Comprehensive Coupled Electrochemical and Thermal Analysis of Proton Exchange Membrane Fuel Cells Under Dynamic Loads

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Abstract. The current work proposes a complete mathematical model of proton exchange membrane fuel cells (PEMFCs) taking into account the processes of electrophysics, thermodynamics, and transients regime. Electrochemical sub-model divides the potential difference into losses according to physical laws governing the process (activation, ohmic, and mass transfer losses). At the same time, an extended thermal model is built, including the heat produced by chemical reactions and losses, sensible heat, latent heat, and convective cooling by the environment. This thermal model is necessary to consider the actual variations in temperature. The model contains elements of non-stationarity, which allows for solving problems associated with rapidly changing loads; the two-layer capacitor model is used to simulate more accurately voltage transients. All the described models have been developed within MATLAB/Simulink. The results of modeling are compared with high-quality experimental data taken from a Ballard Mark V cell. The simulated voltage and temperature profiles match well with the measured ones and this confirms that this configuration is a good representation of the behavior of the PEMFC in real operating conditions and the proposed model can be considered representative.

1 Introduction

Proton Exchange Membrane Fuel Cells (PEMFCs) are among the most promising sources of clean energy for automobiles, trucks, and stationary power applications owing to their efficient operation, fast response time, and negligible emissions [1]. Modeling these cells is crucial for efficient design, reliable control, and system integration, especially under sudden changes in load conditions or strict thermal requirements.
Modeling of thermal management issues has been considered extensively, with coupled electrochemical-thermal models and review papers emphasizing the role of nonuniform

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temperature distributions in impacting the operational, life cycle, and cold start performances of PEMFCs [2]. Dynamic and transient models based on electrochemical-thermal behavior, frequently built using MATLAB/Simulink, also take into consideration the double-layer capacitance effect, aging process, and parasitic elements to realistically simulate the dynamic response in voltage and temperature levels during car operation or network disturbances [3,4].

In this vein, the integrated electrochemical-thermal-dynamic model that we propose and validate against Ballard Mark V stack becomes an ideal tool for analyzing the PEMFC performance under practical conditions, as well as for controlling and energy management applications [5,6].

The membrane fuel cell model describes the production of electrical energy by electrochemical reactions starting with the open circuit voltage and considers the common problems of slow kinetics, internal resistance, and reactant mass transfer restrictions. We have also developed a heat transfer model that involves the heat production and removal through solid conduction, convective heat transfer, and radiation mechanisms [7,8].

Fundamentally, these cells use the charge transfer process to convert the chemical energy of hydrogen into electrical energy, which is the opposite process of electrolysis:

$$H_2(g) + \frac{1}{2}O_2(g) \rightarrow H_2O(l) + \text{electrical energy+Heat} \quad (1)$$

2 Electrochemical Model of the PEM Fuel Cell

The electrochemical model of the PEM fuel cell describes the internal reactions responsible for electricity generation (Figure 1).

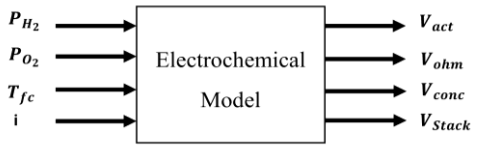

Fig. 1. Electrochemical Model Diagram of Fuel Cell.

2.1 Nernst potential

The open-circuit voltage of a PEMFC is determined from the Gibbs free energy change of the reaction, resulting in the Nernst equation:

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

2.2 Activation overpotentials

A part of the voltage generated by the fuel cell is lost due to activation losses, and these arise from the slow electrochemical kinetics that result in the oxygen reduction process at the cathode needing to be activated. The activation overpotential can be briefly explained using the Amphlett model [9-12].

$$V_{act} = -[\zeta_1 + \zeta_2 T + \zeta_3 T \ln(CO_2) + \zeta_4 T \ln(I_{fc})] \quad (3)$$

