Development of a Mathematical Model for Proton Exchange Membrane Fuel Cells (PEMFCs)

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Abstract. This paper presents the development and validation of a mathematical model for Proton Exchange Membrane Fuel Cells (PEMFCs). The approach developed herein uses both static and dynamic modeling to represent PEMFC performance under different conditions. These include variations in load current, gas pressure, and temperature. The model was built in MATLAB and tested with experimental data from the BAHIA test bench. The results confirm its accuracy in both steady and changing states. The model was also compared with other approaches, such as the MATLAB PEMFC model and the Energetic Macroscopic Representation (EMR) framework. Findings show that the model can predict important electrochemical and physical processes with precision. It also gives useful insights into PEMFC performance and optimization. This work presents a reliable future basis for advanced PEMFC performance studies and emulator development.

1 Introduction

The shift to sustainable energy increases the need for alternatives to fossil fuels. Proton Exchange Membrane Fuel Cells (PEMFCs) are seen as a strong candidate. They are efficient and cause less harm to the environment. A recent review [1] stresses the growing role of PEMFC technology. It also notes their many uses and the need for more research to improve their performance.

PEMFCs create electricity through a reaction between hydrogen and oxygen. This reaction also produces water and heat. For this reason, PEMFCs are viewed as environmentally friendly. As noted in [2], PEMFCs work by splitting hydrogen at the anode. This produces protons and electrons. The protons pass through the membrane. The electrons move through an external circuit and generate an electric current. This

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process is simple but efficient. It forms the core of PEMFC operation. Their flexible and modular design allows them to be adjusted for different power needs. Because of this, PEMFCs are used in many areas. These include stationary power systems, mobile applications, and portable devices [2, 6].

To study PEMFC performance, accurate models are needed. These models also help improve efficiency under different conditions. The model in [7] is based on electrochemical processes. It is designed to support automation. In [9], a dynamic model is introduced to improve energy conversion. Other studies [8, 10] focus on challenges such as water control and heat management. Integrated models, like those in [12], combine electrochemical and thermal aspects. They improve the simulation and prediction of system behavior. This applies to both transient and steady-state conditions. Such models also reduce costs in design and testing. They can simulate many operating situations, such as changes in load current, gas pressure, and temperature [13, 14].

This study introduces a mathematical model for PEMFCs built in MATLAB. The model describes both static and dynamic behavior. It is validated with experimental data from the BAHIA test bench. Its accuracy is checked by comparing it with other models. These include the MATLAB generic PEMFC model and the Energetic Macroscopic Representation (EMR) framework. The results confirm that the model is reliable. They also show its potential to improve PEMFC performance. These findings also strengthen the role of fuel cell systems in sustainable energy solutions.

The remainder of this paper is structured as follows: Section 2 details the model development, Section 3 explains the experimental setup and validation methodology, Section 4 presents the results and analysis, and Section 5 concludes with key findings and suggestions for future research directions.

2 Comprehensive Mathematical Model For PEMFC

This section presents a mathematical model for PEMFCs, combining electrochemical, thermal, and mass transport dynamics. The model integrates key governing equations to simulate PEMFC performance under various operating conditions.

2.1 Electrochemical Model

The PEMFC output voltage V_{cell} is defined by the following equation (1):

$$V_{FC} = E_{nerst} - V_{act} - V_{ohmic} - V_{con} \tag{1}$$

2.1.1 Nernst Potential

This term represents the theoretical maximum voltage of the cell, depending on the temperature and partial pressures of hydrogen and oxygen. It is calculated as:

$$E_{nerst} = E_0 + \frac{RT}{2F} ln\left(\frac{P_{H_2}\sqrt{P_{O_2}}}{P_{H_2O}}\right) \tag{2}$$

The partial pressures are adjusted based on stoichiometry and reactant utilization.

