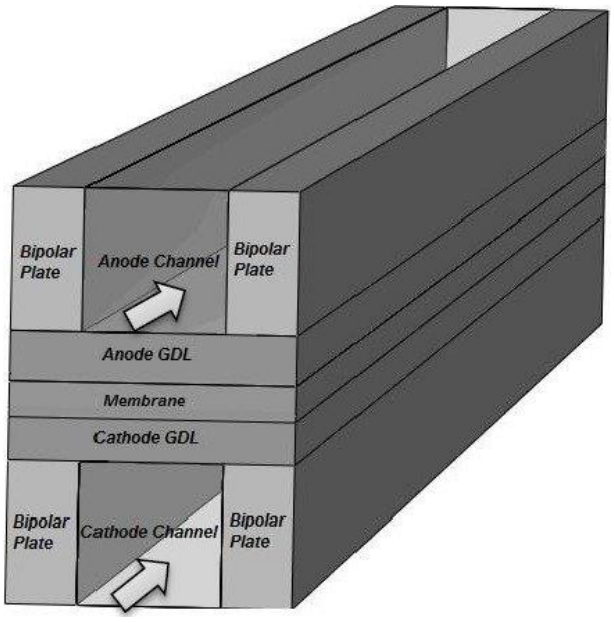

Figure 2. Schematic view of three-dimensional PEMFC model [9].

The combination of thermodynamics, fluid dynamics, and electrochemistry create a complicated system, which is PEMFC. To understand fuel cells' dynamic and static behavior, the mathematical models greatly help estimate control strategies and optimize fuel cells' design. In addition, by applying mathematical models to study fuel cells, there is a reduction in experimental tests, saving time and effort. In these models, the influence of temperature distribution, thermal stress, operating conditions, and other variables could be understood simply through the simulation.

In recent years, modeling has received colossal attention and interest in understanding and studying the fuel cell phenomena. To reduce the time and cost of experiments, fuel cell designers and engineers could get the benefits of using parametric models to predict the fuel cell performance by given operating conditions, geometries, and properties of materials. There are three types of fuel cell models in terms of parametric: empirical/semi-empirical, analytical, and mechanistic. In the following section, these models are described, and the methods that have been applied recently for their optimization are explained. The two other modeling approaches which explain the models in terms of dimensional and phase change are respectively zero to three-dimensional models and multiphase models and are described in this paper.

PEMFC models

Empirical/semi-empirical

There is enormous interest in PEMFC modeling, which saves time and effort as its simulation results will significantly agree with experimental ones [10]. Figure 2 demonstrates a three dimensional PEMFC model. Each application and operating condition has specific features based on experimental data called empirical/semi-empirical models. The details presented by these models are not more than theoretical ones; though, they have a quite favorable advantage in modeling fuel cells and other engineering fields. The empirical/semi-empirical models are designed for particular fields and should be changed for every operating condition or application. For example, the polarization curve of PEMFC, described by 0-dimensional models, are empirical and simple models [11]. Semi-empirical and 0-dimensional models are suitable for beginner researchers trying to find a model for the fuel cell. Simplicity is one of the specifications of empirical/semi-empirical models, and in some fields, these models illustrate better performance than theoretical models [12]. For example, the overpotential of output voltage significantly impacts the reduction factor of fuel cell output [13]. The computation of ohmic overpotential is simplified in empirical/semi-empirical models.The main emphasis of empirical/semi-empirical models is on the correlation between input and output. Besides, these models provide a calculation for the performance of PEMFC in a short time [14]; therefore, the empirical/semi-empirical models are more suitable for problems that focus on controlling.

Analytical models

The analytical models are useful for simple and one-dimensional designs with short-time computing processes and calculating water management and voltage losses [15]. However, the results of analytical models may not be excessively precise. The advantage of analytical models is introducing practical surveys for certain conditions, which provide information easily without requiring a numerical program to run in many cases. However, when the analytical solutions exclusively work for specific elements like catalyst layers and calculate their potential, oxygen concentration, and current density, they neglect the interactions with other parts of PEMFCs [16]. Tafel kinetics and potentials, which are close to open-circuit, are the conditions for achieving the analytical solutions. Furthermore, the analytical approach does not include membrane resistance or mass transport restrictions, which are important for PEMFC performance. By utilizing just mathematical models because of nonlinear problems, it is hard to solve the PEMFC problems, though numerical approaches can solve them. In other words, for every problem, there are computational requirements and a wide range of meshing [17].

Mechanistic models

The difficulty of modeling the PEMFC systems is because they are electrochemical, nonlinear, and multivariable systems [18]. For their explanation, it is necessary to understand internal phenomena at the molecular level of PEMFC. Therefore, the publications aim mainly at the internal phenomena of the PEMFC systems and introduce a model for describing this target. The mechanistic model focuses on thermodynamics, fluid dynamics, and electrochemistry. Being theoretical, these models apply the Stefan-Maxwell, Nernst-Planck, and Butler-Volmer equations for gas phase, species transport, and cell voltage, respectively [19]. In addition, mechanistic models explain the basic actions of a fuel cell, including flow pattern, pressure drop, distribution of current density, and voltage.

The mechanistic models are rigorous in calculations because of the fundamental and partial differential equations they need in a repetitive method to solve a problem. The complexity in mechanistic model confirmation is because it is impossible to compute the pressure, temperature, concentration of species, and other important parameters in a fuel cell with an extreme environment.

By applying electrochemical or physical equations, the operating conditions in PEMFCs occur in mechanistic models. The mechanistic models do not fit applications that aim for control; however, they are suited for optimization and design applications. Furthermore, there are no huge differences between mechanistic and empirical models [19].

Lu [20] indicated that by using both empirical and mechanistic techniques as combination models, predicting the performance of the PEMFCs becomes more effective. The reason to use a hybrid model that consists of mechanistic and empirical approaches is that the usage of both approaches has advantages in improving the model and defeats the disadvantages of each of them. For example, in a hybrid model, the parameters for operation are reduced because of the fewer input dimensions. The other advantages of the combined model over the empirical and mechanistic model are that it can easily be utilized for any operating condition and application without requiring extensive range calculation.

Optimization methods in PEMFC models

System parameters, different flow field designs, and operation conditions affecting the PEMFC's performance can be analyzed using mathematical modeling and computational tools. The complexity of mechanistic fuel cell models is why they are difficult to use in a simulation. However, the precise empirical/semi-empirical models are suitable and easy for simulation.

The results of different studies in recent years show that to examine the PEMFC performance, the effective and suitable model is parametric. Therefore, to achieve the best performance, the precise model parameter identification of PEMFCs is significant and possible by applying different algorithms [21].

The latest researchers have paid huge attention to fuel cell optimization by classifying different parameters and models, like a genetic algorithm (GA) and other evolutionary computation techniques. These techniques increase the precision of model parameter identification in the fuel cell.

Abdi *et al.* [22] presented particle swarm optimization (PSO) as a practical algorithm. The PSO, in comparison with GA, has better and more precise performance in the convergence of problems by providing global and stable optimization solutions. Furthermore, as a straightforward algorithm, the PSO is useful for successfully optimizing the extensive collection of tasks. Similarly, multidimensional elements with velocity and location can be modeled by PSO.

