

MODELING AND SIMULATION OF THE EFFECTS OF OPERATING PARAMETERS ON THE VOLTAGE CHARACTERISTICS OF PEM FUEL CELLS

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Abstract

Proton exchange membrane fuel cells (PEMFCs) have attracted significant attention due to their high efficiency and low emission characteristics. However, the cell performance is strongly influenced by operating conditions and membrane properties, which are difficult to investigate comprehensively by experimental approaches alone. This study develops a complete electrochemical model of a single PEM fuel cell in the MATLAB – Simulink environment based on the voltage loss mechanisms including the Nernst potential, activation overpotential, ohmic losses, and concentration losses. The model is employed to quantitatively investigate the effects of operating temperature, hydrogen partial pressure, oxygen partial pressure, and membrane thickness on the polarization characteristics (I – V curves) of the PEMFC. Simulation results indicate that increasing temperature significantly enhances activation kinetics and improves cell voltage, while elevated oxygen partial pressure yields the most pronounced performance improvement among gas parameters. Conversely, increasing membrane thickness leads to higher ohmic losses and voltage degradation, especially in the high – current – density regime. The proposed model provides an effective numerical tool for teaching, system analysis, and preliminary optimization of PEMFC operating conditions.

Keywords: electrochemical losses; fuel cell simulation; MATLAB – Simulink modeling; operating parameters; PEM fuel cell; polarization characteristics.

1. Introduction

Proton exchange membrane fuel cells (PEMFCs) have attracted increasing global attention as a promising energy conversion technology due to their high efficiency, low emissions, rapid start – up capability, and low operating temperature. As concerns about climate change and energy security intensify, PEMFCs have emerged as a strong candidate for clean transportation, distributed generation, and backup power systems. Compared to conventional internal combustion engines, PEMFCs produce electricity through an electrochemical reaction rather than combustion, offering significantly higher energy efficiency and producing only water as a byproduct. The relatively low operating

temperature of 60 – 80°C also enables compact system integration and fast response dynamics, making PEMFCs suitable for automotive and portable applications.

Despite these advantages, PEMFC performance is highly sensitive to several operating conditions. Temperature, membrane hydration, reactant gas partial pressures, water management, and membrane thickness directly affect electrochemical kinetics, proton transport, and mass transport phenomena. Practical fuel cell systems must therefore operate within a narrow range of optimized conditions to maintain stable voltage output, acceptable efficiency, and long – term durability. However, experimentally evaluating the influence of these parameters is costly and complex. Experimental setups require precise temperature control, high – purity gases, moisture – regulated air supply, and specialized diagnostic equipment. Moreover, varying a single parameter while keeping others constant can be challenging, making systematic analysis difficult.

In recent years, mathematical modeling and simulation have become essential tools for understanding PEMFC behavior and optimizing operating conditions. Models allow researchers to analyze electrochemical mechanisms, predict performance trends, and evaluate parameter sensitivity without requiring expensive test benches. Modeling is also critical for designing control strategies in automotive fuel cell systems, hybrid energy systems, and stack management. A well – constructed model can reveal how activation losses, ohmic resistance, and concentration losses change under different conditions, enabling deeper insights into performance limitations.

The use of MATLAB – Simulink for PEMFC modeling has expanded significantly due to its graphical modeling environment, modular architecture, and ability to integrate dynamic system components. Block – based models allow researchers and students to visualize electrochemical processes, adjust system parameters easily, and expand simulations with control systems. This makes MATLAB – Simulink particularly useful for engineering education and for institutions with limited access to physical fuel cell hardware.

In the international research community, PEMFC modeling has been used to evaluate catalyst performance, membrane hydration, thermal management, water transport, and system – level integration. However, for educational and small – scale research environments, simplified but complete electrochemical models remain valuable because they balance computational efficiency with physical accuracy. Such models typically include four primary voltage – loss mechanisms: the Nernst potential, activation losses, ohmic losses, and concentration losses. Analyzing how each mechanism responds to changing operating conditions provides meaningful insights into the behavior of the fuel cell and helps guide system optimization.

In Vietnam, PEMFC research has grown in recent years, but most efforts focus on membrane – electrode assembly development, hydrogen production, or basic modeling for teaching. Comprehensive simulation – based studies that simultaneously evaluate multiple operating parameters – such as temperature, hydrogen and oxygen partial pressures, and membrane structural characteristics – are still limited. Given the increasing relevance of fuel cell technology in automotive engineering and renewable – energy education, developing a complete and flexible PEMFC simulation model is valuable for universities and research institutions.