2.1.2 Activation Losses

These losses arise from the slow reaction kinetics at the electrodes, particularly at low current densities. They are modeled using the Tafel equation:

$$V_{act} = \frac{RT}{\alpha F}\ln\left(\frac{J}{J_0}\right) \tag{3}$$

J_0 is the exchange current density, which reflects the activity of the catalyst.

2.1.3 Ohmic Losses:

Ohmic losses result from the resistance to ion flow in the membrane and electron flow in the electrodes. They are given by:

$$V_{ohmic} = iR_m \tag{4}$$

The membrane resistance (R_m) depends on membrane thickness, conductivity, and temperature:

$$R_m = \frac{t_m}{\sigma_m}\ ,\ \sigma_m = \sigma_m^0 exp(-\frac{E_\sigma}{RT}) \tag{5}$$

2.1.4 Ohmic Losses:

Concentration losses occur due to mass transport limitations at high current densities, where reactant supply to the electrodes becomes insufficient. They are expressed as:

$$\mathbf{V}_{\mathrm{concentration}} = -\frac{\mathrm{RT}}{\mathrm{F}}\ln\left(1-\frac{\mathrm{J}}{\mathrm{j_{lim}}}\right) \tag{6}$$

The limiting current density (j_{lim}) defines the maximum current the cell can support, based on reactant diffusion rates.

2.2 Thermal Model

The thermal behavior of the fuel cell, which affects its efficiency, depends on the balance between heat generation and dissipation:

$$C_p\frac{dT}{dt} = Q_{gen} - Q_{loss} \tag{7}$$

2.2.1 Heat Generation

Heat is produced from irreversibilities in the electrochemical reactions and resistive losses:

$$Q_{gen} = J(V_{FC} - E_{nerst}) \tag{8}$$

2.2.2 Heat Loss

Heat dissipation occurs through convection and conduction:

$$Q_{loss} = hA_{cell}(T - T_{ambient}) \tag{9}$$

2.3 Mass Transport Model

Mass transport phenomena are essential for maintaining the reactant supply to the electrodes. They are modeled using stoichiometric coefficients and flow rates:

$$\dot{m}_{H_2} = \lambda_{H_2}.J \, , \dot{m}_{O_2} = \lambda_{O_2}.J. \tag{10}$$

2.4 Dynamic Model

In a PEMFC, the dynamic behavior is influenced by the charge double-layer phenomenon, where charged layers at the electrode/membrane interface store electrical energy, behaving like a capacitor. This phenomenon introduces a delay in the activation and concentration potentials as charges redistribute when the voltage changes. This delay can be modeled as a first-order system, with the time constant determined by the equivalent capacitance and resistance. Consequently, activation and concentration voltages exhibit dynamic variations with current before stabilizing at new steady-state values.

According to the recent discussed effects, the circuit model of the studied PEMFC is illustrated in Fig. 1. In this model, the resistances represent the equivalent resistance for various types of fuel cell losses.

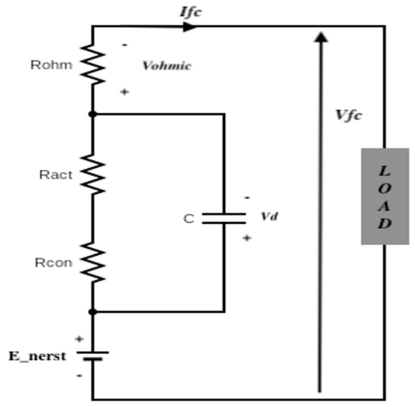

Fig. 1. Fuel cell dynamic model.

This model of fuel cell is described by:

$$\frac{dv_d}{dt} = \frac{1}{C} \times I_{FC} - \frac{1}{\tau} v_d \tag{11}$$

Where v_d represents the equivalent capacitor dynamical voltage, C is the equivalent electrical capacitance; and, τ is the fuel cell electrical time constant depending on the cell temperature given by the equation:

$$\tau = C \times (R_{act} + R_{con}) = C \times (\frac{V_{con}+V_{act}}{I_{FC}}) \qquad (12)$$

2.5 Model Limitations

This model assumes a uniform temperature and gas distribution in the stack, and does not include degradation effects such as aging or membrane drying. It is therefore most accurate for short or medium tests under stable operating conditions.

