Analysis of electrical and thermal models and modeling techniques for polymer electrolyte membrane fuel cells

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A B S T R A C T

Polymeric Electrolyte Membrane Fuel Cell (PEMFC) modeling considering thermal and electrical behavior in a coupled manner is a key aspect when evaluating new designs, materials, physical phenomena or control strategies. Depending on the behavior to be emulated, it is important to choose the modeling technique that best suits the needs required. In this sense, this paper describes the most commonly used PEMFC modeling techniques in the context of analytical-mechanistic approach, semi-empirical approach based on theoretical formulation and empirical correlations, as well as empirical approach based on experimentation with a real system. In addition, an in-depth analysis of PEMFC models at the cell and stack level that emulate the thermal and electrical behavior of these systems in a coupled manner is carried out. A chronological classification of the most relevant models has been made based on the modeling technique used, purpose of the model, state and dimension of the model, and the real system, other developed models or experimental results that have been used to validate the proposed new model. Additionally, guidelines to improve the energy efficiency of PEMFC systems through the development of new models are given.

Key words

Polymer Electrolyte Membrane Fuel Cell (PEMFC), Modeling techniques, Electrical and thermal behavior, Model Development, Review.

1. Introduction

In the current literature, the feasibility of PEMFC (Proton Exchange Membrane Fuel Cell) systems to be used in the field of stationary cogeneration, automotive applications and portable generation has been shown [1], [2], [3]. However, there is still room for improvement in the development of new membranes, catalysts, bipolar plates, collectors, etc., as well as in the management of these systems to be optimally integrated and to increase their energy efficiency and reduce the costs of the system in which they are integrated.

On the one hand, to verify the effectiveness of new materials and designs for the elements that form a PEM type cell, it is necessary to develop models that reproduce with high accuracy the behavior of the desired objective (improvement of mass transport, activation losses, ohmic losses, concentration losses, heat transfer, membrane humidification, etc.) when operating with the new design or material. On the other hand, to optimally operate a PEMFC, it is essential to develop accurate models according to the optimization or operation strategy that will be implemented. In this sense, the modeling of PEMFC systems that

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exactly emulate its operation is a key aspect when studying operation strategies, its integration with other systems or the evaluation of control algorithms aimed at maximizing the energy efficiency of the system. To do this, the model must be able to predict accurately the efficiency of the system based on the energy production of the PEMFC. Besides, the choice of the appropriate modeling technique is a fundamental aspect when modeling a PEM cell or a complete stack. In this sense, to verify the effectiveness of new components, materials or phenomena, it usually involves the use of more complex models that require a higher computational cost. However, if the purpose of the model is to evaluate control strategies at system level or to analyze the behavior of the PEMFC when it operates simultaneously with other generation or storage technologies, the modeling technique will be completely different, so that the user can abstract from the processes that are not related to the variables that take part in the process to be controlled or analyzed.

At present, there are a large number of models that reproduce with sufficient precision the electrical behavior of PEMFC systems in dynamic regime, as well as in steady state [4]-[5]. On the other hand, there is also a wide variety of models that allow studying the thermal behavior of PEMFC systems [6]-[7]. However, since the electrochemical and thermodynamic reactions that occur in a PEMFC are strongly coupled, to emulate the global behavior of a PEMFC, the model necessarily has to contemplate both aspects in a coupled manner. In this context, there are several research works that present non-isothermal models, which integrate the electrical and thermal behavior together and which can be taken as a reference so that the scientific community could improve what has been done so far in terms of evaluating new designs, materials or control strategies.

Taking into account all mentioned above, section 3 of this paper describes the modeling techniques used to develop PEMFC models. Next, section 4 describes the current literature of the PEMFC models that consider coupled electrical and thermal behavior, which are classified in chronological order considering the modeling technique used, the purpose of the model, and the real system or published data used for its validation or comparison, among others. Additionally, section 5 describes the opportunities for improving the energy efficiency of PEMFC systems by developing new models aimed at developing new optimization strategies.

Prior to the description of the models mentioned above, the following section 2 introduces general aspects of PEMFC modeling necessary to facilitate the understanding of the descriptions made in the following sections.

2. General aspects of modelling PEMFC systems

Regarding the modeling of PEMFC systems, there are many characteristics that allow differentiating some models from others. In general, models of PEMFC systems can be classified according to the formulation used (semi-empirical, empirical or analytical-mechanistic), size of the model (zero, one, two or three dimensions), state of the model (stationary, transient) or the limit of the model (cell, complete stack, etc.), among other characteristics. Table 1 shows the general modeling characteristics of PEMFC systems.

Table 1. General modeling characteristics of PEMFC systems

Key aspects	*Options / Characteristics*
Approach	Systemic approach (semi-empirical, empirical) or analytical-mechanistic approach (macroscopic / microscopic)
State	Stationary; dynamic (transient); real time
Limit	A component of a cell; a complete cell; stack; stack including auxiliary systems; Integrated PEMFC.
Computational domain	Single domain; multidomain
Spatial dimensions	Zero (0D); one (1D); two (2D); three (3D). It is also possible to combine the above.
Purpose	Thermal analysis, efficiency analysis, structural analysis, parametric studies, element design (gas and cooling channels, GDL, catalyst, collectors), etc. Integration in control systems, integration in cogeneration and trigeneration systems, hybridization with other technologies, etc.
Complexity	Effects of temperature, two-phase flow, porosity modeling, CO kinetics and poisoning, catalyst degradation, contact resistances, gravitational effects, etc.

In the following subsections, the general aspects shown in Table 1 are introduced in order to facilitate the understanding of the description of the models that can be found in the current literature.

2.1. Approach of the model

Depending on the requirements and the expected functionality, a systemic model (semi-empirical or empirical) or an analytical-mechanistic model can be used.

Models based on an analytical-mechanistic approach are usually very accurate and provide minute details of the operation of the fuel cell at the microscopic or macroscopic level [8]. Its formulation is based on a series of elementary electrochemical and thermodynamic relationships that describe the processes that occur within a PEM (Proton Exchange Membrane) fuel cell. This type of formulation, commonly, addresses three main processes: the electrochemical reactions in the catalytic layers, the migration of protons in the polymeric membrane and the transport of heat and mass in all regions of the cell. The complexity of these models depends on the desired purpose and are generally very difficult to implement due to the highly non-linear nature that describes the behavior of a PEMFC. In this sense, in most cases, due to the highly complex equations on which they are based and the high computational cost required to solve them, these models are not very suitable for use in real-time control systems. Consequently, in most cases they are used as support for the design of components.

Models based on a systemic approach focus on the general behavior of the fuel cell, without going into detail in the processes that occur at the atomic level. Depending on whether part or all of the formulation that describes the behavior of the model is based on empirical relationships, a distinction is made between semi-empirical or empirical models, respectively. This type of formulation is widely used when there are parameters that are not known a priori, such as the diffusivity or conductivity of the membrane, which are described by semi-empirical expressions. The empirical formulation covers a very extensive field, since it allows to identify the behavior of the system through a great variety of identification techniques, such as spectroscopy, voltammetry, interruption of the current, test and error methods, as well as implementation methods, such as the electrical circuits or the black-boxes [4], [9]. These types of models are more suitable for use in operation, control or optimization strategies.

2.2. State of the model

The state of a model differs between steady state and dynamic (transient) state. In the steady state it is assumed that the variables do not change with time, that is, the volumetric flows, entropies, enthalpies, etc., are not a function of time. Commonly, these types of models are used to characterize the polarization curve of a fuel cell, including losses in the activation, ohmic and concentration region. They are also used to study in detail the behavior of the different parts of a PEM cell, such as the GDL (Gas Diffusion Layer), the CL (Catalyst Layer) or the membrane under different operating conditions.

Transient state models include derivatives as a function of time to characterize the behavior of the system dynamically. Generally, time constants are used to characterize the electrochemical behavior of the double layer, the global transfer of heat and mass and the dehydration of the membrane, which usually vary several orders of magnitude [10], [11]. Normally, these types of models are used to analyze the behavior of the system in the event of changes in operating conditions.

2.3. Limit of the model

Depending on the application, the model can be a component of a PEM cell (GDL, CL, membrane, etc.), a complete cell including the MEA (Membrane Electrode Assembly), a stack composed of several cells, or a stack including the auxiliary systems (cooling circuit, coolant pump, air compressor, etc.).

In general, the models developed using an analytical-mechanistic approach focus on components or on a single cell, since simulating a complete stack would require a very high computational cost. On the contrary, models developed with a systemic approach are more suitable for modeling complete stacks.

2.4. Computational domain

A PEMFC model can be based on a single domain or on multiple domains (multi-domain). When a single domain is used, only the source terms (oxygen and hydrogen flow, pressures, velocities and inlet temperatures, etc.) or sink (current density generated, cell voltage, etc.) vary according to the position inside the cell (without internal boundary conditions). In this sense, all the

equations are written in the form of a generic convection-diffusion equation, and all the terms that do not conform to that format are coupled with the source or sink term [12].

Multidomain models use different modeling equations in each domain (GDL, CL, membrane, etc.) and require careful management with border boundary conditions, initial and internal (for example, continuity) and external (pressure, temperature, etc.).

2.5. Spatial dimension

A model of a cell or a stack can be zero (0D), one (1D), two (2D) and three (3D) dimensions. In this sense, a zero-dimensional model is one in which it is assumed that all the magnitudes (temperature, flows, pressures, etc.) are homogeneous in space, considering only the average values of the inputs and outputs of the system. 1D models contemplate variations of physical magnitudes in only one direction, for example, the variation of the temperature through the GDL, the CL and membrane. Following the same line, 2D and 3D models, contemplate variations of magnitudes in a surface and space, respectively.

In the early stages of fuel cell modeling, researchers used 1D models, with varying degrees of complexity, in cross direction assuming the cell arranged as a "sandwich". With this type of models, flows, concentrations, temperatures and electric potentials were analyzed to determine the limit conditions of the cells. These types of models provide enormous information, especially when modeling CLs.

2D models are presented as an improvement of1D models. In this sense, they offer a more realistic view of certain phenomena since spatial variations are considered. These models are usually implemented with the cell in a sandwich arrangement in the x-y direction or in a domain along the channel (design known as along-the-channel) in the y-z direction. The sandwich models are mainly used for flow analysis, heat and mass transfer and concentrations that include the effects of bipolar plate and gas channels. The models with domains along the channel are used, mainly, to analyze the concentrations of the reactants along the gas channels. 1D and 2D models can include the same conservation equations as the 3D models, so they provide a lot of information with sufficient accuracy if the boundary conditions and initial conditions are carefully selected.

3D models (x-y-z directions) are the most appropriate when it is required to study the general behavior of a PEMFC. In practice, it can be interpreted that a 3D model is obtained from the combination of 2D domains, which allows studying the blocking effect of bipolar plates, the detailed distribution of current density, temperature or efficiency of a field flow design.

As an example, Figure 1 shows a schematic illustration of the different dimensions that are contemplated when modeling a PEM cell, based on the selected coordinate axes (1D, direction y; 2D, direction x-y and y-z; 3D, direction x-y-z).

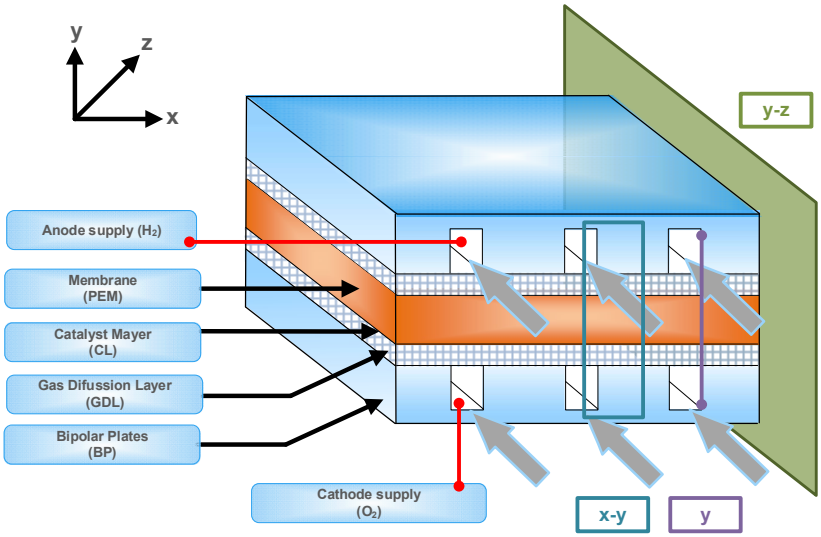

Fig. 1. Schematic illustration of the different dimensions that are contemplated when modeling a PEM cell.