Different modeling techniques and strategies to study the dynamical and statistical performance of fuel cells are changed by varying the purpose of the study. Many of these modeling approaches to examine the

heat and water management, membrane, electrodes, and cathode performance are highly important to the mechanical and chemical phenomenon. By simulating and studying these modeling techniques, the most favorable operating conditions, high and developed performance, and durability of the fuel cell can be achieved. However, because of the complexity of mechanistic models, implementing these models requires quite a huge amount of parameters that indicate the technology and physics of materials engaged.

In fuel cells' procedure to express the electrochemical and physical phenomena, another model depends on empirical/semi-empirical equations. This model is more appropriate for analyzing fuel cell systems. The critical and challenging point for fuel cell application designers is identifying every parameter for each fuel cell. Empirical nature and technological nature are two types of parameters that should be identified for the fuel cell. Because of the difficulty and complexity of the parameters and identification process, some designers apply values for parameters, and the simulation results are achieved with medium quality. Recent years' promising solution is an optimization method that achieves the identifying parameters in fuel cell systems. Intending to solve real problems, modified particle swarm optimization (MPSO), as a nature-inspired algorithm, is suitable for many engineering applications [23]. The optimal result can be attained by applying MPSO and classifying different parameters for a semi-empirical PEMFC model. Furthermore, to gain the results of a simulation with high accuracy is a rigid mission for extensive operation conditions. The MPSO technique can identify and calculate the parameter's value for a PEMFC under different temperatures and normal conditions [23].

For parameter optimization of real problems, a simple and efficient technique is a Hybrid adaptive differential evolution (HADE) algorithm [21]. For identifying the PEMFC model parameters, the HADE algorithm initiates a dynamic crossover possibility and an adaptive scale factor to progress the convergence of the simulation. As a result, the performance of the HADE algorithm in space with high or low dimensions and comparison with GA, PSO, and a standard and adaptive DE algorithm is better and more reliable.

The Simulink technique, which is applied in Matlab-SIMULINK, is suitable for various operating conditions and fuel cell systems. Moreover, it is easy to apply for different applications; because this modeling is simple, and there is no need for extensive time for computation [24].

The best model for designing, developing, optimizing, and calculating the performance of fuel cells is a mathematical model. Several studies are about one or three-dimensional, non-isothermal, and non-isobaric mathematical models and identify separate parameters like liquid water transportation, thermal conduction, and gaseous diffusion. In real-time design control applications, applying these models is problematic and complex because they identify parameters for material structure. A steady model, achieved from mechanistic models and can identify the voltage-current features, is unsuitable for real-time control design. PSO algorithm [25] was developed to suit a model for real-time control design applications. LM algorithm can simply be trapped in the minimum neighborhood. The PSO algorithm is established to solve this problem. The PSO and LM algorithms can be used at the beginning of the global and local search stage. For that reason, a hybrid algorithm that consists of LM and PSO algorithms can be used for optimization. This hybrid algorithm can investigate the PEMFC model with voltage and temperature parameters. The advantage of a hybrid algorithm is that it sets aside both algorithms' disadvantages and failing points and attains the application's aim. Furthermore, the simulation of the dynamic performance of PEMFC by this hybrid algorithm has high reliability and uniformity compared with a physical model. The other advantage of this hybrid algorithm over other models is that it is not complicated and can make the model prediction happen quickly [25].

The polarization curve depicts the fuel cell voltage-current characteristics, showing the fuel cell performance. The parameters that depend on fuel cell voltage-current characteristics are power conditioning design, simulators design for fuel cell systems, operating conditions optimization, and system controller design. These show the significance of the polarization curve for the fuel cell. The physical models of fuel cells use electrochemical or empirical mechanisms. The electrical revolution model for fuel cells, uses an electrical element's circuit to depict voltage-current characteristics. Another model that utilizes mathematical strategies to obtain steady-state and high accurate voltage-current characteristics is the mathematical model. The PEMFC model with dynamic voltage-current characteristics and steady state-integrated mathematical model derives from a technique with the smallest squares by electrochemical equations where other input parameters can be computed. In addition, the modeling can be very effective in optimizing output power, power-conditioning design units, operation points, and simulation of PEMFCs [26].

As the PEMFC performance is studied in a short time, in comparison with experimental study, the

modeling of PEMFC attains much interest among the researchers. But unfortunately, a particular PEMFC has various parameters which are unidentified. This problem causes trouble in illustrating the polarization curve; it needs to identify each parameter for the PEMFC model exactly.

As mentioned before, there are not sufficient and precise statistics and rates for particular PEMFC model parameters, which makes inaccuracy in PEMFC performance in a wide range when comparing the real PEMFC with the model. Therefore, the optimization approaches have developed with parameters identification as a numerical problem to obtain the most precise PEMFC model and solve the problem. Thus, these optimization techniques have recently attained much attention and interest. However, creating a perfect and accurate multi-parameter, combined dynamic system, and complicated nonlinear PEMFC system is not a simple and unimportant task. Furthermore, the parameters of the model affect PEMFC performance, indicating the importance of accurately identifying various parameters of the PEMFC model by investigating the optimization approaches. Therefore, there is an essential need for a precise and accurate model for studying and enhancing the performance of PEMFCI.

DE (differential evolution) [27] is an optimization approach that is not too complicated to implement and has a few parameters. However, its difficulty, which is the prevention of untimely convergence, highly depends on operators and related control parameters. Nevertheless, it is a valuable technique to implement by merging it with added solutions like adaptive differential evolution. ADE adaptive differential evolution characteristics are high equilibrium between examination and discovering high potential. By setting up the control elements and various operators online, ADE becomes the development version of DE. Compared with DE and other optimization techniques, the results obtained by ADE show that it is in good agreement with the experimental model. Therefore, the ADE algorithm can be a promising strategy to create, control, optimize the PEMFC model, and improve the precision [27].

In every PEMFC system, the parameters should independently be categorized. For this explanation, the empirical equation applies. However, there is huge significance in setting up the parameters in the electrochemical module as they are adjusted in steady-state conditions and where the optimizing reliability of models is the next task after tuning the parameters.

The modules of energy balance, mass balance, and electrochemical phenomena are individual in the PEMFC system. The electrochemical model expresses the voltage-current actions of PEMFC. When voltage is lost because of numerous issues, the production of maximum voltage in PEMFC is impossible. Ohmic loss, concentration, and activation overvoltage are different losses in models. The loss terms mentioned above lead to the output voltage of the fuel cell, where the Nernst equation computes the thermodynamic potential. The genetic algorithm in the electrochemical models of PEMFC can provide accurate parameters, which leads to trustworthy outcomes [28].

Nernst equation [12]:

$$E = E^0 + \frac{RT}{2F}\ln\left(\frac{p_{H_2}p_{O_2}^{1/2}}{p_{H_2O}}\right)$$

where p is the partial pressure of H_2, O_2 and H_2O.