3 Materials and Methods

3.1 Experimental Setup

To validate the developed model, experiments were conducted using the BAHIA didactic bench. This platform features 24 PEMFCs with a combined maximum power output of 1.2 kW and an output voltage range of 14 to 22 V, with a nominal current of 65 A. The BAHIA bench is equipped with a Human-Machine Interface (HMI), which allows for the precise configuration of the load current and enables the monitoring of the output voltage from the fuel cell. This setup facilitates a direct comparison between the experimental data and the results predicted by the proposed model.

3.2 Simulation Tools

Simulations were conducted using MATLAB/Simulink to validate the model under consistent conditions. The tools used for this purpose include:

3.2.1 Generic MATLAB PEMFC Model:

The Simscape model gives a detailed, data-based simulation of PEMFC behavior under different operating conditions. The configuration and parameter values used in the model are shown in Table 1. Fig. 2 shows the generic MATLAB model applied for this study.

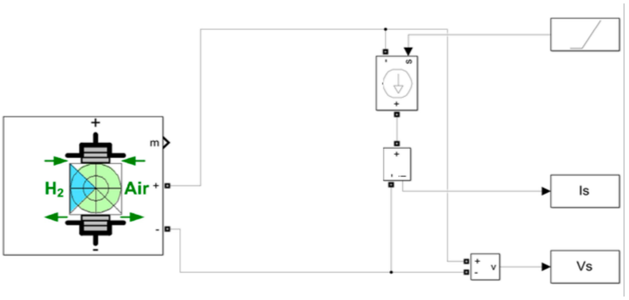

Fig. 2. The generic Simscape MATLAB/Simulink model.

Table 1. Parameters of the generic Simscape Matlab/Simulink fuel cell model

Designation	Value	Designation	Value
Voltage at 0A and 1A	V_0=22.65 V V_1=21 V	Numbers of cellule	N= 24
Nominal operating point	V_{nom}= 15 V I_{nom}=60 A	Nominal supply pressure	PO= 1 bar PH= 1.3 bar
Maximum operating point	I_{end}= 70 A V_{end}= 14.4 V	Operating temperature	T= 75 °C

3.2.2 Energy Macroscopic Representation (EMR) Framework:

The EMR method gives a dynamic view of energy flow in the PEMFC system. It also captures how the system behaves during changes. This model has been well studied in earlier research and is shown in Fig. 3.

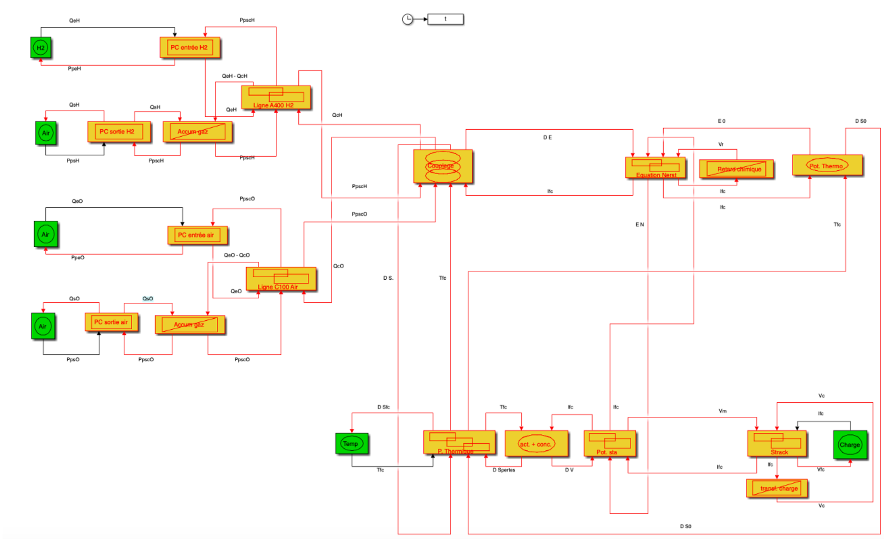

Fig. 3. EMR model of PEMFC

By aligning the operating conditions and parameters, the outputs of the simulation tools were compared with both the experimental data and the proposed mathematical model.