In addition to the mentioned dimensions, it is also possible to combine the previous ones (1 + 1, 2 + 1, 2 + 1/2) when a higher dimension model is coupled with a lower dimension model or when one of the magnitudes of the model is calculated in a different dimension from the global dimension of the model.

2.6. Purpose of the model

The type of modeling chosen is related to the purpose that will be given to the resulting model. In general, 1D designs are used to analyze the limitation of mass and load transport, while 2D or more dimensions are used for thermal analysis, flow analysis, structural analysis, etc. In addition, if the model is oriented to the design of elements (gas and cooling channels, GDL, catalyst, collectors, etc.), the model is implemented with an analytical-mechanistic approach.

When the purpose of the model is to be used to implement a control or optimization strategy, be integrated into a cogeneration system or hybridized with other technologies, zero-dimensional models developed with a systemic approach are usually used (semi-empirical or empirical), although it is also possible to use more complex models depending on the level of details desired. However, for cases in which real-time computation is required, the models are limited to semi-empirical or empirical models of 0D, since the resolution of analytical models of more dimensions supposes a lot of computational time and its implementation would not be viable. for that type of applications [13]. In this context, in [14], to emulate the thermal behavior of a 600 W PEMFC, starting from a 3D computational model, a technique that has allowed converting the 3D model into a 0D model to be implemented in a real time control system has been developed. The fact of developing the 3D model and then converting it to a 0D model provides the combined advantage of both models. In this sense, the 3D model provides high accuracy in the prediction of the temperature profiles of the stack and the refrigeration circuit, and a high speed in computation is obtained by subsequently reducing it to a 0D model.

2.7. Complexity of the model

Thanks to the current computational capacity, simulations with PEMFC models are becoming more complex and demanding and include a high level of detail. In this sense, depending on the level of detail required, computational models can contemplate the effects of temperature, efficiency, two-phase flows, porous media, kinetics and carbon monoxide (CO) poisoning, catalyst degradation, contact resistances, gravitational effects, etc. However, depending on the operating conditions or the desired purpose, a series of assumptions and simplifications are usually established that minimize the complexity of the model [15].

3. PEMFC modeling techniques

One way to classify modeling techniques is based on the method by which a model is implemented. The most complex models that incorporate more details are the models based on the technique of analytical-mechanistic formulation. The models obtained through this technique, also called white-box models, are formulated by means of very complex equations that describe the physic-chemical phenomena that intervene in the functioning of the PEMFC.

When the purpose of a model is to be used in a control strategy or to be integrated with other systems, simplified models can be considered, so that they emulate only the necessary variables that allow their control or integration. These simplified models, commonly known as gray-box models, are developed based on analytical formulation complemented by a prior knowledge of the system (experimental data), so that some very complex mathematical equations are replaced by empirical equations or mapping tables.

Finally, there is another modeling technique in which the relationships between the inputs and outputs of the system are not based on equations or physical laws, but are deduced only through physical experimentation with the real system or throughout experimental databases. Models developed using purely empirical techniques can be classified into two groups: electric models or models based on artificial intelligence. The latter are known by the name of black box models. Fig. 2 shows an outline of the alternatives of modeling approaches, implementation methods, as well as resolution strategies typically used.

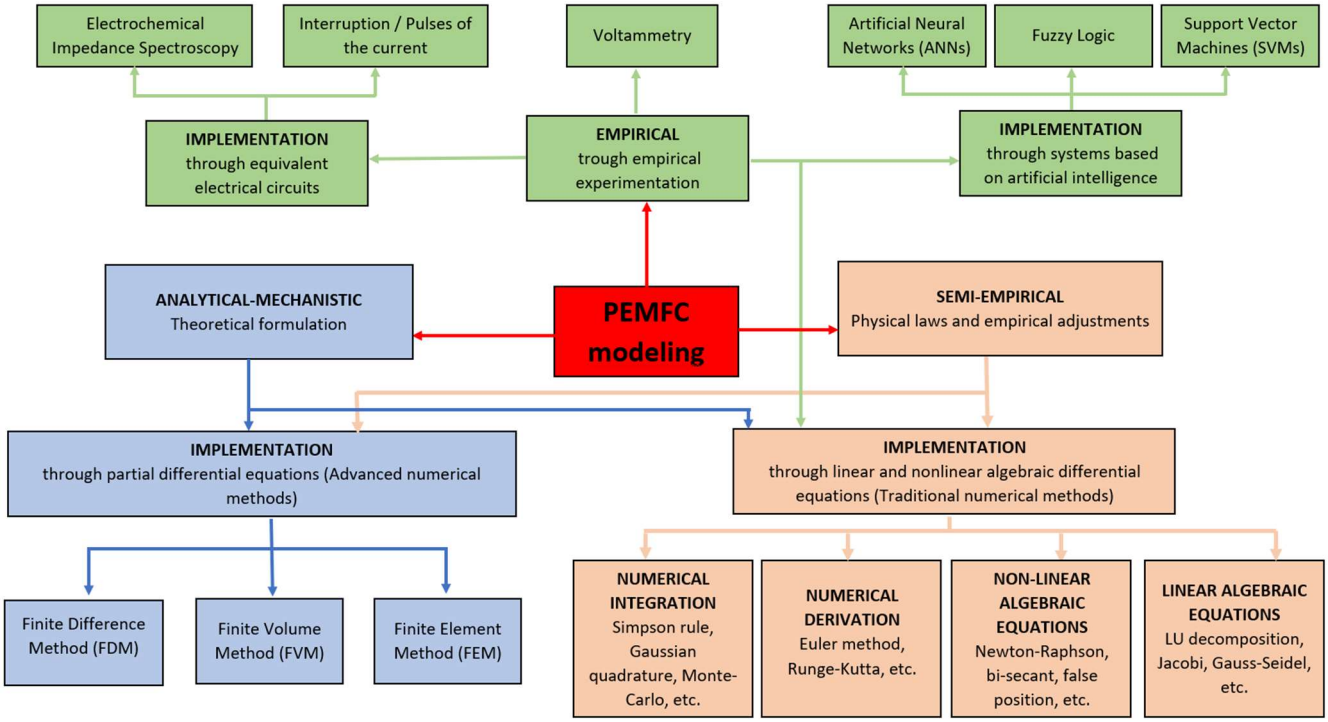

Fig. 2. Outline of the alternatives of modeling techniques, implementation methods, as well as resolution strategies for PEMFC modeling.

In summary, three major groups are distinguished: implementation through analytical-mechanistic formulation, implementation through semi-empirical formulation and implementation through purely empirical methods. Next, these modeling techniques used to model a PEMFC are described.

3.1. Theoretical or analytical-mechanistic modeling techniques

Commonly the models developed using this technique are implemented in a multidimensional domain, considering that physical magnitudes vary in two or three axes of the spatial domain. The analytical-mechanistic formulation typically contemplates the laws of Fick, Nernst-Planck and Butler-Volmer to reproduce the phenomena of charge transport (electric and ionic) and mass transfer [16].

The fist law of Fick relates diffusive flow to concentration assuming a steady state. It is postulated that the flow goes from regions of high concentration to regions of low concentration, with a magnitude proportional to the concentration gradient (spatial derivative), or in simplistic terms the concept that a solute will move from a region of high concentration to a low concentration region through a concentration gradient. Equation (1) shows the formulation of Fick's law, assuming a spatial dimension.

$$J = -D\frac{d\varphi}{dx} \tag{1}$$

where J is the diffusion flow [mol/(m^2·s)] of the substance flowing through an area during a time interval, D is the diffusion coefficient [m^2/s], φ is the concentration of the substance [mol/m^3] and x is the position [m].

The law of Nernst-Planck extends the law of diffusion of Fick assuming that the diffusing particles also move with respect to the fluid due to electrostatic forces. Its formulation is based on the conservation of the mass used to describe the movement of a chemical species charged in a fluid medium. Equation (2) shows the formulation of the Nernst-Planck law.

$$\frac{\partial \varphi}{\partial t} = \nabla \cdot \left[D\nabla\varphi - u\varphi + \frac{Dze}{k_B T}\varphi \left(\nabla\phi + \frac{\partial \mathrm{A}}{\partial \mathrm{t}} \right) \right] \tag{2}$$

where t is the time [s], ∇ represents the gradient, z is the valence of the ionic species, e is the elementary charge [C], k_B is the Boltzmann constant [J/K], T is the temperature [K], u is the velocity vector of the fluid [m/s], ϕ is the electric potential [V] and A is the vector of the magnetic potential [V·s/m].

The law of Butler-Volmer is one of the most fundamental relations in electrochemical kinetics. It describes how the electrical current in an electrode depends on the potential of the electrode, considering that in the same electrode a cathodic, as well as anodic reaction is produced. Equation (3) shows the formulation of the law of Butler-Volmer.

$$j = j_0 \cdot \left(exp\left[\frac{\alpha_a z F}{RT} \right] (E - E_{eq}) - exp\left[\frac{\alpha_c z F}{RT} \right] (E - E_{eq}) \right) \tag{3}$$

where j is the current density at the electrode [A/m^2], j_0 is the exchange current density [A/m^2], E is the electrode potential [V], E_{eq} is the equilibrium potential [V], z is the number of electrons involved in the reaction, F is the Faraday constant [C/mol], R is the universal gas constant [J/(mol·K)], and α_a and α_c are the coefficients of anodic and cathodic charge transfer, respectively.

The way to solve this type of models based on the formulation described above, in multidimensional domains, is based on the use of advanced numerical methods. The first computer programs based on advanced numerical methods are known as Computational Fluid Dynamics (CFD) programs, which is a computerized tool to simulate the behavior of systems that contemplate fluid flow, heat transfer and other related physical processes. This software works by solving the equations that describe the flow of the fluid over a region of interest, with boundary conditions previously specified in the limit of that region. Currently, there is software that is based on advanced numerical methods and combines the simulation of mechanical, thermal, electrical and fluid-mechanical properties, allowing to completely model virtually any system, including all the parts involved in a PEMFC. Two of the most complete commercial software packages that include multiphysics packages are ANSYS and COMSOL Multiphysics.

The methodology of calculation by means of this type of methods consists of the following points:

- *Pre-processing*. During pre-processing, the geometry of the problem to be solved is defined by CAD (Computer-Aided Design) software. Once the geometry is developed, the domains of each element are established. For example, in the case of an MEA, the gas channels, the GDL, the CL, the PEM, etc.

- *Meshing*. In the meshing stage, the volume occupied by each domain is divided into smaller subdomains formed by primitive geometries, forming a mesh. This mesh can be uniform or non-uniform, structured or unstructured. The geometries commonly used are based on hexahedrons, tetrahedra, prisms, pyramids and polyhedrons.
- *Physical model definition.* Once the complete geometry is meshed, the fundamental equations that describe the problem to be solved are defined. For example, the equations that describe the movement of the fluid, the heat transfer, the conservation of chemical species, etc.
- *Definition of boundary conditions*. By defining the boundary conditions, the behavior of the fluid and the properties on all the delimiting surfaces of the fluid domain are specified. For transient problems, the initial conditions are also defined.
- *Simulation*. During simulation, the equations that describe the physical problem are solved iteratively for the type of study contemplated. In this sense, simulations of steady state or transitory regime can be performed (based on the equations described when defining the physical modeling). Another option is to perform parametric studies, performing several simulations (in stationary or transitory regime) and changing one or more variables that intervene in the equations.
- *Post-processing*. In the post-processing stage, the results of the simulation are visualized and an analysis of them is carried out.

Depending on how the complete geometry is discretized in small subdomains and how the differential equations are solved, three main methods are distinguished to solve the problem: Finite Difference Method (FDM), Finite Volume Method (FVM) and Finite Elements Method (FEM).

Finite Difference Method (FDM)

The FDM is one of the first methods used in the resolution of problems based on CFD and is easy to program. This method is based on solving differential equations by approximating them with equations of first order differences, in which the finite differences approximate the derivatives. In (4) the typical formulation used in the FDM is shown.

$$\frac{\partial Q}{\partial t}+\frac{\partial F}{\partial x}+\frac{\partial G}{\partial y}+\frac{\partial H}{\partial z}=0 \tag{4}$$

where Q is the vector of the conserved variables, and F, G and H represent the flows in the directions x, y and z, respectively. Traditional FDM codes cannot handle discontinuities, which is a big problem in the CFD field, where there are commonly sharp fronts [17], [18]. Another problem with FDM is that the mass is not rigorously preserved. Although accuracy can be improved by reducing the time and grid size and using a higher order of approximation, the calculation time also increases [17], [19].