The concentration of (H_2, O_2) is expressed as a function of its pressure according to Henry's law [2]:

$$C_{O_2} = \frac{P_{O_2}}{5{,}08.10^6.e^{-\frac{498}{T}}} \quad (4)$$

$$C_{H_2} = \frac{P_{H_2}}{1{,}09.10^6.e^{\frac{77}{T}}} \quad (5)$$

2.3 Ohmic losses

Ohmic losses occur due to the resistance encountered when protons are transported through the electrolyte membrane and the resistance encountered between the different parts of the cell such as the electrodes, bipolar plates, and interfaces [10,12]. The resultant voltage drop follows Ohm's law and can be expressed as:

$$V_{ohm} = I_{fc}(R_m + R_c) \quad (6)$$

R_m is calculated from the membrane's specific resistivity ρ_M, its thickness l, and cross-sectional area A.

$$R_m = \rho_m \frac{\ell}{A} \quad (7)$$

The specific resistivity of the membrane $[\rho_M]$[10] is determined by Equation (8):

$$\rho_m = \frac{181{,}6\left(1+0{,}03\frac{I_{fc}}{A}+0{,}062\left(\frac{T}{303}\right)^2\left(\frac{I_{fc}}{A}\right)^{2{,}5}\right)}{\left(\lambda-0{,}643-3\left(\frac{I_{fc}}{A}\right)\right)e^{\left[\frac{4{,}18(T-303)}{T}\right]}} \quad (8)$$

2.4 Concentration losses

In case the rate of depletion is higher than the rate of arrival of the reactants (hydrogen or oxygen), then there is the formation of local concentration gradients in the fuel cell. The following are the major sources of such losses: restricted diffusion of the gases through the electrodes, constrained transport through the electrolytes, or insufficient dissolution of the reactants/products, they are expressed as:

$$V_{conc} = -B\ ln\left(1 - \frac{j}{j_{lim}}\right) \quad (9)$$

2.5 Global voltage equation

Theoretically, the voltage generated in a PEM fuel cell at standard conditions is about 1.23 volts, but due to losses incurred in the processes of activation, ohmic, and concentration, the cell voltage drops. Hence, the final cell voltage may be represented as:

$$V_{Cell} = E_{Nernt} - V_{act} - V_{ohm} - V_{conc} \quad (10)$$

3 Thermal Model of the PEMFC

The thermal model of a PEMFC accounts for heat generation and dissipation during operation, which is essential for performance analysis (Figure 2).

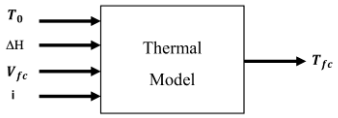

Fig. 2. Thermal Model Block Diagram of the Fuel Cell

3.1 Energy Balance Submodel

The thermal behaviour of the PEM fuel cell follows the law of energy conservation [12]. All heat and energy exchanges occurring within the stack satisfy the following balance:

$$q_{Cell} = q_{chimi} - q_{elec} - q_{sens+latent} - q_{loss} \quad (11)$$

3.2 Chemical Heat Generation

Thermal generation of electricity in PEM fuel cells through an electrochemical process originates from the difference between the enthalpy of the electrochemical reaction involving hydrogen and oxygen and the available electrical energy generated by the stack [12]. This thermal component, which is referred to as reaction heat or irreversible chemical heat, represents the portion of the energy that was not converted to electricity and can be expressed as:

$$q_{chimi} = \dot{N}_{H_2,cons} \Delta H \quad (12)$$

3.3 Electrical Heat Generation

Some amount of energy is lost as electrical heat resulting from the irreversible electrochemical reaction and ohmic loss in the cell elements [12]. The electrical heat production, q_{elec}, may be given as:

$$q_{elec} = V_{fc}.I_{fc} \quad (13)$$

3.4 Sensible Heat

Sensible heat refers to the amount of heat energy transferred via the inlet and outlet of the anode gas flow and the cathode gas flow due to temperature differences [12]. The formula for calculating the sensible heat is:

$$q_{sens+latent} = (\dot{N}_{H_{2(g)}}.C_{p,H_2} + \dot{N}_{O_{2(g)}}.C_{p,O_2} + \dot{N}_{H_2O(g)}.C_{p,H_2O})(T - T_0) + H_V.\dot{N}_{H_2O(g)} \quad (14)$$