3.3 Validation Parameters

The validation process tested the model under both static and dynamic conditions:

- **Static Testing:** Steady-state polarization curves were compared. This was done to test how well the model predicted voltage at different current densities.
- **Dynamic Testing:** Step changes in load current were applied to see if the model could predict transient voltage responses, including effects such as the charge double-layer and thermal behavior.

The comparison of simulation and experimental results was used to confirm the model's predictive capability and to ensure its robustness under different conditions.

4 Results and Discussion

This section presents the validation of the proposed mathematical model. The analysis includes both static and dynamic behavior. It shows how accurate the model is and how well it can predict system performance.

4.1 Static Performance Analysis

The static behavior of the PEMFC was studied using polarization curves under steady-state conditions, as shown in Fig. 4. The voltage responses of the proposed model, the MATLAB generic model and the EMR model were compared with experimental data. The results show a strong match between the proposed model and the experimental data, especially at low and medium current densities. All models were able to show the three main regions of the polarization curve:

- **Activation Region:** At low current densities, the activation losses dominate, and the model accurately predicts the voltage drop due to sluggish reaction kinetics.
- **Ohmic Region:** At intermediate current densities, the voltage drop due to ohmic losses is linear and closely matches experimental data.
- **Concentration Region:** At high current densities, the proposed model accurately represents the impact of concentration losses arising from mass transport limitations.

The Root Mean Square Error (RMSE) values for each model are shown in Table 2. They confirm that the proposed model reaches a level of accuracy similar to the MATLAB generic and EMR models. The RMSE differences are small and confirm good agreement.

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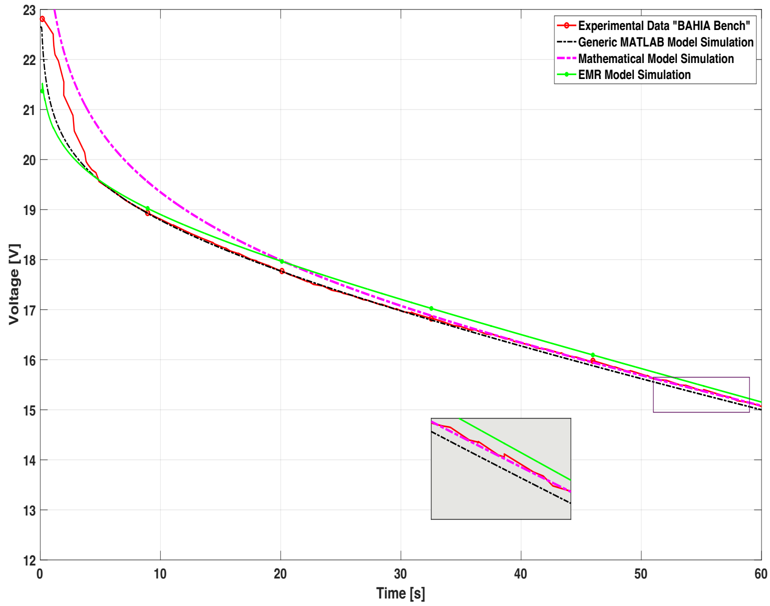

Fig. 4. Comparison of Static Voltage Response of PEMFC Models with Experimental Data

Table 2. Root Mean Square Error (RMSE) for PEMFC models compared to experimental data

Model	RMSE
MATLAB Model	0.1561
Mathematical Model	0.2078
EMR Model	0.1405

4.2 Dynamic Performance Analysis

The dynamic behavior of the PEMFC was tested by applying step changes in the load current. Fig. 5 shows the transient voltage response for the experimental data, the proposed mathematical model, and the simulations from the MATLAB generic and EMR models.