Finite Volume Method (FVM)

In FVM, the governing PDEs (Partial Differential Equations) (typically the Navier-Stokes equations, the mass and energy conservation equations and the turbulence equations) are reformulated in a conservative way and then resolved on discrete control volumes. This discretization guarantees the conservation of flows through a particular control volume [20]. In (5) the typical formulation used in the FVM is shown.

$$\frac{\partial}{\partial t}\int\int\int QdV + \int\int FdA = 0 \tag{5}$$

where Q is the vector of the conserved variables, F is the vector of the flows, V is the volume of the volume control element and A is the surface of the volume control element. The FVM has the advantage of using less memory than the FDM and good computing speed, especially for large problems, high Reynolds number turbulent flows and source-dominated flows, such as combustion [21].

Finite Element Method (FEM)

In FEM, the complete geometry is subdivided into small domains called finite elements. In this way, the EDPs that control the physical ones are converted into simple algebraic equations that model these finite elements [22]. Then, these finite elements are assembled obtaining a system of equations that model the complete domain. In this sense, the method provides approximate values of the variables under study in a discrete number of points on the complete domain [22]. The FEM uses variational calculation methods to approximate a solution by minimizing an associated error function. In the expression (6) the typical formulation used in the FEM is shown.

$$R_i = \int\int\int W_i Q dV^e \tag{6}$$

where R_i is the residue of the equation corresponding to the vertex of element i, W_i is the weight factor, Q is the conservation equation expressed on the basis of an element, and V^e is the volume of the element. This method is commonly used in the structural analysis of solids, but it is also applicable to fluids. Although the FEM formulation requires special care to ensure a conservative solution and requires more memory and computing time, it is much more stable than the FVM [23].

In addition to these advanced methods, to solve the algebraic equations obtained as a result of applying the advanced numerical methods, traditional numerical methods are used. Among the latter, there are numerical integration methods (Simpson's rule, Gaussian square, Monte-Carlo, etc.), numerical derivation methods (Euler, Runge-Kutta, etc.), linear algebraic equation solving methods (LU and Cholesky decomposition, Jacobi, Gauss-Seidel, etc.) and the methods of solving non-linear algebraic equations (Newton-Raphson, bisection, secant, etc.).

3.2. Semi-empirical modeling techniques

The ways to convert a white box model to a gray box model are those based on empirical adjustments for the simplification of some complex equation or the identification of parameters that describe the behavior of some physical phenomenon related to the behavior of the PEMFC.

The implementation of a model from semi-empirical modeling techniques typically combines differential and algebraic equations that describe the theoretical formulation with empirically determined relationships. These equations can be solved by traditional numerical methods (derivation and numerical integration, etc.). Depending on the size and degree of complexity of the resulting model, it may also be necessary to resort to advanced numerical methods to solve the formulated equations. In practice, when the use of empirical correlations is minimal, it is difficult to differentiate an analytical model from a semi-empirical model of this type, since the line that separates them is very thin.

Generally, empirical relationships are used when physical phenomena are difficult to model, when the theory governing these phenomena is not fully understood or simply because a level of detail about the phenomenon in question is not required.

The following are some typical examples of empirical adjustments on the analytical formulation:

- Correlation of the conductivity of the membrane and porosity of the electrodes with the water content in the membrane [24].
- Correlation of partial pressures and dissolved oxygen and hydrogen concentrations, with temperature, current density and molar fractions in the gas channels [25].
- Correlation of the reversible voltage of the cell, overpotentials of activation and resistance of the cell with the temperature, partial pressures, dissolved oxygen and hydrogen concentrations and current density [25].
- Empirical relationships to estimate the activation and ohmic losses, as well as transport limitations in the cathode reactive region [25].
- Estimation of a factor to determine the fraction of CO that occupies the surface of the anode catalyst [26].
- Correlation of the porosity of the cathode gas with the current density [27].

3.3. Empirical modeling techniques

The implementation of a model based on empirical methods implies real experimentation with the system to be modeled. In general, PEMFC models based on empirical methods can be classified according to the modeling technique used, among which are those based on parameter identification techniques, and those based on artificial intelligence, such as ANN (Artificial Neural Networks), fuzzy logic and SVM (Support Vector Machine) systems.

3.3.1. Parameter identification

The techniques of parameter identification are based on experimenting with the real system in order to obtain certain parameters that will serve to evaluate an empirical expression or construct an electrical circuit, which will emulate the behavior of the PEMFC. One of the most used techniques to extract data and evaluate an empirical expression is voltammetry. For the case of the identification of parameters to construct an electrical circuit equivalent of the fuel cell, the EIS (Electrochemical Impedance Spectroscopy) and the current interruption or pulse are the most used techniques. [28].

A) Voltammetry

This method consists of measuring the current as the potential of a cell or a stack varies, which allows obtaining the polarization curve V-I. The identification of the V-I curve is generally obtained by keeping the operating conditions of the fuel cell constant (such as temperature, stoichiometry, humidity, etc.) constant and measuring the stabilized voltage and current corresponding to each voltage value. Once the V-I curve is obtained, it can be characterized by empirical equations, as can be seen in [29]-[30], resulting in a mathematical equation that describes the behavior of the fuel cell. By way of example, expression (7) shows the empirical equation developed by J. Kim *et al.* [29].

$$E = E_0 - b \cdot log\ i - R \cdot i - m \cdot exp(n \cdot i) \tag{7}$$

where E is the cell voltage [V], E_0 is the open circuit voltage under standard conditions [V], b represents the parameters of the Tafel slope [V/dec] for oxygen reduction, R represents the ohmic resistance of the membrane [Ω/m^2], i is the intensity provided by the cell [A] and, m [V] and n [m^2/A], are constants used to characterize the overpotential of mass transport as a function of current. The constants m and n are obtained by linear regression from expression (8).

$$\Delta E = m \cdot i^{\,n} \tag{8}$$

In addition to linear regression, there are several methods to adjust the experimental data obtained by voltammetry in order to obtain an empirical system, for example, non-linear regression methods (exponential, logarithmic and polynomial), least squares method, Box-Jenkins method, Hammerstein-Wiener structures, Uryson structures, look-up tables, etc. Some examples of this type of empirical adjustment are shown in [31]-[32].

B) Electrical circuits

The implementation of a PEMFC model using equivalent electrical circuits is a modeling approach used to describe the dynamic behavior of the fuel cell in terms of energy. The components of the equivalent electric circuit reflect a macroscopic view of the local physical-chemical phenomena that occur in the fuel cell. In some cases, they even allow to describe the electrochemical behavior by means of frequency components. Therefore, these dynamic models maintain a link with physical phenomena, presenting the advantage of being able to be executed in simulators of electrical circuits used in the field of electrical engineering, such as PSPICE or PSIM.

The most used techniques for the identification of circuit parameters are:

- Electrochemical impedance spectroscopy (EIS). This technique consists of imposing a sinusoidal voltage (or current) of low amplitude on a fuel cell, while operating at a specific point of the polarization curve I-V. Under these conditions, the impedance is calculated by measuring the phase and the amplitude of the current (or voltage) response. To obtain a spectrum of the total impedance (mapping the entire dynamic response range), a frequency sweep is carried out (typically from 10 mHz to 100 kHz). This technique allows to identify the different fuel cell loss mechanisms due to the association of the ionic resistance of the membrane, the resistance of the load transfer and the mass diffusion and transport losses with certain frequency ranges [33]. Some examples that use this identification technique are those presented in [33]-[34]. Fig. 3 shows an example of an equivalent electrical circuit of Randle, which represent the impedance spectrum obtained by means of the EIS technique. The resistance R_m represents the ohmic losses, the resistance R_{ct} and the so-called Warburg impedance Z_W represent the charge transfer losses and the capacitor C_{dl} characterizes the phenomenon of charge accumulation in the double layer [9].

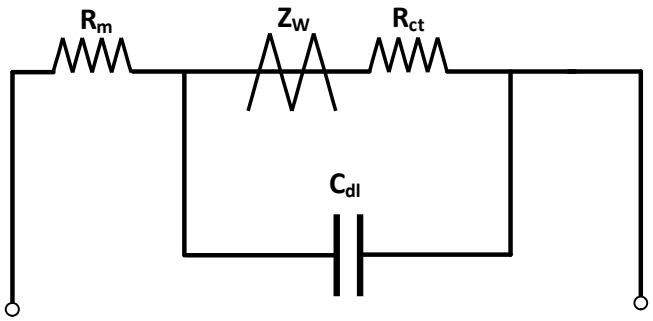

Fig. 4. Equivalent electrical circuit of Randle.

- The method of pulses or interruption of the current. This technique consists of measuring the transient voltage of a fuel cell before a step change in the demanded current. A variation of this method involves subjecting the fuel cell to a short duration current pulse. This technique allows to obtain the ohmic resistance associated to the ohmic losses, calculated from the instantaneous change of the voltage, and the loss of load transfer (activation losses), obtained from the gradual change of the voltage until reaching the value of steady state, as shown in the Fig. 4. Some examples that use this identification technique are those presented in [35]-[36].

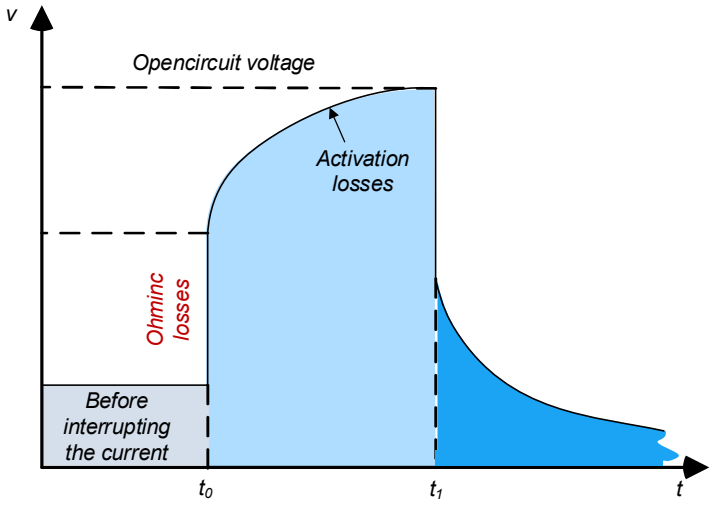

Fig. 5. Cell voltage during an interruption in the current.

3.3.2. Artificial Intelligence systems (AI)

Artificial intelligence systems are systems that try to emulate the processes of human intelligence through machines, especially computerized systems. In a generalized way, these processes include learning (acquiring information and rules on how to use that information), reasoning (how to use the rules to achieve a certain objective) and self-correction (adjusting the rules acquired when the desired objective is not achieved).

There are several ways to implement an artificial intelligence system, among all, Support Vector Machines (SVM), fuzzy logic systems and Artificial Neural Networks (ANN) are the most popular in the field of modeling PEMFC systems [9].

A) Support Vector Machines (SVM)

The SVMs belong to the group of supervised learning models used in problems of classification and regression. From a set of training examples (samples) labeled in classes, by means of an SVM training algorithm, a model that predicts the class of a new sample is obtained.

In general, an SVM can be defined as a model that represents the samples in space, separating the classes into two spaces by means of a separation hyperplane defined as the vector between the two points (of the two classes) closest to each other. This vector is known as a support vector. In this way, a model based on SVM can classify the new samples depending on the spaces to which they belong, in one class or another. In addition to the linear classification, the SVMs can perform non-linear classifications efficiently using a kernel, mapping their entries in high-dimensional spaces [37]. Fig. 6 shows the concept of mapping made by a SVM, which consists of mapping a non-linear function in a linear function through the kernel function, thus allowing to separate the input samples in two classes.

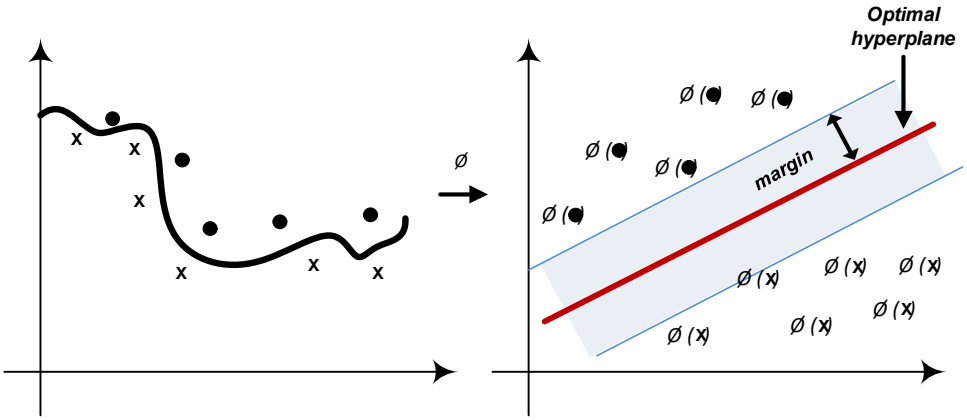

Fig. 7. Illustration of the mapping of a nonlinear function to a linearly separable function.