3.5 Heat Loss

Losses due to heat are mainly because of the exterior surfaces of the stack, resulting from conduction, convection, and radiative effects [5]. In the current model, the heat loss from the PEM fuel cell occurs mainly because of convection by air at the exterior surfaces of the stack. The heat flow from the hot surfaces into the air is given by Newton's law of cooling:

$$q_{loss} = h.A.(T - T_0) \quad (15)$$

3.6 Global Thermal Model of the PEMFC

Thermal model of the entire system is based on energy generation and energy loss within the stack due to chemical, electrical, sensible, latent, and convective loss [12]:

$$m_{stack} C_{p,stack} \frac{dT}{dt} = q_{chimi} - q_{elec} - q_{sens+latent} - q_{loss} \quad (16)$$

4 Model Implementation in MATLAB/Simulink

4.1 Thermal Model architecture

Thermal model structure is illustrated in Figure 3, showing how the energy balance sub-modules interact and interconnect, describing the process of heat generated through chemical reactions (q_{chimi}), electrical heat (q_{elec}), heat exchanges ($q_{sens+latent}$), and convection heat losses (q_{loss}). It is important to note that this model stresses the temporal evolution of temperatures using input variables such as stack current, gas flow rates, and environmental conditions, thus allowing for real-time predictions of PEMFC thermal dynamics.

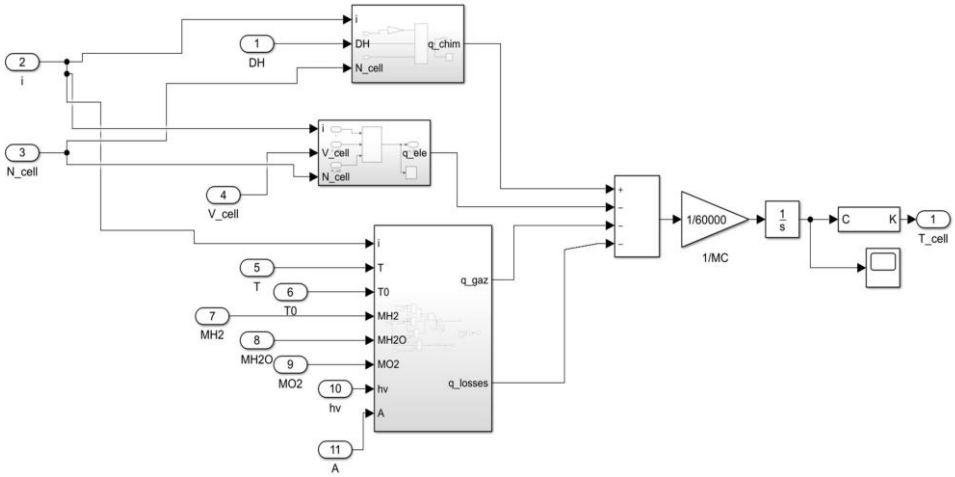

Fig. 3.Thermal Model of PEMFC

4.2 Electrochemical Model architecture

Figure 4 shows the electrochemical cell model architecture that incorporates E_{Nernst}, V_{act}, V_{ohm}, and V_{conc} into computing the cell voltage. Some key elements include gas concentration based on Henry's law, resistance based on membrane properties, and current-based losses. These form the basis for obtaining an accurate steady-state polarization curve simulation that is consistent with Ballard Mark V performance results.