The PEMFCs need a precisely adjustable model to design steady-state, dynamic, and control simulations because the output voltage of PEMFCs is not regulated. The typical modeling strategy is to achieve an accurate thermal PEMFC model by considering the fuel cell's mass and momentum's conservation, thermodynamics, and physical power concepts. However, in real-time studies, because of some parameters in nature that cannot be computed in the model, these classic models are unsuitable for such applications. Therefore, to develop models to achieve high accurate performance results in comparison with real PEMFCs, it is necessary to identify the values of parameters in the models precisely.

Different meta-heuristic approaches have been investigated in recent years for identifying parameters in the PEMFC models. The dragonfly algorithm, genetic algorithm, Multi-verse optimizer, differential evolution, particle swarm optimization, and many other optimization approaches are examples of meta-heuristic methods for accurate parameter identification in PEMFCs. Although these meta-heuristic methods are more capable of enhancement, they are trendy because they produce highly accurate results in PEMFCs. The benefits of this algorithm are the closeness of the parameter values to the actual computed values and the short convergence time. Therefore, the PSO [29] is a secure, capable, precise, and valid optimization approach for PEMFC.

A predictive control system is essential for output power to achieve the best effectiveness of fuel cells by optimizing humidity, the pressure of reactants in the membrane, and temperature. The support vector regression machine (SVRM) benefits nonlinear system modeling and makes it valuable in time sequence applications. Furthermore, this optimization approach is part of statistical learning and is sustained by mathematical theory. Therefore, the control system of

PEMFC's output power can be developed by this approach.

In nonlinear population-based optimization applications, PSO is appropriate to apply. The PSO approach needs a small number of parameters, and its implementation is effortless. By modeling the control system for the output power of PEMFC on SVRM and combining it with the PSO algorithm for the optimization process, the produced PEMFC model is more accurate. The need for a short time and short memory in PSO optimization makes this approach suitable and easy to implement. Besides, the mathematical operators that apply in this method are uncomplicated. In results of the studies, which use this optimization approach, are validated, qualified, and successful. In the PEMFC optimization process, it is significant to design a control system to improve the output power by setting up the relative hydrogen humidity [30].

Nowadays, in studies to identify parameters in PEMFCs, bio-inspired optimization approaches achieve much interest and attention. One of the new methods with the features like simple implementation and few parameters is the seagull optimization algorithm (SOA) [31], which is used in nonlinear modeling problems of PEMFCs for parameter identification. Moreover, a balanced SOA (BSOA) can be used instead of the standard SOA to improve the convergence of the application. In modeling complicated nonlinear PEMFCs, this technique promises accurate and precise results [32].

Zero to three dimensional PEMFC models

In terms of dimensions, there are four models for PEMFC. The evaluation of the inner quantities of PEMFC because of its spatial dimensions is not a simple task. Computational fluid dynamics (CFD) is a suitable approach to examining every part's temperature gradients, pressure distribution, and species concentrations. The dimensions of the problem, which should be zero, one, two, or three-dimensional, depend on the number of independent spatial variables of the differential equations.

Zero dimensional models

The simplest fuel cell modeling can be achieved by neglecting the spatial alterations, taking time into account, and is called the zero-dimensional or lumped-parameter model. Based on illustrating the polarization curve of PEMFC, zero-dimensional models, which are usually empirical, are uncomplicated in discovering the different losses that occur in the system, comparing them with each other, and concluding the kinetic parameters. Therefore, zero-dimensional and semi-empirical PEMFC models are simple and helpful for examiners at the start point [11].

To explain the state of health of a PEMFC based on the degradation of the cathode catalyst layer, a zero-dimensional PEMFC model was investigated by Schneider *et al.* [32]. The developed model is suitable for PEMFC design and control because it is fast and reliable and can understand the degradation mechanisms in the cathode catalyst layer. Du *et al.* [33] investigated a method for parametrizing control-oriented zero-dimensional PEMFC. A two-step parameterization method was introduced by separating the model into two sub-models. This method reduces the solution space significantly. Furthermore, parametrizing a fuel cell model with measurement demonstrates an advantage in the sensitivity analysis.

One dimensional model

One dimensional model is the first model that researchers established to study the fuel cell. It was a complicated model with a sandwich domain in the y-direction. These models give massive details in different operating conditions for fuel cells by examining the temperatures, mass concentrations, electrical potentials, and fluxes. A one-dimensional, semi-empirical, and steady-state model of an HT-PEMFC fed with a gas mixture is developed by Nalbant *et al.* [34] to study the effects of different cell temperatures, Pt loading, phosphoric acid percentage, and different binders on the performance of the fuel cell were examined.

In the precise calculation of the PEMFC performance by Sohn *et al.* [35], a one-dimensional PEMFC model has been developed. Instead of three-dimensional with more detailed models, they preferred a macro-scale one-dimensional PEMFC model, which consists of control volumes for the cathode catalyst layer to compute the liquid water production and fuel concentration.

The characteristics and mechanisms of cold start must be understood; therefore, Jiang *et al.* [36] developed a one-dimensional PEMFC model to simulate the PEMFC cold start to improve fuel cells' startup ability and durability. Salva *et al.* [37] used a one-dimensional analytical model to simulate a PEMFC stack to validate the experimental data. Mass transfer of reactants and electrochemistry are the parameters considered in this work.

Two dimensional model

The Sandwich model in the *y-z* or *x-y* directions is a two-dimensional, upgraded version of the one-dimensional model. These two-dimensional sandwich models could examine the influence of channel geometry, bipolar plates, heat, mass transfer, and

fluxes on fuel cells. Like three-dimensional models that significantly contribute to fuel cell modeling studies with their precise and accurate results, both one and two-dimensional models can contain conservation equations by choosing boundary conditions cautiously to achieve results with a high range of exactness.

Liu *et al*. [38] developed a PEMFC with two-dimensional analytical models with the dead-end anode to study the effect of cathode parameters on PEMFC performance. Their results show the model's importance in guiding the practical work of PEMFC with a dead-end anode.

Liu *et al*. [39] examined the reactants' mass transfer, gas flow in channels, and electrochemical reactions on the electrodes by developing a two-dimensional analytical model of PEMFC. The results illustrated that the concentration of hydrogen and oxygen in the direction of flow along the channel and in the catalyst layers decreased. They presented that improving PEMFC performance could improve oxygen mass transfer from the cathode channel to the cathode catalyst layer. A two-dimensional model of a low-temperature PEMFC was used to study the effect of bipolar plate geometry on mass transport, current density, and PEMFC performance by Ionescu *et al*. [40].

Three dimensional model

The most appropriate model to analyze PEMFC in every detail, for instance, current density distribution, the influence of flow field design on fuel cell performance, or bipolar plate blockage impact, is the three-dimensional model, which is in the *x*-*y*-*z* direction.

Saco *et al*. [41] developed a three-dimensional model to examine the flow field design influence on PEMFC performance. Because of fast water removal from the gas channels, minimum pressure drop, better proton conductivity, and better hydrogen and oxygen consumption, they introduced the straight zigzag flow field with the best performance among serpentine zigzag, serpentine parallel, and straight parallel flow fields.