In the expression (9) the general formulation of a classifier based on SVM is shown.

$$f_{SVM}(x) = w^T \Phi(x) + b \tag{9}$$

where parameters w and b represent the weight vector and the bias, respectively, that are determined during the training process by minimizing a cost function, and $\Phi(\cdot)$ represents the non-linear mapping function to map the input vector x in a space of higher dimension, in order to be able to easily separate the data contained in x by a linear hyperplane (Fig. 8).

Starting from the fact that a training sample (x_i, y_i) is a support vector if it satisfies $y_i f_{SVM}(x_i) \leq 1$, and denoting the support vectors extracted by $s_k \in [1, K]$, the function of the SVM can be represented according to the expression (10).

$$\begin{cases} f_{SVM}(x) = \sum_{k=1}^{K} K(x, s_k) + b \\ K(x, s_k) = \Phi^T(x)\Phi(s_k) \end{cases} \tag{10}$$

where $K(\cdot,\cdot)$ represents the kernel function to be implemented to represent the non-linear mapping of $\Phi(\cdot)$. The most commonly used kernel functions are linear, polynomial and RBF (Radial Base Function) [38]. Some examples of PEMFC models based on SVM are those presented in [39], [40].

B) Fuzzy Logic systems

Fuzzy logic systems focus on fixed and approximate reasoning as opposed to fixed and exact reasoning. A variable in fuzzy logic can take a range of true values between 0 and 1, instead of taking "true" or "false" values as in traditional binary sets. Since the true value is a range of values of the total set, fuzzy logic systems can only partially handle the truth.

A model based on fuzzy logic maps inputs to outputs combining three components: if-then rules, membership functions and logical operators, that is, AND and OR [41]. Numerical data are converted into linguistic variables through membership functions that define how well a variable belongs to the output, that is, an evaluation between 0 and 1 [41]. For the correct definition of

these functions or rules, unlike the ANNs, prior knowledge of the user is required, which does not allow to abstract from the physical behavior of the problem to be modeled [9]. Some examples of PEMFC modeling based on fuzzy logic are those presented in [42], [43].

C) Artificial Neural Networks (ANN)

Like SVMs and systems based on fuzzy logic, ANNs are systems that can be used to solve classification problems. ANNs are inspired by biological neural networks, and have proved to be a powerful tool for the modeling of non-linear systems [44]. Fig. 6 shows the standard model of an artificial neuron, which was described by D.E. Rumelhart and J.L. McClelland [45], [46].

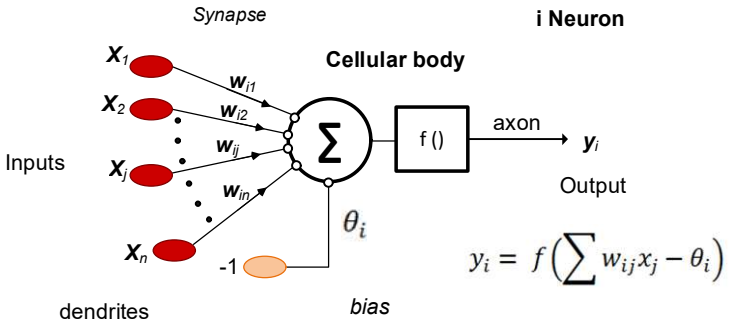

Fig. 6. Standard model of an artificial neuron.

A biological neuronal system is composed of millions of neurons organized in layers. In the emulation of said biological neural system, a hierarchical structure similar to that existing in the brain can be established by means of an artificial neural system. The essential element will be the artificial neuron, which will be organized in layers. Several layers will constitute a neural network. Finally, a neural network together with the input and output interfaces will constitute the neuronal system (Fig. 7).

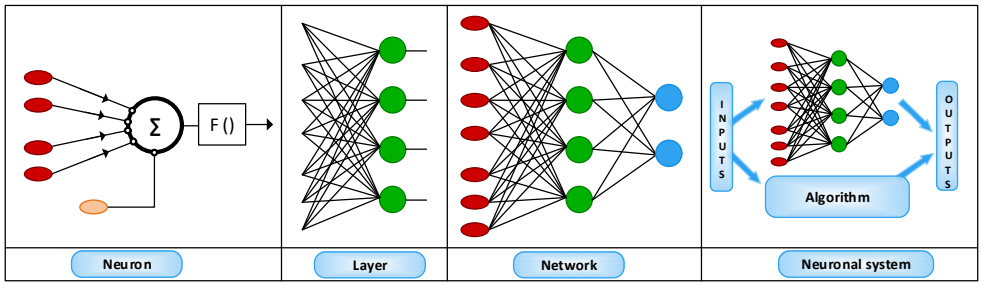

Fig. 7. Global structure of a neuronal system.

There are several models of neural network (linear associator, simple perceptron, Adaline, multilayer perceptron, etc.), architectures (unidirectional, feedback, monolayer, multilayer, etc.) and learning algorithms (Hebbian algorithm, Rosenblatt algorithm, Widrow-Hoff algorithm, backpropagation algorithm, etc.). However, due to the limitations of some of the neural network models and architectures when emulating very complex non-linear systems, within the PEMFC context, the most used model and architecture corresponds to the MLP (Multi-Layer Perceptron) with feedback. The architecture of the MLP has

become so popular because, with a single hidden layer, this neural network model can approximate any continuous function in a range up to the desired level [47].

The MLP model is usually trained through the BP (Back Propagation) algorithm. That is why in the current literature, this architecture can commonly be found under the name of backpropagation network. Fig. 8 shows the structure of the MLP with a single hidden layer, as well as the activation function used in the multilayer perceptron, which is a sigmoid function.

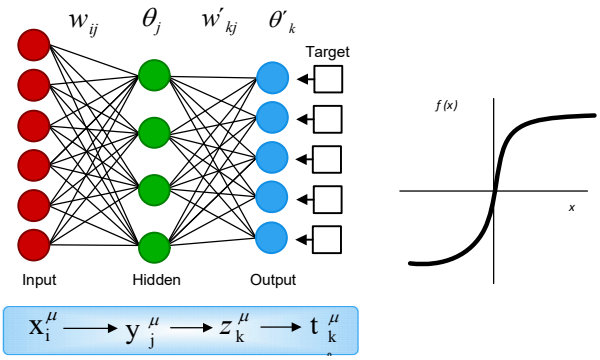

Fig. 8. Structure (left) and activation function (right) of a MLP.

The operation performed by a multilayer perceptron with a single hidden layer and activation functions of the hidden layer and output layer of sigmoid and linear type, respectively, can be defined according to the expression (11).

$$z_k = \sum_{j=1}^{o} w'_{kj} y_j - \theta'_k = \sum_{j=1}^{o} w'_{kj} f\left(\sum_{i=1}^{n} w_{ji} x_i - \theta_j\right) - \theta'_k \tag{11}$$

where x_i are the n inputs of the network, y_j are the o outputs of the hidden layer and z_k are the s outputs of the output layer (those that have to be compared with the targets t_k). w_{ji} and θ_j represent the weights and biases of the hidden layer, respectively, and w'_{kj} and θ'_k represent the weights and biases of the output layer, respectively. f represents a function of sigmoid type.

Considering a three-layer MLP (Fig. 4), that is, including a single hidden layer, and with the inputs, outputs, weights and biases of the neurons defined above, given an input pattern $x^r (r = 1, \dots, N)$, the global operation of this architecture for each of the k output neurons with $(k = 1, \dots, s)$ can be defined by means of (12).

$$z_k^r = \sum_{j=1}^{o} w'_{kj} y_j^r - \theta'_k = \sum_{j=1}^{o} w'_{kj} f\left(\sum_{i=1}^{n} w_{ji} x_i^r - \theta_j\right) - \theta'_k \tag{12}$$

The commonly used cost function is the MSE (Mean Square Error), being for the case of the MLP the expressed in (13) and (14).

$$E(w_{11}, \dots, w_{on}, \dots, w'_{1s}, \dots, w'_{os}, \theta_1, \dots, \theta_o, \theta'_1, \dots, \theta'_s) \quad where\ E \in \Re^{(n \times o)+(o \times s)+o+s} \tag{13}$$

$$E(w, w', \theta, \theta') = \frac{1}{2}\sum_{r=1}^{N}\sum_{k=1}^{s}(t_k^r - z_k^r)^2 \quad (14)$$

There are several methods for the minimization of (14), although the most effective are the Levenberg-Marquardt, Bayesian Regularization and Conjugate Gradient methods [48]. Some examples of PEMFC modeling based on ANNs are those presented in [44], [49].

4. PEMFC systems modeling: electrical and thermal behavior

This section includes a compilation of the models that can be found in the current literature, which emulate both electrical and thermal behavior of PEMFC systems. Models that at least emulate the voltage and temperature variation as a function of current density are considered. In this sense, it should be noted that only non-isothermal models that consider the temperature as an output variable and not as an input variable are considered. Besides, only stack or cell domain models are considered,

As seen above, there are several ways to classify a model (approach, regime, domain, etc.). To classify all the models contemplated in this section, a classification based on the dimension of the model has been considered.

4.1. Zero-dimensional models (0D)

Among the first research works contemplated in this section that present zero-dimensional models is the model proposed by S. Busquet *et al*. [50]. The model presented is a novel empirical model for accurately calculating the V-I characteristic of a PEM fuel cell, an electrolyzer or a reversible fuel cell. The empirical adjustment is made through experimentation with a PEMFC of 4 kW. Additionally, the new methodology presented allows to adjust the model through experimentation to any PEMFC or electrolyzer. The model is mathematically coherent and convergent near zero, allowing to interpolate the experimental results of the PEMFC when the model is operated in regions where the current density does not cross the mass transfer limitations. The same year, A. Kazim [51], presents a comprehensive exergy analysis of a 10 kW PEM fuel cell at variable operating temperatures, pressures, cell voltages and air stoichiometry. The analysis is carried out by varying the temperature and pressure, cell voltage and stoichiometry of the air, in order to determine the effect of these variations on the efficiency of the fuel cell. The results obtained highlighted the importance of the operating temperature, pressure, cell voltage and air stoichiometry on the exergy efficiency of the fuel cell. However, they recommend to operate the fuel cell at stoichiometric proportions below 4 to maintain the RH (Relative Humidity) level in the air and to prevent the membrane from drying out at high operating temperatures.

One of the first zero-dimensional models implemented by electrical circuits is found in the work of X. Kong *et al.* [52], in which a fuel cell model that is able to characterize the steady state behavior of the fuel cell, as well as the transient behavior is presented. To make the empirical adjustment of the model, a Ballard Nexa of 1.2 kW of electric power is used. The proposed model shows good behavior (93% accuracy) when validating it with the experimentation results in steady and dynamic state. Later, in [53], an

update of the model implemented with electrical circuits in [52] is proposed, in such a way that the dynamics of the system using an ANN based on the MLP is calculated. The ANN is composed of two hidden layers with 30 neurons per layer. By means of this technique it is managed to reduce to half the MSE of the model based on the Nexa Ballard equivalent circuit. In [54], K.C.S. Wang *et al.* propose a model based on electrical circuits developed in Pspice environment to model the dynamic behavior of a Nexa Ballard of 1.2 kW of electrical power. In the study, it is put special emphasis on the dynamic behavior during the cold start of the stack, as well as on the temperature evolution in time. The simulation results show consistency with the experimental results.

In [55], Z. Zhang *et al.* present a dynamic model of an equivalent electrical circuit for the Nexa Ballard of 1.2 kW, considering the characteristics of the temperature and the equivalent internal resistance. The results of the model show that the developed model can accurately represent the experimental results in a wide range of load conditions. M. Miansari *et al.* [56], develop a model of a PEM cell to study the effect of different operating conditions, such as temperature, pressure and air stoichiometry on the exergetic efficiencies and the irreversibilities of the cell. The effect of the depth of the anode and cathode channels on efficiency is also calculated. In this sense, the highest efficiencies for a channel depth of 1.5 mm for the anode and 1 mm for the cathode are obtained. ME. Youssef *et al.* [57], propose a model of zero dimensions, oriented to the study of the effect of temperature, pressure, stoichiometry, thickness of the membrane and thickness of the gas diffusion layer on the behavior of the cell. The results obtained with the model are compared with the results presented by A.R. Maher *et al.* [58].