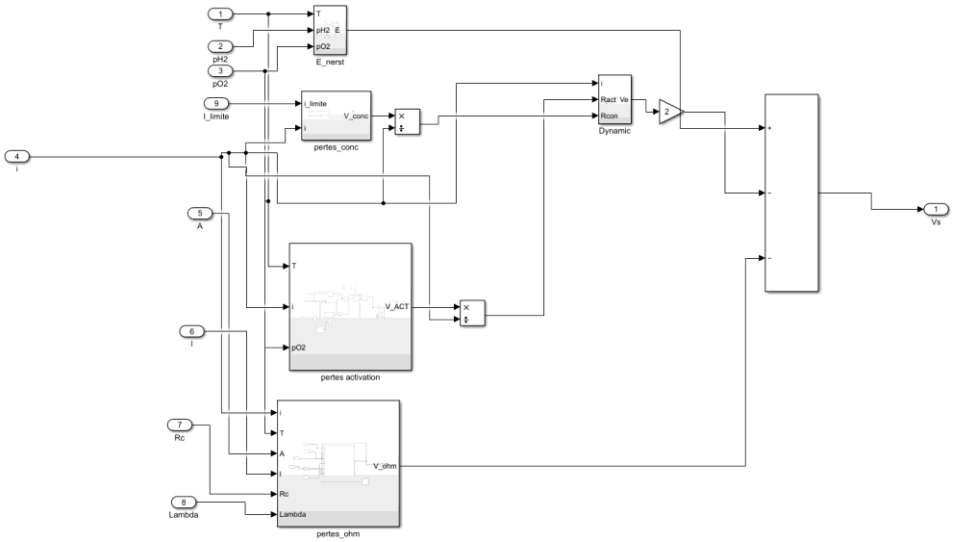

Fig. 4. Electrochemical Model of PEMFC

5 Dynamic Model of the PEMFC

Fuel cell dynamics is the transient behavior of a fuel cell that changes under rapid changes in loading and operation (Figure 5). Electrochemical processes, including losses due to activation, concentration, and resistance, as well as double layer effect, are accounted for in this model [10,12].

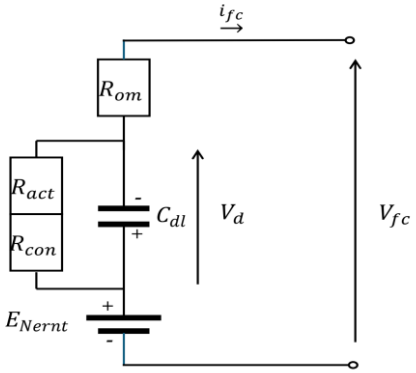

Fig. 5. Dynamic Electrical Equivalent Circuit of a PEM Fuel Cell

The current of the circuit is described as:

$$i_{fc} = \frac{V_d}{(R_{act}+R_{con})} + C_{dl}\frac{dV_d}{dt} \quad (17)$$

The voltage variation over time is described as:

$$\frac{dV_d}{dt} = \frac{1}{C_{dl}}\left(i_{fc} + \frac{V_d}{(R_{act}+R_{con})}\right) \quad (18)$$

The output voltage of the fuel cell can be expressed as:

$$V_{fc} = E_{Nernt} - V_d - R_{om}.i_{fc} \quad (19)$$

6 Simulation Results and Discussion

Following the table presents an example of the simulation parameters for the BALLARD MARK V,

Table 1. Simulation parameters of the BALLARD MARK V fuel cell [9,11]

Parameters	values	Parameters	values
A	50,6 cm^2	ζ_1	−1.12
L	178µm	ζ_2	$3{,}57*10^{-3}$
P_{H_2}	1 atm	ζ_3	$8{,}01*10^{-3}$
P_{O_2}	1 atm	ζ_4	$-15{,}9410^{-5}$
B	0,015 V	λ	22
R_c	0,1 mΩ	j_{max}	1500 mA/cm^2
i_{max}	75,9 A	C_{dl}	0,8 F

The output voltage response of the Ballard Mark V fuel cell is shown in Figure 6. From the simulation, the model can describe voltage drops in relation to current flow by taking into consideration both physical and dynamic parameters. This is because the physical parameters account for the activation and ohmic losses, while the dynamic parameters, like the double layer capacitance, make the model able to describe transient behavior in the event of sudden load changes.

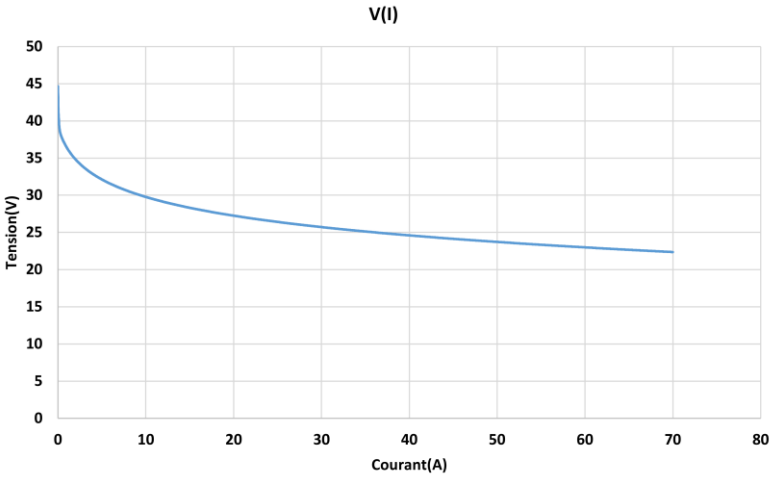

Fig. 6. Polarization behaviour of the Ballard Mark V fuel cell.