To study the influence of membrane geometry on PEMFC performance, a three-dimensional PEMFC model has been investigated by Jourdani *et al*. [42]. The numerical results indicated that higher current density could be obtained by a thinner membrane, hydrogen and oxygen consumption, and high water production.

Caglayan *et al*. [43] developed a three-dimensional model for a PEMFC with a 1000 °C–1800 °C range of temperature. Their result showed that because of high membrane proton conductivity and fast reaction kinetics, the increase in temperature improves the PEMFC performance. In addition, they suggested that the current density is uniform in high operating voltage.

Multiphase flow

Fluid flows, which contain two or three phases, including gas-solid flow, liquid-solid flow, gas-liquid flow, and liquid-liquid flow, are different types of two-phase flow. Three-phase flows are gas-liquid-solid flows, gas-liquid-liquid flows, gas-oil-water flows, and solid-liquid-liquid flows. The mass, momentum, and energy transfer occur in the interface that divides different phases. In the PEMFC, the liquid water production and the phase change processes develop by multiphase transport.

The gas phase consists of hydrogen, water vapor, oxygen, and nitrogen. The liquid phase is liquid water in a two-phase PEMFC model study. VOF model, multiphase mixture, multi-fluid, and some other models have been used in the multiphase flow PEMFC modeling studies.

VOF model

The interface in the gas-liquid flow, as shown in Figure 3, is detected and transported by the VOF model. This model recreates the interface profile; then, the interface transportation occurs in the velocity field. The VOF model can record the surface tension as a significant force in the micro-channel flows. The disadvantage of the VOF model is that it is only examined with a gas-liquid interface [9,44,45]. Zero and one, respectively, are the volume fraction for the gas and liquid phase in the VOF model. The continuity, mass, and momentum equations are as follows [9]:

Continuity equation:

$$\nabla \vec{U} = 0$$

Mass conservation:

$$\frac{\partial \gamma}{\partial t} + \nabla\left(\vec{U}_{\gamma}\right) + \nabla\left[\vec{U}_{r}\,\gamma\left(1-\gamma\right)\right] = 0$$

Momentum conservation:

$$\frac{\partial\left(\rho \vec{U}\right)}{\partial t} + \nabla\left(\rho \vec{U}\,\vec{U}\right) - \nabla\left(\mu \nabla \vec{U}\right) - \left(\nabla \vec{U}\right)\nabla\mu = -\nabla P_{d} - \vec{g}\,\vec{x}\,\nabla\rho + f_{s}$$

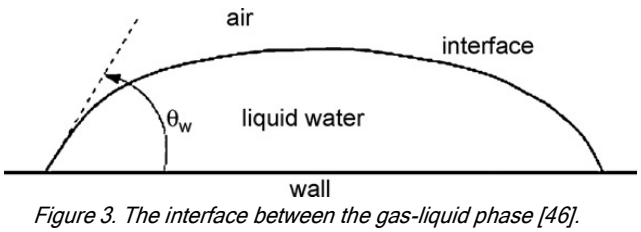

Figure 3. The interface between the gas-liquid phase [46].

Multiphase mixture model

The multiphase mixture model examines a mix of phases instead of separated phases. There is one set of conservation equations for the mixture phase. Among various phases, relative velocity, density, and other mixture quantities are estimated afterward [9].

Mass conservation:

$$\nabla\left(\rho\vec{V}\right)=0$$

Momentum conservation:

$$\vec{V}=-\frac{k}{\rho\mu}\nabla P$$

The density and velocity of the mixture are as follows:

$$\rho=s\rho_1+(1-s)\rho_g$$

$$\rho\vec{V}=\vec{V}_1\rho_1+\vec{V}_g\rho_g$$

Species conservation:

$$\nabla\left(\gamma_k\vec{Vc}_k\right)=\nabla\left(D_{kg,eff}\nabla c_{kg}\right)-\nabla\left[\left(\frac{w_{kl}}{M_k}-\frac{c_{kg}}{\rho_g}\right)\vec{J}_l\right]+S_k$$

where the convection correction factor γ is a function of the liquid saturation.

Applying the multiphase mixture model is more proficient in the pressure of the gas phase than the pressure of the liquid phase.

Multi-fluid model

The equations for mass and momentum of every phase in the multi-fluid model are solved separately. However, the two phases are coupled because of phase change and relative permeability [9].

Mass conservation:

$$\nabla\left(\varepsilon\rho_g\vec{V}_g\right)=S_{PC}$$

$$\nabla\left(\varepsilon\rho_l\vec{V}_l\right)=S_{PC}$$

Momentum conservation:

$$\vec{V}_g=-(1-s)\frac{K_g}{\mu_g}\nabla P_g$$

$$\vec{V}_l=-s\frac{K_l}{\mu_l}\nabla P_g-D(s)\nabla_s$$

In high conditions of saturation, the multi-fluid model works effectively. However, the multi-fluid model tends to be unstable because of the coupled phases and variables in high amounts.

Figure 4. Visualization of two-phase flow in PEMFC channels [47].

Two-phase flow models

Various models based on the water flow in MEA and the gas channels have been investigated to understand water transport within PEMFC [48]. A visualization of two-phase flow in PEMFC channels is illustrated in Figure 4. For example, a steady-state, non-isothermal, and single and two-phase flow PEMFC model, with various temperatures on anode and cathode and extension in cross-section ratio of channel geometry, has been investigated to improve the fuel cell performance [49]. High temperature apparently affects kinetics rise and liquid water reduction and increases PEMFC's performance. The other factors that enhance PEMFC's performance are the gas channel cross-section and the anode side's temperature.

The single and two-phase flow PEMFC model performance are close to each other at low current densities because of the consequence of low transportation of mass and slow reaction rate. High current density causes a reduction in cell voltage. It is detected that mass transport resistance enhancement makes a fast reduction of current density at low voltages. To achieve highly accurate polarization curve estimation, two-phase models are better than single-phase ones.

Zhang *et al.* [50] employed a three-dimensional mathematical model to study the influence of temperature, operating pressure, and relative humidity on PEMFC performance. Also, for processing the liquid water transport in PEMFC, the non-isothermal two-phase flow was simulated. According to the findings in their study, high operating pressure and temperature improve the PEMFC performance. Moreover, two things improve the water removal process: 1) increasing the contact angle at the interface of the GDL/channel and 2) adding the baffles in the cathode channel. Zhang *et al.* [51] presented a multiphase three-dimensional PEMFC model that includes a detailed study of two-phase flow in the PEMFC. The influence of gravity, surface tension, wall adhesion, pressure drop, and mass transport were studied in this simulation. According to their study, there is an improvement in the water removal process by adding baffles in the cathode channel and increasing the contact angle at the interface of the GDL/channel.

CFD software for fuel cell modeling

The measurement of internal quantities of

PEMFC is not a simple task because of its spatial dimensions. However, examination of pressure distribution, temperature gradients, and species concentrations in every part of PEMFC is achievable by utilizing computational fluid dynamics (CFD). Furthermore, the PEMFC performance could be predicted by implementing CFD in various operating conditions.