K. Hyun-il *et al.* [59], present a model to characterize the slow transient response of PEMFC. In the work, the estimation of the necessary parameters to obtain the behavior in static, as well as in dynamic regime is presented. The model is validated with experimental results carried out with a Nexa Ballard of 1.2 kW. R. da Fonseca *et al.* [60], present a stack-level model, oriented to applying a control strategy using the theory of differential flatness. The model responds to the control signals that regulate the most important variables in the air supply subsystem: oxygen stoichiometry and cathode pressure. The model is based on a stack of 5 kW of electrical power composed of 80 cells.

In [61], I. San Martín *et al.* develop a model of the Ballard Nexa 1.2 kW in the MATLAB/Simulink environment, obtaining the parameters that emulate the behavior of the electrochemical and thermodynamic phenomena empirically. The model is validated in static and dynamic regime. The behavior of the model is validated forming a micro-grid with 4 fuel cells of the same type. R. Salim *et al.* [62], present a technique with a heuristic approach to estimate up to 18 parameters to model a Nexa Ballard of 1.2 kW. The identification algorithm is based on PSO (Particle Swarm Optimization). The resulting model shows good accuracy and requires few mathematical relationships. M.M. Barzegari *et al.* present in [63] a stack level PEMFC model to investigate the temperature effect on performance of dead-end cascade PEMFC stack with an integrated humidifier and separator. The equations are posed using a semi-empirical approach and are solved using a fourth-order Runge-Kutta method. The model can predict the

bulk humidifier and PEMFC temperatures and the stack voltage. Besides, cascade PEMFC operation in a dead-end mode is compared with an open-end mode. Authors propose the obtained model for system identification and control purposes.

F.J. Asensio *et al.* develop in [64] a 0D stack level model of a 600 W PEMFC to evaluate the electrical and thermal efficiency of the system, including power electronics. The model is implemented using ANNs and is developed in MATLAB/Simulink environment. The model provides the temperature and the hydrogen consumption as a function of electrical and thermal demand with good accuracy. Later, same authors present in [65] an improvement of the model by adding the cooling fluid flow rate as an input variable to the model. The temperature of the cooling fluid is calculated using a 3D model in COMSOL Multiphysics environment and a dynamic look-up table is developed to couple the thermodynamic model to the previously developed ANN-based model, resulting in a 0D model more accurate. Authors propose the model to develop real-time control, optimization strategies and to optimally manage the cooling system of the PEMFC.

In [66], X. Chen *et al.* show a thermodynamic model of a PEMFC that includes the main auxiliary components. In this sense, the model contemplates a heat exchanger, a water tank, a cooling pump, as well as the input gas processing components (humidifier and compressor). A parametric study is carried out to study the electrical and thermal efficiency of the PEMFC and the efficiency of the total system. The PEMFC is controlled with MOEA/D (Multi-Objective Evolutionary Algorithm based on Decomposition) to optimize the operating parameters of the system, aimed at maximizing the efficiency and power of the system. The model is obtained by formulating semi-empirical relationships. In [67], A. Kheirandish *et al.* propose an AI-based model using FCMs (Fuzzy Cognitive Map) to describe the behavior of a fuel cell of 250 W for a power electric bicycle system. Authors use fuzzy rules to explain the cause and effect between concepts. C. Ziogou *et al.* present in [68] a PEM cell model aimed to apply MPC (Multivariable Predictive Control) strategies. The model is developed using semi-empirical formulation and gPROMS software. Authors show how using the model and strategy implemented fuel cell system operates economically and at a stable environment regardless of the varying operating conditions.

J. Chen *et al.* propose in [69] a dynamic scalable model of PEMFC systems considering two-phase water flow. The model is developed in MATLAB/Simulink environment using the toolbox Simscape. Simulation results show reasonable distributions of current density, temperature, pressure, and two-phase water flow at both the steady state and dynamic operations. Authors highlight that the pattern reconfigurability and the segmentation scalability of the proposed model meet the requirements for both controller design and system analysis for fuel cells. K. Sankar *et al.* present in [70] a PEMFC system level 0D model aimed at evaluating a nonlinear MSMC (Multivariable Sliding Mode Control) strategy. In addition to the electrochemical and thermodynamic behavior of the PEMFC, the model developed is capable of emulating the behavior of the air compressor, air cooler, primary manifold, supply manifold, humidifier and return manifold. All equations involved are implemented in MATLAB/Simulink environment.

4.2. One-dimensional models (1D)

One of the most relevant one-dimensional models can be found in the work presented by J.C. Amplhett *et al.* [71], in which a PEMFC model designed to predict electrical and thermal behavior, both in steady state and in transitory regime is presented. To do this, the transient characteristics of heat and mass transfer are incorporated into an electrochemical model to form a general model that predicts the transient responses of a PEMFC. The developed model is based on the Ballard Mark V system, which is a PEMFC system of 5 kW of electrical power, formed by 35 fuel cells. Through experimentation with this equipment, a thermal model of the stack based on the conservation of mass and energy balance was developed. The thermal characterization of the stack includes the determination of sensible heat changes in anode, cathode and water circulation flows, the theoretical energy derived from the reaction, the electrical energy produced by the fuel cell, and the heat released through the surface of the stack. The thermal model is coupled to an electrochemical model, relating the power produced by the stack and the temperature of the stack with the amount of heat that must be extracted from the stack. The electrochemical model calculates the electrical power produced by the stack by predicting the cell voltage based on a complex expression involving the operating current, the temperature of the stack, and partial flow rates and pressures of hydrogen and oxygen.

A. Rowe *et al.* [72], present a one-dimensional model of a PEM cell on which the effect of designing and operating conditions on cell efficiency, thermal response and water management is researched. It is shown how the water phase change in the electrodes affects the temperature profile, especially for unsaturated reactants and at low operating temperatures. The simulation results obtained are compared with the experimental results presented by E.A. Ticianelli *et al.* in [73] and [74]. N. Djilali *et al.* [75], present a work in which a theoretical model of transport phenomena is formulated for a PEM fuel cell. The model considers the diffusion of humidified fuels and oxidizing gases through the porous electrodes, the transport of water through the electrodes and the membrane, as well as the gradients of heat transfer and gas pressure in the fuel cell. The micro-hydrodynamic phenomena associated with the low permeability of the electrodes are also considered. The model is implemented in a one-dimensional code, and a parametric study is performed, comparing the results obtained with those presented in the work carried out by D.M. Bernardi *et al.* [76] and E.A. Ticianelli *et al.* [77]. In this sense, it is verified that, unlike the isothermal and isobaric models, the non-uniform temperature and pressure distributions have a great impact on the flows of liquid water and in the form of simulated vapor in the anode and cathode diffusion layers. In particular, the results indicate that water management requirements (i.e., humidification or removal of water) to prevent possible dehydration of the membrane or flooding of electrodes are much more conservative than when assuming isothermal conditions. It is shown that, in the permeability range of the porous electrodes used in the PEMFC (10-16 – 10-17 m^2), the Knudsen diffusion must be considered when modeling the gas transport.

In the work presented by X. Xue *et al.* [78], a dynamic model at PEMFC system level that emulates the temperature, the gas flow through the channels and the capacitance formed by the double charge layer in the MEA is presented. To quantify the dynamic interactions, the PEMFC system is divided into three control volumes: the anode channel, the cathode channel and the

fuel cell body; developing the respective dynamic models with grouped parameters. The resulting model is simulated in Simulink environment and validated by comparing the results obtained with those derived from [71]. It is concluded that the model is useful to be used in the optimization and real-time control of PEM fuel cells installed in automotive or stationary applications. Y. Shan *et al.* [79], propose a model that is constructed based on the layers of a PEM cell, considering the following factors: dynamics of the temperature gradient across the cell, dynamics in the redistribution of water concentration in the membrane, dynamics of the concentration of protons in the catalyst layer, and dynamics in the redistribution of the concentration of reactants in the GDL of the cathode. For the construction of the model, they are based on the parameters presented in [80], [81]. In the work, the results obtained in transitory regime, during the start of the PEMFC and in steady state are shown.

C. Wang *et al.* [82], present the development of a dynamic model for PEM fuel cells using electrical circuits implemented in MATLAB/Simulink and Pspice environments. The model contemplates the effect of double layer charge and the thermodynamic characteristic within the cell. The model responses obtained in steady state and transient conditions are validated by experimental data acquired from the PEMFC Avista Labs SR-12 of 500 W of electric power. The authors propose the model to be used in PEM fuel cell control studies. In [83], S. Kjelstrup *et al.* present a model for a PEM cell aimed at studying the rate of production of local entropy in various parts of the fuel cell. Authors present five sets of transport equations for a one-dimensional heterogeneous steady-state cell (compatible with the second law of thermodynamics) and solve them by an iterative process. For the implementation of the model, data found in the literature on cells that use the membrane based on Nafion 115 is used.

In [84], A.Z. Weber *et al.* present a one-dimensional model of a PEM cell based on the membrane Nafion 112, which is used to compare the behavior of it in an isothermal and non-isothermal situation. P. Sang-Kyun *et al.* [85], present a PEMFC model for studying the effect of water variation (contemplating one and two phases) and the temperature distribution along the stack at variable loads on the behavior of the stack. Authors include the cooling circuit in the model. For the construction and validation of the model, an PEMFC of 80 W composed of two cells of 140 cm^2 is used. From the developed model, several starting strategies for a PEMFC composed of 20 cells are shown. A.A. Shah *et al.* propose in [86] a two-phase model that includes a complex kinetic mechanism to describe the electrode reactions. The model is aimed at studying the sulfide poisoning in PEMFCs and is developed in COMSOL Multiphysics environment. Obtained results are compared with experimental data published in [87]. Authors conclude that the kinetic mechanism in the anode is intimately linked with the temperature and the water activity, which yield a wider influence on performance, through the form of the reaction rates. These reactions cause a reduction on the water levels in the anode, which reduce the current density and restricts back diffusion of water via proton migration.

P. Hu *et al.* [88], present an ANN-based model aimed at characterizing the non-linear dynamic behavior of a PEMFC of 1.5 kW of electrical power. For the implementation of the ANN authors use a hybrid algorithm based on PSO and LM (Levenberg-Marquardt). The architecture of the ANN is based on MLP with feedback, and consists of 3 neurons in the input layer, 11 in the hidden layer and 3 in the output layer. The model shows good accuracy compared to the real system. S. M. Sharifi *et al.* [89]

present a model aimed at emulating the dynamic response of a PEMFC to variations in the load. The innovation of the model is that it calculates the water content in the membrane and considers the presence of water vapor in the cathode channel. The model is validated with experimental results from several real systems (SR-12, Ballard Mark V and BCS 500), obtaining good correlation with them. In [90], F. Tiss *et al.* propose a non-isothermal model that takes into account the double layer effect, the geometric capacity and the temperature gradient. The model is developed to operate in a dynamic regime and the results obtained are compared with the isothermal model presented in the work of A. Haddad *et al.* [91]. Authors conclude that the effect of the temperature distribution significantly influences the cell voltage and the gas flow rate.

N. Noguer *et al.* [92], present a one-dimensional and two-phase model, aimed at developing a method to evaluate the reliability of a PEMFC. The method combines physical modeling with statistical analysis. The model is developed with the Modelica-Dymola software and allows analysis in transitory regime with time constants greater than 0.1s. In [93], J.A. Salva *et al.* develop a one-dimensional, two-phase model of a 50 cm^2 PEM cell to emulate the cell voltage and water content in the membrane. For the resolution of non-linear equations, they use the software EES 9.705-3D. The model is validated with a novel technique based on neutron images. Subsequently, in [94], authors use the model to emulate the behavior of a stack composed of 3, 5 and 7 PEM cells.

4.3. Two-dimensional models (2D)

The first modeling based on two dimensions, is found in the work presented by T.V. Nguyen *et al.* [95], in which a two-dimensional and single-phase model of heat and mass transfer for a PEM fuel cell is presented. To developed the model, the electro-osmotic coefficient is assumed to be constant. The model is developed as a designing tool for the development of PEM-type cell humidification systems. Subsequently, authors present in [96] an update of the model with updated data on the commercial Nafion membranes of that time, in order to investigate several techniques of membrane humidification. In the same line, in [97] T.F. Fuller *et al.* develop a model that allows quantifying the amount of heat to be extracted from the cell.