Figure 7 shows the relationship between the theoretical value (V_{sim}) and experimental values (V_{exp}) for the polarization curve of the Ballard Mark V fuel cell, demonstrating the dependence of the generated voltage on the varying currents. It can be seen that both curves have the same trend with an RMSE value of 4.89% percent, showing that the model used is effective. It is also evident that there is a significant match between the curves in the current values of 20-50 A.
Figure 8 shows the change in temperature with the increase in fuel cell currents, where it is evident that the temperature increases sharply at the beginning and reaches stability levels at around 348-350 K.

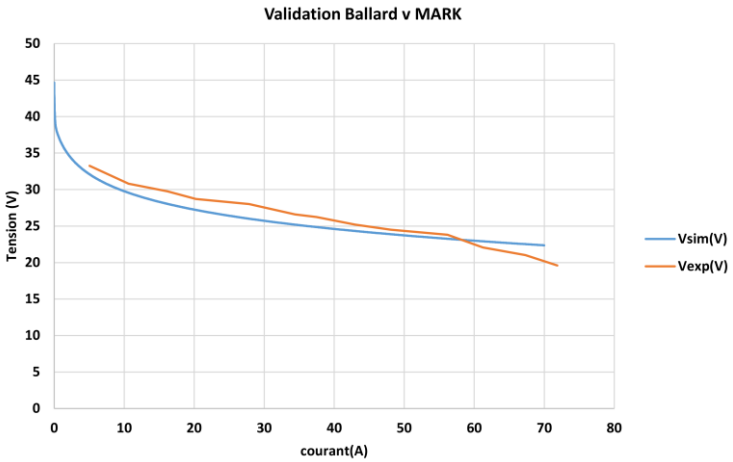

Fig. 7. Model validation using experimental data of Ballard Mark V.

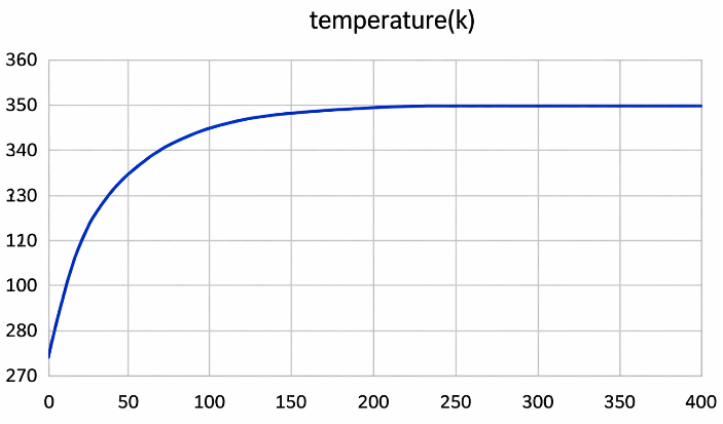

Fig. 8: Fuel cell temperature versus current.

7 Conclusion

In this work, we have developed a combined electrochemical-thermal-dynamic model of PEMFCs. In this way, the relationship between voltage production and heat generation/heat dissipation processes is made clear. By combining loss mechanisms like activation, ohmic, and concentration losses with a detailed thermal analysis, which considers chemical reactions, electrical losses, sensible and latent heats, and heat transfer to the surrounding atmosphere, our proposed model can predict power generation and temperature behavior realistically. To validate the proposed model, MATLAB/Simulink software was used, and experimental data from Ballard Mark V were compared with the results obtained using the developed model. It was found that the predictions made by the model had excellent correlations with the experimental data based on the low RMSE value. Among other things, the thermal part of the model is quite interesting, demonstrating how the temperature first increases rapidly before reaching a stable condition of quasistationarity. Such a development makes our research useful for stack cooling studies.

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