Fuel cell modeling combines electrochemistry and thermodynamics in porous media over transportation phenomena to the science of material [52]. Improvement of recent computers' calculation abilities and parallel computation make the CFD simulation on a large scale achievable. In fuel cell system investigation, CFD models – influential design devices – have an important role in enhancing robust, effective, powerful, and modern solver algorithms. One fuel cell modeling software with influential pre- and post-processing options is Fluent. By using different solvers, it is possible to apply single or double-precision infinite volume computations. Comsol Multiphysics (FEMLAB), another CFD software, can solve multidimensional PEMFC models by applying chemical engineering modules and using finite elements. MATLAB/Simulink is another suitable software for small-scale fuel cells and parallel computing on a multicore processor. CFD-ACE+, OpenFOAM, and STAR-CD are CFD software based on the finite volume method and suitable for multidimensional fuel cells. NADigest FDEM also provides durable solutions based on a strong error estimation method.

There are several conditions in PEMFC simulation to improve the system's performance. First, one uses different flow field designs [53–55]. Flow field design greatly affects reactants' mass transport and liquid water removal in the gas channels. Therefore, uniform mass transport and distribution of reactants in the flow channel and water transport in the gas channel improve the performance of the PEMFC. Figure 5 is demonstrated four different PEMFC flow field designs.

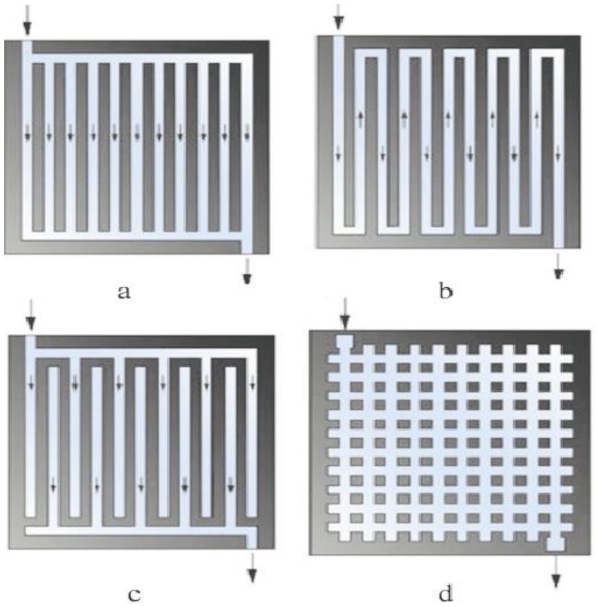

Figure 5. Various types of flow field design, a) Straight channel, b) Serpentine channel, c) Interdigitated channel, d) Pin type channel [56].

The other significant concern that influences PEMFC performance is water management. Different water formation in PEMFC flow channel is illustrated in Figure 6. The amount of water in the PEMFC is a crucial subject; excess water is the reason for flooding in the gas channel, catalyst layer, and gas diffusion layer and causes a problem in reactants transportation. While proton conductivity depends on membrane hydration, inadequate water in the membrane is the reason for membrane dehydration, resulting in a reduction in proton conductivity. There must be a balance between flooding and hydration to enhance PEMFC performance [57]. Figure 7 is shown different sites of PEMFC that are possible for flooding.

Many studies have investigated water management to improve the PEMFC performance and proposed some solutions, for instance, optimization of

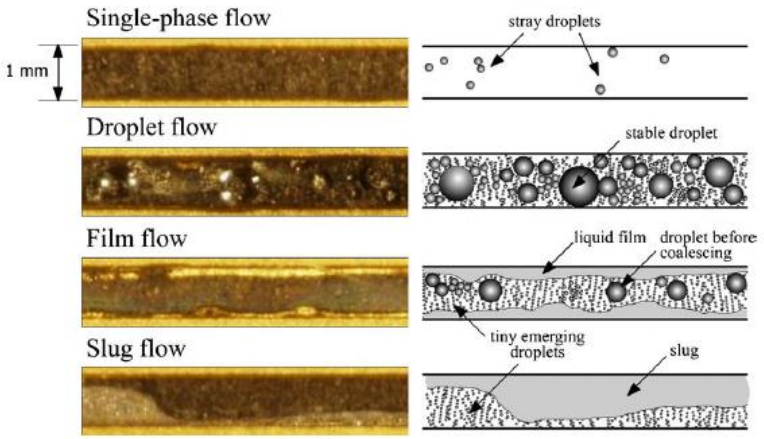

Figure 6. The various form and distributions of liquid water in the flow channel [58].

porous media of gas diffusion layer, catalyst layer, and bipolar plate. The results of the partial flooded two-dimensional PEMFC model [59] presented that one of the factors in decreasing the chance of flooding is high temperature. Partial flooding makes the distribution of current density uneven, and it has an unfavorable influence on PEMFC performance. Mammar et al. [60] investigated a fuzzy logic technique to study the membrane's hydration level.

Intending to study water flooding and how to solve this problem in PEMFC, Li *et al.* [61] have evaluated several studies in the field of water management in PEMFC. Modifying the structure and the material of membrane electrode assembly and system design and engineering are two strategies to reduce the flooding issue in PEMFC.