J.H. Lee *et al.* develop in [98] a technique to numerically model a MEA in two dimensions, in order to be integrated as part of a PEMFC dynamic model. The MEA model includes processes, losses and electrical characteristics. The equations used for the construction of the model are based on the previous works developed by J. Kim *et al.* [99] and J.H. Lee *et al.* [100]. For the development of the numerical models, authors use a MEA of 350 cm^2 and a stack composed of 125 cells. The simulation results show that the model developed using the proposed numerical technique is especially useful to study the effect of temperature, pressure, humidity, and variations in oxygen concentration on the efficiency of the MEA.

Based on a semi-empirical formulation technique, V. Gurau *et al.* present in [101] a model for a two-dimensional PEM cell with two-phase flow, to study the distribution of oxygen and water vapor in the GDL for various current densities. Authors also study the water content in the membrane and several aspects that influence the efficiency of the cell. The equations are solved by means

of SIMPLE algorithm for the resolution of CFD systems, developed by S.V. Patankar [21]. The simulation results of the implemented model are compared with the results of the work presented by E.A. Ticianelli *et al.* [73]. In [102], M. Noponen *et al.* present a two-dimensional model in which the current density in the active layer of the cathode is modeled assuming an agglomerated material. The model is developed in the environment of COMSOL (FEMLAB 2.3) and validated using a segmented PEM cell.

E. Biergersson *et al.* propose in [103] a two-phase two-dimensional model developed in COMSOL (FEMLAB 2.5), with which the effect of contact resistances between cell components and the effect of different capillary pressures are studied. The catalyst layer is treated as a reactive limit. Authors conclude that heat transfer by convection is negligible under the given operating conditions. S. Litster *et al.* present in [104] a model for studying heat and mass transfer on the cathode side of a PEM cell. The model, which includes the cooling system, is solved using the CFX software and the SIMPLEC algorithm. The computational domain consists of more than 30,000 mesh elements for the air domain and 580 mesh elements for both electrodes.

In [105], J.J. Hwang develops a two-dimensional model to characterize the electrochemical behavior and heat transfer of a PEM cell in a coupled manner. The model contemplates a single phase of water status. The resulting mesh consists of 8,789 elements and the coupled equations are solved by the Newton-Rapshon algorithm. The polarization curve of the model is validated with the work presented in [106].

M. Acosta *et al.* present in [107] a two-dimensional two-phase model to study the performance of the flow field. In the work emphasis is placed on physical parameters and capillary saturation pressure, and the results are compared with experimental investigations. A saturation level of liquid water of 60% is predicted for low cell voltages. The computational domain consists of the GDL and the CL treated as a thin layer (6,400 elements of equal size). To solve it, authors use the software MUFTE_UG. In [108], H. Wu *et al.* present a two-dimensional model designed to emulate the dynamics of water transport (in a single phase) in PEM cells under non-isothermal temperature conditions. In the work done, authors focus on studying the effect of membrane width (Nafion 117) on the efficiency of the cell. Authors conclude that the thermal effect has a great impact on the transient behavior of the cell.

In [109], Y. Zhang *et al.* develop a model in two dimensions to study the atmospheric air intake in a PEM cell with an active area of 6 cm^2. The effects of the orientation of the cell, the operating conditions and the geometrical parameters are analyzed. Fluent software is used to solve the model together with user-defined subroutines, consisting of 5,748 elements. The results of the model are compared with the experimental results presented in the technical report presented in [110]. In the same research line, B.P.M. Rajani *et al.* present in [111] a two-dimensional model aimed at studying the cell respiration. Despite being a two-dimensional model, the catalyst layer is considered very thin and is treated as a single dimension. Authors also use Fluent and user-defined subroutines to study various effects. In the work authors show that most of the dynamic response processes are within few seconds.

In [112] H. Meng proposes a two-dimensional model and two-phase flow to study the transient phenomena of liquid water transport and heat transfer in a PEM cell before a change in cell voltage. The domain is implemented and solved in Fluent, using a step time of 0.01s and incrementing it gradually during the simulation. Z. Belkhiri *et al.* present in [113] a 2D transient model of a PEMFC to study the effect of permeability on the dynamic behavior of the velocity and pressure profiles in the parallel flow field of the fuel cell. The equations are solved considering the FVM. Obtained results demonstrate the difference between the flow in a continuous medium and a porous medium.

In [114], B. Randrianarizafy *et al.* present a 2D model to investigate the competition between current collection and oxygen supply. Authors propose the model as a design tool to obtain an optimal channel with a varying width. Model is based on semi-empirical formulation and is implemented using COMSOL Multiphysics. Obtained results are compared to the results obtained in the AutoStack-CORE project [115]. N.T. Truc *et al.* propose in [116] a 2D, non-isothermal and single-phase model to investigate the reactant gas crossover effect in a PEM cell. The model is developed in the opensource software FreeMem++, and is validated with experimental data. Results from simulations show that gas diffusion coefficient as a function of temperature and RH. Authors conclude that simulating the effect of the temperature seems more complicated due to a significantly effect of crystalline region at higher temperature range of 80–100 °C.

4.4. Three-dimensional models (3D)

One of the first models of PEMFC presented in three dimensions corresponds to the model proposed in [117] by T. Berning *et al.*, in which using semi-empirical formulation, present a computational model for a three-dimensional PEM cell that contemplates the whole cell with the MEA and the GDL flow channels. Except the phase change, the model includes all the most important transport phenomena. The software used to develop the model is the CFX-4.3. The model is compared with the results of the model proposed by J.S. Yi *et al.* in [118]. Later, in [119], present a parametric study using the same model, with which the effect of the temperature and pressure of the gases on the efficiency of the cell is studied. The simulation results are compared with the experimental results of the work presented by A. Parthasarathy *et al.* [120].

In [121], S. Mazumder *et al.* present a three-dimensional model including the phase change as an equilibrium process. The transport of liquid water is determined by pressure, surface tension, gravity and electro-osmotic resistance. The results show that the inclusion of liquid water transport greatly improves the predictive capacity of the model. The results of the model are compared with the experimental results of the work presented by E.A. Ticianelli *et al.* [73].

L. Pei-Wen *et al.* present in [122] a three-dimensional model for a PEM cell in which authors simultaneously solve the mass / heat transfer processes and the electrochemical reactions by means of the SIMPLE algorithm. In addition, the latent heat of steam condensation in the cathode channel and the effect of heat conduction on bipolar plates is contemplated. The model is used to predict the efficiency of the cell as a function of the humidity of the anode gas. The simulation results are compared with the

model developed by Springer *et al.* [24]. In [123], P.T. Nguyen *et al.* propose a model for a PEM cell in three dimensions developed in CFX-4.3, in which a new algorithm that relates the voltage and current to calculate the local activation fields is developed. The coupling of the local activation overpotential distribution and the reactant concentration allows them to predict the local current density distribution with greater precision. The model is validated with the experimental results presented by L. Wang *et al.* [124].

In [125], B.R. Sivertsen *et al.* develop a three-dimensional model using Fluent 6.1. The model is very complete and is used to predict the concentration of species, the convective and diffusive transport, the ionic and electrical potential, the local overpotential distribution and the maximum current densities of a PEM cell. The model is validated with the experimental results presented by L. Wang *et al.* [124]. H. Ju *et al.* present in [126] a two-phase three-dimensional model to study the efficiency, current density and temperature gradients of a PEM cell. Authors use the Star-CD software with UDFs (User Defined Functions). The model consists of 140,000 elements and is solved using a single PC (2 GHz) in 3-4 h.

Y. Wang *et al.* study in [127] the two-phase flow in a non-isothermal model using a multiphase mixture formulation. Authors represent the saturation of water in liquid phase, velocity fields and temperature gradients. For the development of the model, FLUENT software and the SIMPLE algorithm together with user-defined coding are used. The computational domain of straight channel consists of 120,000 elements of mesh and the results are verified on the balance of species, requiring an imbalance lower than 1% and residues of equations less than 10^{-6}. Subsequently, in [128] they publish a large-scale analysis for a non-isothermal single-phase model with a detailed 200 cm^2 MEA. Authors use more than 23 million computational elements, requiring 600 iterations with a global mass balance of less than 1% and residues of the equation of species less than 10^{-6}. The calculations are made with FLUENT, the SIMPLEC algorithm and the parallel computation method based on AMG (Auxiliary algebraic Multigrid). The problem was solved using a PC-cluster in approximately 20 h (2.8 GHz Pentium IV, 1 GB DDRRAM). G. Hu *et al.* present in [129] a three-dimensional model to describe the transient process and dynamic characteristics of a 25.32 cm^2 PEM cell with a serpentine-shaped fluid channel. The model consists of 170,560 elements, is developed in Fluent and is solved with the SIMPLE algorithm and UDFs. The step time used in the simulation is 0.02s.

F. Mueller *et al.* present in [130] a model of a quasi-three-dimensional PEM cell developed in MATLAB/Simulink environment and using semi-empirical formulation. The model is based on the discretization of the cell in control volumes (FVM) and is validated with the experimental results of a 25 cm^2 PEM cell that uses a Nafion 112 type membrane. The dynamic model is proposed as a candidate to be used to develop strategies for PEM battery control. In [58], R. Maher *et al.* propose a 3D model that is able to accurately calculate the local activation overpotentials, which result in a better prediction of the local current distribution. Authors perform a parametric sweep to study the effect of temperature, pressure, stoichiometry, depth of gas channels, thickness, porosity and conductivity of the GDL and the thickness of the membrane on the behavior of the stack. The

new methodology presented is proposed as a computer-assisted tool designed to optimize high-power fuel cells. The results obtained are contrasted with the experimental data presented by L. Wang *et al.* [124].

Y. Wang *et al.* present in [131] a combined model of two and three dimensions aimed at studying the dynamics of dehydration of the GDL and its impact on the efficiency of a PEM cell. Authors use the Fluent software together with the FLOOR algorithm to solve the model. The step time used for the simulations is 0.1s. In [132], K. Jiao *et al.* propose a multiphase model to study the cold start processes in PEMFCs. The model is developed in Ansys Fluent environment and includes the water freezing in the membrane, the non-equilibrium mass transfer between the water in the ionomer and the water in the pore region of the CL, and the water freezing and melting in the CL and GDL. A starting at different subzero temperatures (-10 ºC, failed cold start; -3 ºC, successful cold start) is simulated and obtained results are compared to experimental data published in [133] showing good agreement with the model predictions. Authors conclude that water production rate is higher than the water diffusion rate in the ionomer due to the low diffusivity at subzero temperatures, thus increasing the ionomer fraction in the cathode CL has more significant effects than increasing the thickness of the membrane in reducing the amount of ice formation. Subsequently, same authors present in [134] an in-depth study in which cold starting is analyzed at various operating and initial conditions, considering cell voltages, initial water contents and distributions, anode inlet RH, surrounding heat transfer coefficients, and cell temperatures. Authors found that the heating-up time can be significantly reduced by decreasing the cell voltage and conclude that an effective purge is critical for PEMFC cold start.

H. Wu *et al.* present in [135] a 3D non-isothermal model that fully couples multi-species and multi-phase transport, electrochemical kinetics, and heat transfer processes. The model is aimed at studying the effect of non-equilibrium phase transfer and is developed based in FVM using Fluent 6.3.26. The validation is carried out using experimental data from [136]. Obtained results show that compared to the liquid production modeling the dynamic response of PEM fuel cells in vapor production modeling is significantly overestimated owing to the sluggish condensation process. H. Heidary *et al.* propose in [137] a 3D, multiphase, non-isothermal model of a single 9-layer counter-flow PEM fuel cell to analyze the effect of in-line and staggered blockages in parallel flowfield channels. The model is developed in Ansys Fluent environment using the SIMPLE algorithm and is validated using previously published results in [138]. Authors conclude that blockages cause higher y-direction velocity to produce better heat transfer and that blockages improve performance, with the staggered configuration being better than in-line and baseline cases.

In [139], Y.T. Mu *et al.* present a non-isothermal 3D transient two-fluid model to investigate water removal processes in a PEMFC during the gas purging prior to its shutdown. The dryness in the sub-regions of the PEMFC and the effects of the operation conditions (such as the gas flow rate, RH and temperature) are explored. The model is developed in Ansys Fluent environment using UDFs and is validated using experimental data from [140] and numerical results from [141]. Authors conclude

that effective gas purge protocols can be established by engineering material properties or purge conditions that enhances water vapor diffusion.