The model accurately represents dynamic phenomena, including:

- **Charge Double-Layer Effect: The** model accurately predicts the initial voltage drop and recovery, which are characteristic of the capacitive behavior at the electrode/electrolyte interfaces.
- **Thermal Effects:** The impact of temperature on the cell's dynamic response is well-represented, particularly during sustained load changes.
- **Mass Transport Delays:** The model effectively captures the transient effects caused by the delayed diffusion of reactants to the catalytic sites.

The close match between the model predictions and the experimental data confirms its reliability. It shows that the model can simulate the transient behavior of PEMFCs under practical operating conditions.

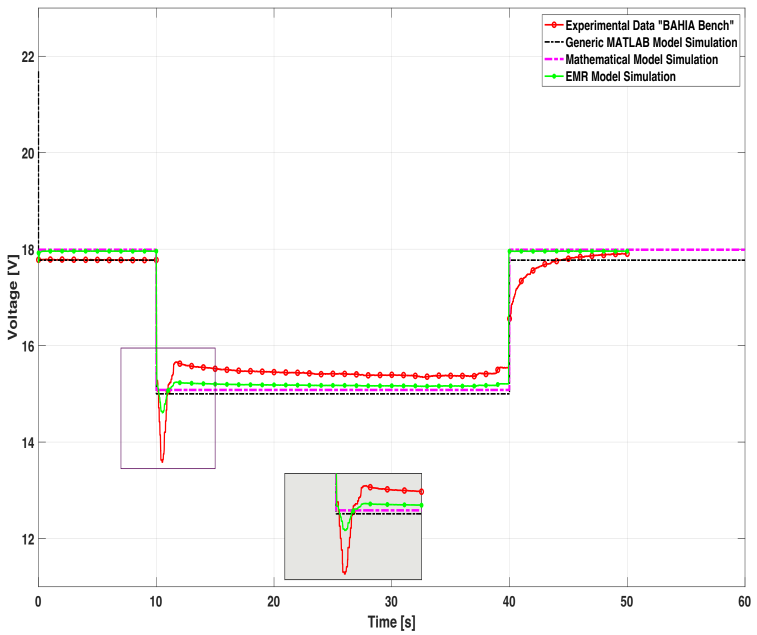

Fig. 5. Comparison of Dynamic Voltage Response of PEMFC Models with Experimental Data

The developed PEMFC mathematical model was tested against experimental data from the BAHIA test bench. It gave accurate results for both steady and changing conditions. The model captures key electrochemical and physical processes, such as voltage responses and system transitions under different operating states. Its performance was compared with the MATLAB generic PEMFC model and the Energetic Macroscopic Representation (EMR) framework. The results show very small differences and strong predictive accuracy.

The comparison shows that the model is effective as a simulation tool. It can handle complex electrochemical, thermal, and mass transport processes. The findings prove that the model is useful for improving PEMFC performance in different conditions. It can also support the design of better fuel cell systems.

5 Conclusion

This study develops and validates a detailed mathematical model for Proton Exchange Membrane Fuel Cells (PEMFCs). The model includes electrochemical, thermal, and mass transport processes and was tested with experimental data from the BAHIA test bench. Its performance was also compared with the MATLAB generic PEMFC model and the Energetic Macroscopic Representation (EMR) framework.

The results show that the model accurately predicts key performance indicators such as voltage response, polarization curves, and transient behavior. The strong agreement with both experimental and simulation data confirms its reliability and suitability for performance analysis and optimization.

This work provides a solid foundation for future studies. The model can be used for real-time emulation and control testing of PEMFC systems, particularly in vehicle and energy-storage applications. Future improvements will focus on integrating degradation effects and optimizing control strategies for long-term operation.

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