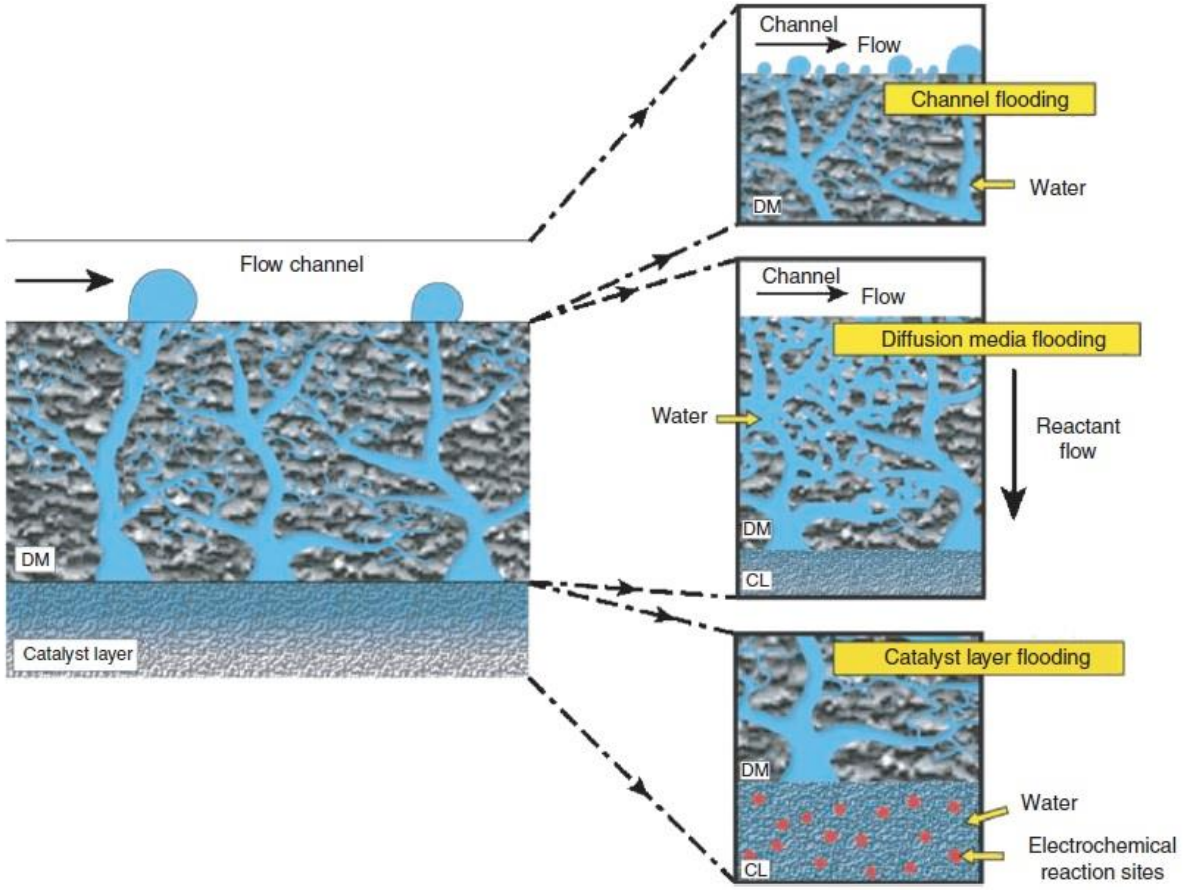

Figure 7. The possible sites of flooding in a PEMFC [62].

CONCLUSION

In recent years, modeling has attracted tremendous attention and interest in understanding PEMFC phenomena. To reduce the time and cost of experiments, fuel cell designers and engineers could get the benefits of using parametric models to predict the fuel cell performance by given operating conditions, geometries, and properties of materials. This review summarizes the different modeling methods for PEMFC and explains their characteristics.

The empirical/semi-empirical models are designed for particular fields and should be changed for every operating condition or application. These models provide a calculation for the performance of PEMFC in a short time; therefore, the empirical/semi-empirical models are more suitable for problems that focus on controlling. The analytical models are helpful for simple designs with short-time computing processes and calculating water management and voltage losses. The analytical approach does not include membrane resistance or mass transport restrictions, which are important for PEMFC performance. Mechanistic models focus on thermodynamics, fluid dynamics, and electrochemistry and explain a fuel cell's basic actions, including flow pattern, pressure drop, distribution of current density, and voltage. The mechanistic models are suited for optimization and design applications.

Hybrid models have better performance and overcome the pure models' disadvantages. The reason to use a hybrid model that consists of mechanistic and empirical approaches is that the usage of both approaches have advantages in improving the model and defeats the disadvantages of each of them, and

improves the performance of the PEMFCs. Furthermore, in a hybrid model, the parameters for operation are reduced because of the fewer input dimensions. The other advantages of the combined model over the empirical and mechanistic model are that it can be utilized for any operating condition and application and easily does not need extensive range calculation. This review illustrates optimization methods for parametric PEMFC models by applying different algorithms, like GA, PSO, etc.

The zero-dimensional model is uncomplicated in discovering the different losses that occur in the system, comparing them with each other, and concluding the kinetic parameters and general ohmic resistance from data. One dimensional model is the first model that researchers established to study the fuel cell. It was a complicated model with a sandwich domain in the y-direction. These models give massive details in different operating conditions for fuel cells by examining the temperatures, mass concentrations, electrical potentials, and fluxes. The Sandwich model in the *y-z* or *x-y* directions is a two-dimensional, upgraded version of the one-dimensional model. Two-dimensional sandwich models could examine the influence of channel geometry, bipolar plates, heat, mass transfer, and fluxes on fuel cells. A three-dimensional model in the *x-y-z* direction is the most appropriate model to analyze PEMFC in every detail, for instance, current density distribution, the influence of flow field design on fuel cell performance, or bipolar plate blockage impact. It also presents the multiphase flow; there are two and three-phase flow in the PEMFC. Some models, such as the VOF model, have used multiphase mixture and multi-fluid to examine phase change and water production in PEMFC. The interface in the gas-liquid flow can be detected and transported by the VOF model. The VOF model can record the surface tension as a significant force in the micro-channel flows. The multiphase mixture model examines a mix of phases instead of the separated phases. Applying the multiphase mixture model is more proficient in the pressure of the gas phase than the pressure of the liquid phase. The multi-fluid model works effectively in high saturation conditions, although the multi-fluid model tends to be unstable because of the coupled phases and variables.

The characterization of PEMFC simulation has an essential part. This review shows that the influence of different parameters on PEMFC performance can be identified more easily by applying CFD coding. Hence, other CFD softwares are also explained in PEMFC modeling.

Flooded models are important to examine water management in PEMFC. These models can investigate the water in the PEMFC and present solutions to improve the performance.

ACKNOWLEDGMENTS

This work is supported by the National Science Fund for Distinguished Young Scholars of China under Grant 61625304 and the National Natural Science Foundation of China under Grant 61973208.

List of Abbreviations

ADE	Adaptive Differential Evolution
AFC	Alkaline Fuel Cell
BSOA	Balanced Seagull Optimization Algorithm
CFD	Computational Fluid Dynamics
DE	Differential Evolution
DMFC	Direct Methanol Fuel Cell
GA	Genetic Algorithm
GDL	Gas Diffusion Layer
HADE	Hybrid adaptive differential evolution
LM	Levenberg-Marquardt
MCFC	Molten Carbonate Fuel Cell
MEA	Membrane Electrolyte Assembly
MPSO	Modified Particle Swarm Optimization
PAFC	Phosphoric Acid Fuel Cell
PEMFC	Proton Exchange Membrane Fuel Cell
PSO	Particle Swarm Optimization
PTFE	Poly Tetra Fluoro Ethylene
SOA	Seagull Optimization Algorithm
SOFC	Solid Oxide Fuel Cell
SVRM	Support Vector Regression Machine
VOF	Volume of Fluid

Greek Letters

γ	Convection correction
σ	Conductivity (S m^{-1})
ρ	Density (kg m^3)
μ	Dynamic viscosity (Pa s)
Φ	Electric potential (V)
α_m	Mass accommodation coefficient
ε	Porosity

List of symbols

c_P	Specific heat capacity (J g^{-1} K^{-1})
D	Diffusivity (m^2 s^{-1})
D	Diameter (m)
E	Cell potential (V)

F	Faraday's constant (96485 C mol^{-1} e^{-1})
K	Permeability
R	Universal gas constant (8.314 J mol^{-1} K^{-1})
P	Pressure (Pa)
p	Partial pressure (Pa)
$\vec{U}$	Velocity (m s^{-1})
S_m	Mass conservation
S_M	Momentum conservation
S_k	Species conservation
S_E	Energy conversion
S_e	Electrical charges
S_i	Ionic charges
T	Temperature (K)
t	Time (s)
$\vec{V}$	Velocity (m s^{-1})
w	Mass fraction