In [142], S.M. Rahgoshay *et al.* present a 3D non-isothermal model to study the cooling flow fields effect on PEMFC performance. Authors compare the results obtained with cooling flow fields and without cooling flow field (isothermal). Results show that the serpentine cooling flow field compared with parallel one, has better cooling performance and that the coupling effect of temperature distribution on the catalyst surface leads to results closer to the real conditions. In the same research line, M. Ghasemi *et al.* propose in [143] a 3D model also to numerically study the cooling flow fields effect on PEMFC performance. In this case, authors compare six configurations for the flow fields: conventional serpentine, typical multi-pass serpentine, typical serpentine, parallel-serpentine, conventional spiral and conventional parallel. Authors conclude that conventional spiral flow fields have the lowest IUT (Index of Uniform Temperature). In both works, the obtained models were validated using experimentally obtained data presented in [144]. M.A. Akbar *et al.* propose in [145] a 3D, non-isothermal and parallel flow model to study reactants distribution, current density and final power in PEMFCs for various square tubular configurations: simple, DPIE (Double Parallel Intermediate Electrode), DBIE (double bisectors intermediate electrode) and TPIE (triple parallel intermediate electrode). The model is developed in Ansys Fluent 14 environment using SIMPLE algorithm and is validated using experimental data from [124]. Authors conclude that DPIE configuration show better performance compared to the DBIE and that adding more than one intermediate electrode layer decreases the net output power.

J.C. Kurnia *et al.* propose in [146] a model developed in Ansys Fluent to study the performance of a PEM fuel cell stack with variable inlet flows under simulated driving cycle conditions. In the study, six cases representing possible scenarios for dynamic inlet flow conditions are evaluated: steady inlet flows, all inlet flows vary, anode inlet flow varies, cathode inlet flow varies, anode-cathode inlet flow varies, and coolant inlet flow varies. Authors found that the highest gross power density is achieved with steady inlet flows. On the other hand, when all inlet flows vary, it results in the highest net power over the entire driving cycle time and has comparable thermal, water and gas management with the steady inlet flow case. In [147], E.E. Kahveci *et al.* also present a 3D single-phase model to investigate the performance of PEMFCs. The model is developed in Ansys Fluent and is validated with the experimental results presented in [124]. Among others, authors show the effect of humidification and cell temperature on the power density of the fuel cell. It is concluded that increasing oxygen flow rate does not cause a significant change in the performance and that maximum power density is reached at 0.6 GDL porosity, RHa = 100% and 3 atm pressure.

In [148], S. Li *et al.* present a 3D, non-isothermal, two-phase flow mathematical model to study the effects of agglomerate model parameters on transport characterization and performance of PEM fuel cells. From this work, it is concluded that current density is greatly improved when the agglomerate radius is decreased and the volume fraction is increased. Later, same authors present in [149] a 3D, non-isothermal, two-phase flow mathematical model to investigate the effect of the GDL deformation on transport phenomena and performance of PEM fuel cells with interdigitated flow fields. Authors found that the thickness and porosity of

GDLs are decreased due to the deformation and that the cell performance is improved but with a high pressure drop penalty. Both models are developed using Ansys Fluent 16.2 and UDS (User Defined Scalar) equations and are validated using experimental data published in [150].

M. Abdollahzadeh *et al.* propose in [151] a 3D multiphase model to investigate the steady polarization curves and long-term stability of a poisoned PEM cell, as well as evaluate the performance of various commercial GDLs. The model is developed in Ansys Fluent environment and considers the electrochemical and transport mechanisms in catalyst layers and the membrane and includes: full description of mass, charge and thermal energy transport equations in the multi-phase system, the non-equilibrium mass transfer between the ionomer and the water (vapor, liquid), the full kinetic models for CO poisoning and mass-diffusion limitations in the catalyst layer. The model developed is validated using experimental data from a 25 cm^2 PEM cell, as well as reported data from [152] and [153]. Authors conclude that even low CO concentration in the anode fuel, leads to a considerable degradation of the fuel cell output current density. Besides, Among the tested gas diffusion layers, results showed that the ones with the highest thickness presented worst performance of the PEMFC. Additionally, results showed, that high tortuosity and low contact angle (hydrophobicity) of the gas diffusion layer, decreases the performance of the PEM cell.

4.5. Summary of models for the electrical and thermal study of PEMFCs

Table 2 shows a summary of the models for the electrical and thermal study of LT (Low Temperature) PEMFC systems. The papers presented are classified in chronological order. In the table presented, the dimension D (0D, 1D, 2D and 3D), modeling technique (theoretical, semi-empirical and empirical), state (stationary or transient), purpose, software/method used and system or data used for validation or comparison for each proposed model is shown.

Table 2. Summary of models for electrical and thermal study of PEMFCs.

Ref.	Year	D	Modeling technique	State	Purpose	Software/ method	Validation/ Comparison
[95]	1989	2D	Theoretical Non-linear equations	Stationary	Design tool for the development of PEM-type cell humidification systems	Runge-kutta Newton Raphson Algorithm	PEM cell
[96]	1993	2D	Theoretical Non-linear equations	Stationary	Investigate several membrane humidification techniques	Newton Raphson Algorithm	PEM cell
[97]	1993	2D	Theoretical Non-linear equations	Stationary	Identify the amount of heat that needs to be extracted from the fuel cell		PEM cell
[71]	1996	1D	Semi-empirical Non-linear equations	Stationary/ Transient	Prediction of electrical and thermal behavior in static regime and with variations in the load		Ballard Mark V (5 kW)
[98]	1998	2D	Semi-empirical Non-linear equations	Stationary/ Transient	To model a MEA and apply it to large-scale systems		Stack of 125 cells (MEA 350 cm^2)

[101]	1998	2D	Semi-empirical FEM	Stationary	Study the distribution of oxygen and water vapor in the GDL for various current densities. Study the water content in the membrane	SIMPLE Algorithm	Comparison with [73]
[72]	2001	1D	Semi-empirical Non-linear equations	Stationary	Investigate the effect of design and operating conditions on cell efficiency, thermal response and water management	BAND(J) Newman Algorithm	Comparison with [73]-[74].
[75]	2002	1D	Theoretical Non-linear equations	Stationary	Test the effects of temperature and pressure variation on the fuel cell	Iterative algorithm with sub-relaxation	Comparison with [76]
[117]	2002	3D	Semi-empirical FEM	Stationary	Emulate all transport phenomena of a PEM cell (without phase change)	CFX-4.3 (AEA Technology)	Comparison with [118]
[119]	2003	3D	Semi-empirical FEM	Stationary	Verify the effects of the temperature and pressure of the gases on the efficiency of the cell by means of parametric study	CFX-4.3	Comparison with [120]
[121]	2003	3D	Semi-empirical FEM	Stationary	Improve prediction of water transport in a PEM cell	Software CFD (generic)	Comparison with [73]
[122]	2003	3D	Semi-empirical FEM	Stationary	Predict the efficiency of the cell as a function of the humidity of the anode gas	SIMPLE Algorithm	Comparison with [24]
[51]	2004	0D	Semi-empirical Non-linear equations	Stationary	Predict the effects of temperature, pressure, cell voltage and stoichiometry on the efficiency of the PEMFC		PEMFC of 10 kW
[78]	2004	1D	Semi-empirical Non-linear equations	Stationary	Use for real-time control in automotive or stationary applications	MATLAB/ Simulink (OD23S)	Comparison with [71]
[50]	2004	0D	Empirical Non-linear equations	Stationary	Provide a replicable model to other PEMFC and PEM type electrolyzers	MATLAB/ Simulink	PEMFC of 4 kW
[123]	2004	3D	Semi-empirical FEM	Stationary	Predict local current distributions accurately	CFX-4.3	Comparison with [124]
[102]	2004	2D	Semi-empirical FEM	Stationary	Emulate the current density in the active layer of the cathode considering agglomerated materials	COMSOL Multiphysics (FEMLAB 2.3)	Segmented PEM cell
[103]	2005	2D	Semi-empirical FEM	Stationary	Study the effect of contact resistances between cell components and the effect of different capillary pressures	COMSOL Multiphysics (FEMLAB 2.3)	Comparison with [102]
[126]	2005	3D	Semi-empirical FEM	Stationary	Study the efficiency, current density and temperature gradients in a PEM cell	Start-CD	Comparison with results calculated theoretically
[125]	2005	3D	Semi-empirical FEM	Stationary	Predict the concentration of species, convective and diffusive transport, ionic and electric potential, local overpotential distribution and maximum current densities	Ansys Fluent 6.1	Comparison with [124]
[52]	2005	0D	Empirical Electrical circuit	Stationary/ Transient	Characterize the stationary and transitory regime of a PEMFC	MATLAB C code	Nexa Ballard of 1,2 kW
[79]	2005	1D	Semi-empirical Non-linear equations	Stationary/ Transient	Predict the behavior of the cell during variations in the load. Special emphasis on thermal response		Parameters presented in [80], [81].
[82]	2005	1D	Empirical Electrical circuit	Stationary/ Transient	Use in external PEMFC controllers	MATLAB/ Simulink and Pspice	PEMFC Avista Labs SR-12, 500 W

[54]	2005	0D	Empirical Electrical circuit	Stationary/ Transient	Characterize the dynamic behavior during the cold start and the evolution of the temperature.	Pspice	Nexa Ballard 1,2 kW
[83]	2005	1D	Theoretical Non-linear equations	Stationary	Determine the local entropy rate in a PEM cell	MATLAB 6.0.088	Nafion 115-based membrane cell
[127]	2006	3D	Semi-empirical FEM	Stationary	Study the phenomena of transport, saturation of the liquid phase of water, fields of velocities and temperature gradients.	Ansys Fluent 6.0.1.2 SIMPLE Algorithm	Validation considering balance of species
[104]	2006	2D	Theoretical FEM	Stationary	Study heat and mass transfer on the cathode side of a PEM cell	CFX SIMPLEC Algorithm	Validation considering local Nusselt numbers
[128]	2006	3D	Semi-empirical FEM	Stationary	Large-scale study of a 200 cm^2 MEA	Ansys Fluent 6.0.1.2 SIMPLE Algorithm	200 cm^2 MEA
[84]	2006	1D	Semi-empirical Non-linear equations	Stationary	Compare the thermal and non-isothermal effects on the behavior of water transport in the cell		Nafion 112-based PEM cell
[105]	2006	2D	Theoretical FEM	Stationary	Characterize electrochemical behavior and heat transfer in a coupled manner	Newton Raphson Algorithm and Gaussian elimination	Comparison with [106]
[53]	2006	0D	Empirical ANN	Stationary/ Transient	Update the proposed model in [52] implementing the dynamics of the PEMFC by using ANNs	DSpace	Nexa Ballard 1,2 kW (Comparison with [52])
[55]	2006	0D	Empirical Electrical circuit	Stationary/ Transient	Emulate the dynamic behavior of the Nexa Ballard 1.2 kW by means of the internal equivalent resistance		Nexa Ballard 1,2 kW
[107]	2006	2D	Semi-empirical FEM	Stationary	Oriented to simulate PEM cells with conventional and interdigitated gas distributors	MUFTE_UG	Célula PEM con electrodo ELAT-DS de E-TEK inc.
[129]	2007	3D	Theoretical FEM	Transient	Describe the transient process and the dynamic characteristics of a PEM cell with a fluid channel in the form of a coil.	Ansys Fluent and SIMPLE Algorithm	21,32 cm^2 PEM cell
[130]	2007	~ 3D	Semi-empirical Non-linear equations	Stationary/ Transient	Oriented to apply control strategies in PEM-based stacks	MATLAB/ Simulink	Nafion 112-based 25 cm^2 PEM cell
[58]	2007	3D	Semi-empirical FEM	Stationary	Use as a computer-assisted tool to optimize fuel cells with high power density and lower cost	Software CFD	Comparison with [124]
[108]	2007	2D	Semi-empirical FEM	Stationary/ Transient	Study the dynamic characteristics of the cell and the influence of the width of the membrane on the efficiency	COMSOL Multiphysics	Nafion 117-based PEM cell
[109]	2007	2D	Semi-empirical FEM	Stationary	Investigate the behavior of a PEM cell that runs on hydrogen fed at the anode and air supplied by natural convection at the cathode	Ansys Fluent	Comparison with [110]
[111]	2007	2D	Semi-empirical FEM	Stationary	Study the respiration of a PEM cell under atmospheric conditions of 23 °C and 20% of RH.	Ansys Fluent	6 cm^2 PEM cell
[112]	2007	2D	Theoretical FEM	Transient	Study the effects of liquid water transport and heat transfer phenomena on the transient responses of a PEM cell during a change in cell voltage	Ansys Fluent	PEM cell
[131]	2007	2D 3D	Semi-empirical FEM	Stationary/ Transient	Study of the dynamics of GDL dehydration and its impact on the efficiency of a PEM cell	Ansys Fluent 6.0.12 PISO Algorithm	Comparison with [104]

[85]	2008	1D	Semi-empirical Non-linear equations	Stationary/ Transient	Study the effect of water variation (two phases) and heat to variable loads on the behavior of the stack		PEMFC of 80 W composed of two cells of 140 cm^2
[86]	2008	1D	Semi-empirical FEM	Stationary	Investigate the effects of hydrogen sulfide contaminant on performance of PEMFCs	COMSOL Multiphysics	Comparison with [87]
[56]	2009	0D	Semi-empirical Non-linear equations	Stationary	Study the effect of stoichiometry, temperature, pressure and air on the exergetic efficiency and irreversibilities of a PEM cell		25 cm^2 PEM cell
[132]	2009	3D	Semi-empirical FVM	Transient	Study the cold start processes in PEMFCs	Ansys Fluent 6.3 UDFs PISO Algorithm	Comparison with [133]
[88]	2010	1D	Empirical ANN	Transient	Characterize the nonlinear dynamic behavior of a PEMFC	MATLAB R2008a	PEMFC of 1,5 kW composed of 28 cells of 232 cm^2
[89]	2010	1D	Semi-empirical Non-linear equations	Stationary/ Transient	Study the dynamic response of the PEMFC to variations in the load	MATLAB/ Simulink	SR-12 Ballard Mark V BCS-500
[57]	2010	0D	Semi-empirical Non-linear equations	Stationary	Study of the effect of temperature, pressure, stoichiometry, thickness of the membrane and thickness of the gas diffusion layer on the behavior of a PEM cell	MATLAB	Comparison with [58]
[59]	2010	0D	Semi-empirical Non-linear equations	Stationary/ Transient	Oriented to characterize the slow transient response of a PEMFC.	Excel Runge-Kutta of order 4	Nexa Ballard 1,2 kW
[135]	2010	3D	Semi-empirical FVM	Stationary/ Transient	Study the effect of non-equilibrium phase transfer	Ansys Fluent 6.3.26	Experimental results presented in [136].
[90]	2013	1D	Semi-empirical Electrical circuit	Transient	Study of the behavior of a PEM cell in non-isothermal and transitory conditions	Mathcad	Comparison with [91]
[60]	2014	0D	Empirical Electrical circuit	Transient	Oriented to apply control techniques on the air subsystem (oxygen stoichiometry and cathode pressure)	MATLAB/ Simulink	PEMFC of 5 kW composed of 80 cells
[61]	2014	0D	Empirical Electrical circuit	Stationary/ Transient	Emulate the stationary and transient behavior of a micro-grid formed by 4 PEMFC	MATLAB/ Simulink	Nexa Ballard 1,2 kW
[62]	2015	0D	Empirical Non-linear equations	Stationary/ Transient	Experimental methodology Identify up to 18 parameters of the model experimentally	MATLAB fourth-order Runge-Kutta method	Nexa Ballard 1,2 kW
[92]	2015	1D	Semi-empirical Non-linear equations	Stationary/ Transient	Oriented to develop a method to evaluate the reliability of a PEMFC	Modelica-Dymola	220 cm^2 PEM cell manufactured by CEA LITEN
[113]	2015	2D	Semi-empirical FVM	Transient	Study the effect of permeability on the dynamic field in the PEM fuel cell	FVM-based software	Generic PEM cell
[63]	2016	0D	Semi-empirical Non-linear equations	Transient	Investigate the temperature effect on performance of dead-end cascade PEMFC stack with integrated humidifier and separator. Model suitable for system identification and control purposes.	Fourth-order Runge-Kutta method	PEMFC stack composed of 4 cells of 225 cm^2

[93]	2016	1D	Semi-empirical Non-linear equations	Stationary	Emulate the cell voltage and the water content in the membrane (new validation technique based on neutron images)	EES 9.705-3D	50 cm^2 PEM cell
[94]	2016	1D	Semi-empirical Non-linear equations	Stationary	Emulate static behavior at stack level	EES 9.705-3D	50 cm^2 PEM cell
[137]	2017	3D	Semi-empirical FVM	Stationary	Investigate the effect of a blockage in the flowfield channel of a PEM fuel cell on mass transfer of reactant gas from the channel into the catalyst layer	Ansys Fluent SIMPLE Algorithm	Previously published results in [138]
[64]	2017	0D	Empirical ANN	Stationary/ Transient	Emulate the hydrogen consumption and temperature as a function of the electrical and thermal load	MATLAB/Simulink	PEMFC of 600 W
[139]	2017	3D	Semi-empirical FVM	Transient	Investigate the water removal processes in a PEMFC during the gas purging prior to its shutdown	Ansys Fluent and UDS equations	Validated using experimental data [140] and numerical data [141]
[66]	2017	0D	Semi-empirical Non-linear equations	Stationary	Apply a multi-objective optimization algorithm (MOEA/D) aimed at maximizing the energy efficiency of the system		PEMFC of 5 kW composed of 75 cells
[142]	2017	3D	Theoretical FVM	Stationary	Study the cooling flow fields effect on PEMFC performance	Ansys Fluent	PEM cell presented in [144]
[67]	2017	0D	Empirical Fuzzy logic	Transient	Determine de behavior of a fuel cell electric bicycle system	Fuzzy Cognitive Map Rule-based FCM	22 cell air-cooled stack of 250 W
[143]	2017	3D	Theoretical FVM	Stationary	Study the cooling flow fields effect on PEMFC performance	Ansys Fluent	PEM cell presented in [144]
[145]	2017	3D	Semi-empirical FVM	Stationary	Study reactants distribution, current density and final power in PEMFCs for four square tubular configurations (simple, DPIE, DBIE and TPIE)	Ansys Fluent 14 SIMPLE algorithm	Validated using data reported in [124]
[146]	2017	3D	Semi-empirical FVM	Stationary/ Transient	Evaluate the performance of a PEM fuel cell stack with variable inlet flows under simulated driving cycle conditions	Ansys Fluent 15 UDFs Scalars in C code	PEMFC of 320 cells and 1,600 cm^2 of active catalyst area
[65]	2018	0D	Theoretical FEM Empirical ANN	Stationary/ Transient	Provide a tool to develop new optimization strategies in real time applications	COMSOL Multiphysics MATLAB/Simulink	PEMFC of 600 W
[68]	2018	0D	Semi-empirical Non-linear equations	Transient	Apply a multivariable model predictive control (MPC) strategies for PEM fuel cells.	gPROMS software	6 W PEM cell
[147]	2018	3D	Semi-empirical FVM	Stationary	Investigate the performance of a PEMFC.	Ansys Fluent 16.2	Validated using data reported in [124]
[148]	2018	3D	Semi-empirical FVM	Stationary	Study the effects of agglomerate model parameters on transport characterization and performance of PEM fuel cells	Ansys Fluent and UDS equations	Validated using data reported in [150]

[114]	2018	2D	Semi-empirical FEM	Stationary	Investigate the competition between current collection and oxygen supply. Used for rib/channel design.	COMSOL Multiphysics	Comparison with results from AutoStack-CORE project [115]
[69]	2018	0D	Semi-empirical Non-linear equations	Stationary/ Transient	Develop a dynamic scalable segmented model of PEMFC systems with two-phase water flow	MATLAB/Simulink Simscape	
[151]	2018	3D	Semi-empirical FVM	Stationary	Investigate the steady polarization curves and long-term stability of poisoned PEMFC, as well as evaluate the performance of various commercial GDLs.	Ansys Fluent and UDF equations	Validated using data reported in [152] and [153] and a 25 cm^2 PEM cell
[149]	2018	3D	Semi-empirical FVM	Stationary	Determine the effects of GDL deformation and obtain the transport characteristics in PEMFCs with interdigitated flow fields	Ansys Fluent and UDS equations	Validated using data reported in [150]
[70]	2018	0D	Semi-empirical Non-linear equations	Stationary/ Transient	Develop a Nonlinear multivariable sliding mode control for a reversible PEM fuel cell integrated system	MATLAB/Simulink	PEMFC composed of 35 cells
[116]	2018	2D	Semi-empirical FEM	Stationary	Investigate the reactant gas crossover effect in a PEM cell	FreeMem++	PEM cell

5. Opportunities to improve energy efficiency through new model developments

An important aspect when modeling a PEMFC system is that the developed model must contemplate the effect that temperature has on the efficiency of the system. In this context, it would be interesting if models would consider the electrical and thermal behavior of the PEMFC emulate as precisely as possible the effect that temperature has on the speed at which the electrochemical reactions occur. Since the operating temperature is directly related to the amount of heat extracted through the cooling circuit, a key aspect to keep into account is that the model has to consider the thermal management of the system. In this sense, among all research works that can be found in the current literature, only a small group of them focuses on models that include the thermal management of the system through the refrigeration circuit. However, most models that include in detail the effect of heat extraction through the cooling system are developed by a complex formulation, which does not allow to use the model to evaluate real-time control strategies or optimization strategies, for which a very reduced calculation time is required.

Considering all mentioned above, the need to develop zero-dimensional models of PEMFC that contemplate the regulation of the flow rate of the cooling fluid as an input variable to the model is detected. This will allow to establish the optimal reference of electrical and thermal production of the fuel cell in order to maximize the electrical efficiency of the system and to minimize the production costs. This aspect is especially important if it is considered that a PEMFC could operate connected to the power grid and that other auxiliary electrical and / or thermal generation devices could be integrated with the PEMFC in a microgrid. In this way, the model developed could be used to predict the behavior of the system in different situations (for predicted electrical and thermal load profiles), which in turn will allow establishing the optimum operating reference that maximizes efficiency and

minimizes operating costs. of the system based on the hourly prices of electricity, prices of the fuels used by other generators, as well as all the operation and maintenance costs of all the devices

6. Conclusions

In this paper the general modeling aspects of the PEMFCs have been introduced. Likewise, a search was made of the state of the art of the PEMFC models that emulate in a coupled manner the thermal and electrical behavior, at cell and stack levels, contemplating a total of 78 research works. It has been possible to verify how approximately 80% of the models developed in the last 5 years (2014-2018) correspond to zero-dimensional and three-dimensional models, practically in the same proportion.

Due to the existing computational capacity, it has been proven how simulations with PEMFC models are becoming more complex and exigent and include a high level of detail. In this sense, the global modeling of PEMFC has evolved from steady to dynamic, from one-dimensional to complex three-dimensional models, from isothermal to non-isothermal, from single-phase to multi-phase and recently from straight channels to field structures with more complex flow, such as serpentine or interdigitated flow fields.

It has been detected that, to use a PEMFC model in real-time control or optimization strategies, it is usually necessary to resort to zero-dimensional system models to avoid the high computational cost involved in the inclusion of details and phenomena that occur at a microscopic level inside a PEM cell. In this sense, it has been detected that MATLAB is the most used engineering tool by the research community in terms of modeling PEMFCs in zero dimensions. In terms of multidimensional modeling, Ansys Fluent (based on FVM) has been shown as the most widely used multiphysics software, followed by COMSOL Multiphysics (based on FEM).

In the context of zero-dimensional systemic modeling, the modeling approach based on empirical techniques has been more widely used, due to the good relationship between simplicity and precision that it provides. Among these techniques, the identification of parameters through EIS and their subsequent implementation using equivalent electrical circuits has been shown as one of the most suitable alternatives to emulate the dynamic characteristics of the electrical behavior of the PEMFCs. However, to contemplate the coupled behavior, electrical and thermal, it has been found that artificial intelligence based on ANNs show a great potential in the modeling of these electrochemical devices of a highly non-linear character.

Finally, it has been verified that, among all the models that have been identified in the scope of the application of operation and optimization strategies, the works that have considered the flow of the refrigerant as a control variable from the point of view of energy efficiency are very limited. Since the operating temperature of the PEMFC is directly related to the efficiency of the stack, and which in turn, the operating temperature is related to the amount of heat extracted from the PEMFC, it is detected the need to implement optimization strategies to control PEMFC systems that will take the regulation of the cooling flow as a control variable to maximize the electrical and thermal efficiency of the system. In addition to the efficiency of the system, the

optimization strategy could be implemented as a multi-objective strategy that would contemplate the minimization of operating and maintenance costs and harmful emissions.

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