REFERENCES

[1] U. Lucia, Renewable Sustainable Energy Rev. 30 (2014) 164–169. https://doi.org/10.1016/j.rser.2013.09.025

[2] J. Macedo-Valencia, J.M. Sierra, S.J. Figueroa-Ramírez, S.E. Díaz, M. Meza, Int. J. Hydrogen Energy 41 (2016) 23425–23433. https://doi.org/10.1016/j.ijhydene.2016.10.065

[3] T. Elmer, M. Worall, S. Wu, S.B. Riffat, Renewable Sustainable Energy Rev. 42 (2015) 913–931. https://doi.org/10.1016/j.rser.2014.10.080

[4] Y. Chang, Y. Qin, Y. Yin, J. Zhang, X. Li, Appl. Energy 230 (2018) 643–662. https://doi.org/10.1016/j.apenergy.2018.08.125

[5] N. Limjeerajarus, P. Charoen-amornkitt, Int. J. Hydrogen Energy 40 (2015) 7144–7158. https://doi.org/10.1016/j.ijhydene.2015.04.007

[6] P. Pei, H. Chen, Appl. Energy 125 (2014) 60–75. https://doi.org/10.1016/j.apenergy.2014.03.048

[7] S.A. Atyabi, E. Afshari, J. Therm. Anal. Calorim. 135 (2019) 1823–1833. https://doi.org/10.1007/s10973-018-7270-3

[8] J.P. Kone, X. Zhang, Y. Yan, G. Hu, G. Ahmadi, J. Comput. Multiphase Flows 9 (2017) 3–25. https://doi.org/10.1177/1757482X176923

[9] N. Ahmadi, S. Rezazadeh, A. Dadvand, I. Mirzaee. J. Renewable Energy Environment 2 (2015) 36-46. https://doi.org/10.30501/jree.2015.70069

[10] A.A. El-Ferganya, H.M. Hasanien, A.M. Agwa, Energy Convers. Manage. 201 (2019) 112197. https://doi.org/10.1016/j.enconman.2019.112197

[11] D. Hao, J. Shen, Y. Hou, Y. Zhou, H. Wang, Int. J. Chem. Eng. 2016 (2016) 4109204. https://doi.org/10.1155/2016/4109204

[12] Y. Akimoto, K. Okajima, J. Energy Technol. Policy 1 (2014) 91–96. https://doi.org/10.1080/23317000.2014.972480

[13] M. Pan, C. Li, J. Liao, H. Lei, C. Pan, X. Meng, H. Huang, Energy 207 (2020) 1–13. https://doi.org/10.1016/j.energy.2020.118331

[14] M. Ohenoja, A. Sorsa, K. Leiviskä, Computers 7 (2018) 60–72. https://doi.org/10.3390/computers7040060

[15] A.U. Thosar, H. Agarwal, S. Govarthan, A.K. Lele, Chem. Eng. Sci. 206 (2019) 96–117. https://doi.org/10.1016/j.ces.2019.05.022

[16] J.X. Liu, H. Guo, F. Ye, C.F. Ma, Energy 119 (2017) 299–308. https://doi.org/10.1016/j.energy.2016.12.075

[17] R.K.A. Rasheed, Q. Liao, Z. Caizhi, S.H. Chan, Int. J. Hydrogen Energy 42 (2017) 3142–3165. https://doi.org/10.1016/j.ijhydene.2016.10.078

[18] B. Grondin-Perez, S. Roche, C. Lebreton, M. Benne, C. Damour, J.A. Kadjo, Engineering 6 (2014) 418–426. https://doi.org/10.4236/eng.2014.68044

[19] E.J.F. Dickinson, G. Hinds, J. Electrochem. Soc. 166 (2019) 221–231. https://doi.org/10.1149/2.0361904jes

[20] J. Lu, Ph.D. Thesis, James Cook University, North Queensland, Australia, (2013). https://researchonline.jcu.edu.au/40440/

[21] Z. Sun, N. Wang, Y. Bi, D. Srinivasan, Energy 90 (2015) 1334–1341. https://doi.org/10.1016/j.energy.2015.06.081

[22] H. Abdi, N.A. Messaoudene, L. Kolsi, M.W. Naceur, J. Therm. Anal. Calorim. 144 (2021) 1749–1759. https://doi.org/10.1007/s10973-020-10370-1

[23] M. Sarvi, I. Soltani, Int. J. Comput. Sci. Eng. Technol. 3 (2012) 285–378. https://ijcset.com/docs/IJCSET12-03-08-036.pdf

[24] S.Z. Chen, Z.G. Bao, Y.C. Wang, Appl. Mech. Mater. 740 (2015) 474–478. https://doi.org/10.4028/www.scientific.net/AMM.740.474

[25] P. Hu, G. Cao, X. Zhu, J. Li, Simulation Model. Pract. Theory 18 (2010) 574–588. https://doi.org/10.1016/j.simpat.2010.01.001

[26] A. Omran, A. Lucchesi, D. Smith, A. Alaswad, A. Amiri, T. Wilberforce, J.R. Sodr´, A.G. Olabi, Int. J. Thermofluids 11 (2021) 100–110. https://doi.org/10.1016/j.ijft.2021.100110

[27] J. Cheng, G. Zhang, Int. J. Electr. Power Energy Syst. 62 (2014) 189–198. https://doi.org/10.1016/j.ijepes.2014.04.043

[28] K. Priya, T.S. Babu, K. Balasubramanian, K.S. Kumar, N. Rajasekar, Sustain. Energy Technol. Assess. 12 (2015) 46–52. https://doi.org/10.1016/j.seta.2015.09.001

[29] Y. Cao, X. Kou, Y. Wu, K. Jermsittiparsert, A. Yildizbasi, Energy Rep. 6 (2020) 813–823. https://doi.org/10.1016/j.egyr.2020.04.013

[30] Y. Li, Z. Ma, M. Zheng, D. Li, Z. Lu, B. Xu, Membranes 11 (2021) 1–16. https://doi.org/10.3390/membranes11090691

[31] Y. Cao, Y. Li, G. Zhang, K. Jermsittiparsert, N. Razmjooy, Energy Rep. 5 (2019) 1616–1625. https://doi.org/10.1016/j.egyr.2019.11.013

[32] P. Schneider, C. Sadeler, A. C. Scherzer, N. Zamel, D. Gerteisen, J. Electrochem. Soc. 166 (2019) F322. https://doi.org/10.1016/j.egyr.2019.11.01310.1149/2.0881904jes

[33] Z.P. Du, C. Steindl, S. Jakubek, Processes 9 (2021) 713. https://doi.org/10.3390/pr9040713

[34] Y. Nalbant, C.O. Colpan, Y. Devrim, Int. J. Hydrogen Energy 43 (2018) 5939–5950. https://doi.org/10.1016/j.ijhydene.2017.10.148

[35] Y. Sohn, S. Yim, G. Park, M. Kim, S. Cha, K. Kim, Int. J. Hydrogen Energy 42 (2017) 13226–13233. https://doi.org/10.1016/j.ijhydene.2017.04.036

[36] H. Jiang, L. Xu, H. Struchtrup, J. Li, Q. Gan, X. Xu, Z. Hu, M. Ouyang , J. Electrochem. Soc. 167 (2020) 1–18. https://doi.org/10.1149/1945-7111/ab6ee7

[37] J.A. Salva, A. Iranzo, F. Rosa, E. Tapia, Int. J. Hydrogen Energy 41 (2016) 20615–20632. https://doi.org/10.1016/j.ijhydene.2016.09.152

[38] S. Liu, T. Chen, Y. Xie, Int. J. Green Energy 17 (2020) 255–273. https://doi.org/10.1080/15435075.2020.1722133

[39] J.X. Liu, H. Guo, F. Ye, C.F. Ma, Energy 119 (2017) 299–

308. https://doi.org/10.1016/j.energy.2016.12.075
[40] V. Ionescu, N. Buzbuchi, Energy Procedia 112 (2017) 390–397. https://doi.org/10.1016/j.egypro.2017.03.1085
[41] S.A. Saco, R.T.K. Raj, P. Karthikeyan, Energy 113 (2016) 558–573. https://doi.org/10.1016/j.energy.2016.07.079
[42] M. Jourdani, H. Mounir, A. Marjani, Int. J. Multiphys. 11 (2017) 427–442. https://doi.org/10.21152/1750-9548.11.4.427
[43] D.G. Caglayan, B. Sezgin, Y. Devrim, I. Eroglu, Int. J. Hydrogen Energy 41 (2016) 10060–10066. https://doi.org/10.1016/j.ijhydene.2016.03.049
[44] A. d'Adamo, M. Haslinger, G. Corda, J. Höflinger, S. Fontanesi, T. Lauer, Processes 9 (2021) 688. https://doi.org/10.3390/pr9040688
[45] Z. Niu, J. Wu, Z. Bao, Y. Wang, Y. Yin, K. Jiao, Int. J. Heat Mass Transfer 139 (2019) 58–68. https://doi.org/10.1016/j.ijheatmasstransfer.2019.05.008
[46] A. Di. Le, B. Zhou. J. Power Sources 182 (2008) 197–222. https://doi.org/10.1016/j.jpowsour.2008.03.047
[47] A. Di. Le, B. Zhou. J. Power Sources 182 (2008) 197–222. https://doi.org/10.1016/j.jpowsour.2008.01.047
[48] N.S.M. Hassan, W.R.W. Daud, K. Sopian, J. Sahari, J. Power Sources 193 (2009) 249–257. https://doi.org/10.1016/j.jpowsour.2009.01.066
[49] L. Xing, X. Liu, T. Alaje, R. Kumar, M. Mamlouk, K. Scott, Energy 73 (2014) 618–634. https://doi.org/10.1016/j.energy.2014.06.065
[50] Z. Zhang, W. Liu, Y. Wang, Int. J. Hydrogen Energy 44 (2019) 379–388. https://doi.org/10.1016/j.ijhydene.2018.05.149
[51] G. Zhang, L. Fan, J. Sun, K. Jiao, Int. J. Heat Mass Transfer 115 (2017) 714–724. https://doi.org/10.1016/j.ijheatmasstransfer.2017.07.102
[52] C. Siegel, Energy 33 (2008) 1331–1352. https://doi.org/10.1016/j.energy.2008.04.015
[53] J. Shen, Z. Tu, S. H. Chan. Appl. Therm. Engineering 149 (2019) 1408–1418. https://doi.org/10.1016/j.applthermaleng.2018.12.138
[54] Y. Shen, B. Zhao, T. H. Kwan, Q. Yao. Energy Convers. Manage. 213 (2020) 112840–112855. https://doi.org/10.1016/j.enconman.2020.112840
[55] J. Shen, Z. Tu, S. H. Chan. Appl. Therm. Engineering 164 (2020) 114464–114473. https://doi.org/10.1016/j.applthermaleng.2019.114464
[56] M. Sauermoser, N. Kizilova, B. G. Pollet, S. Kjelstrup. Frontiers in Energy Research 8 (2020). https://doi.org/10.3389/fenrg.2020.00013
[57] Z. Liu, Z. Mao, C. Wang. J. Power Sources 158 (2006) 1229–1239.https://doi.org/10.1016/j.jpowsour.2005.10.060
[58] I. S. Hussaini, C. Y. Wang. J. Power Sources 187 (2009) 444–451. https://doi.org/10.1016/j.jpowsour.2008.11.030
[59] J. Shen, L. Xu, H. Chang, Z. Tu, S. H. Chan. Energy Convers. Manage. 207 (2020) 112537–112545. https://doi.org/10.1016/j.enconman.2020.112537
[60] K. Mammar, F. Saadaoui, S. Laribi. Renewable Energy Focus 30 (2019) 123–130. https://doi.org/10.1016/j.ref.2019.06.001
[61] H. Li, Y. Tang, Z. Wang, Z. Shi, S. Wu, D. Song, J. Zhang, K. Fatih, J. Zhang, H. Wang, Z. Liu, R. Abouatallah, A. Mazza. J. Power Sources 178 (2008) 103–117. https://doi.org/10.1016/j.jpowsour.2007.12.068
[62] E.C. Kumbur, M.M. Mench, in Encyclopedia of Electrochemical Power Sources, J. Garche Ed., Elsevier B.V., (2009), p. 828-847. ISBN 978-0-444-52745-5.

SAHRA HAMDOLLAHI
LUO JUN

School of Mechatronic Engineering and Automation, Shanghai University, Shanghai, China

PREGLEDNI RAD

MODELOVANJA VODONIČNE GORIVNE ĆELIJE: PREGLDENI RAD

Gorivne ćelije su elektrohemijski uređaji koji pretvaraju hemijsku u električnu energiju. Među njima, vodonična gorivna ćelija se smatra jednim od najperspektivnijih kandidata za izvore energije sledeće generacije zbog svoje velike gustine snage, nulte emisije i niske radne temperature. Poslednjih godina modelovanje je dobilo ogromnu pažnju i interesovanje za razumevanje i proučavanje fenomena vodoničnih gorivnih ćelija. Ovaj pregledni rad prikazuje nedavni napredak u modelovanju vodoničnih gorivnih ćelija. Empirijski, polu-empirijski, analitički i mehanistički modeli, nulto do trodimenzionalni modeli i modeli višefaznog toka, kao što su višefazne smeše, multifluidni i VOF modeli, su različite vrste pristupa modelovanju vodoničnih gorivnih ćelija u smislu parametarskog, dimenzionalnog i dvo- ili trofaznog protoka. On osvetljava važnost kombinovanja različitih strategija modelovanja i identifikacije parametara u modelima vodoničnih gorivnih ćelija, kako bi se postigli precizni modeli koji smanjuju vreme i troškove eksperimenata.

Ključne reči: vodonična gorivna ćelija, modelovanje, performanse gorivne ćelije, empirijski/polu-empirijski model, model višefaznog toka.