This study aims to contribute to this direction by developing a MATLAB – Simulink – based PEMFC model that incorporates key electrochemical loss mechanisms and allows

systematic parameter variation. The model provides a practical framework for analyzing how temperature, reactant gas pressures, and membrane thickness affect voltage – current characteristics. By evaluating these parameters quantitatively, the study offers insights that can assist in optimizing PEMFC operation for applications such as electric vehicles, stationary power systems, and laboratory instruction.

The primary contributions of this study are as follows:

- (1) The development of a block – structured PEMFC model integrating the Nernst equation, activation overpotentials, ohmic resistance, and concentration losses;
- (2) A quantitative investigation of how operating temperature, oxygen partial pressure, hydrogen partial pressure, and membrane thickness influence the polarization behavior of a single PEM fuel cell;
- (3) The provision of a simulation framework that supports engineering education, parameter analysis, and preliminary system design.

Overall, the study provides an accessible and physically meaningful modeling approach suitable for academic and research environments, offering both pedagogical and technical value for further PEMFC – related investigations.

2. Literature Review

Proton exchange membrane fuel cells (PEMFCs) have been extensively investigated due to their high efficiency, low operating temperature, and suitability for automotive and portable power applications. Accurate modeling of PEMFC performance is essential for understanding the influence of operating parameters and supporting system optimization.

Early mechanistic modeling efforts were established by Amphlett et al. (1995), who developed a comprehensive electrochemical framework for the Ballard Mark IV PEMFC. This model incorporated reversible voltage, activation losses, ohmic losses, and concentration losses, forming the basis for many subsequent PEMFC performance models. Bernardi and Verbrugge (1991) further contributed by proposing a detailed mathematical model for gas diffusion electrodes bonded to polymer electrolytes, emphasizing mass transport and electrochemical kinetics within porous electrodes.

Springer et al. (1991) introduced a widely adopted PEMFC model that explicitly accounts for membrane hydration effects on proton conductivity. Their work highlighted the strong dependence of ohmic losses on membrane water content and thickness, which has been confirmed in later studies. Building upon these foundations, Rowe and Li (2001) presented a generalized mathematical model capable of predicting polarization characteristics under various operating conditions, making it suitable for system-level simulations.

With the advancement of numerical tools, system-oriented and simulation – based PEMFC models have been increasingly developed. Musio et al. (2011) implemented a PEMFC system model in the MATLAB – Simulink environment, enabling dynamic analysis and integration with auxiliary components. Such approaches are particularly useful for parametric studies and control – oriented applications.

Mass transport phenomena and water management at the cathode have also received significant attention. Wang and Chen (2001) investigated two – phase flow and transport in the air cathode of PEM fuel cells, demonstrating the critical role of liquid water accumulation on oxygen transport and voltage losses at high current densities.

More recently, research has focused on improving PEMFC operational efficiency through system – level optimization strategies. Studies by Do and Chen (2022) and Do et al. (2024) analyzed the influence of fan speed on open – cathode PEMFC performance, highlighting the trade – off between electrochemical efficiency and parasitic power consumption. Further investigations by Do et al. (2025, 2026) explored cathode purge strategies and data – driven optimization methods, demonstrating the growing role of intelligent modeling techniques in PEMFC performance enhancement.

Despite the extensive literature on PEMFC modeling, there remains a need for simplified yet physically meaningful models that can clearly illustrate the effects of key operating parameters on polarization behavior. In this context, the present study develops a MATLAB – Simulink – based PEMFC model to systematically investigate the influence of temperature, reactant gas partial pressures, and membrane thickness on cell voltage characteristics.

3. Materials and Methods

3.1. Model Structure

The PEMFC model developed in this study consists of four major computational blocks implemented in MATLAB – Simulink: (i) reversible voltage (Nernst potential), (ii) activation losses, (iii) ohmic losses, and (iv) concentration losses. The cell voltage is expressed as:

$$V_{cell} = E_{Nernst} - \eta_{act} - \eta_{ohmic} - \eta_{conc} \quad (V) \quad (1)$$

Where E_{Nernst} is the reversible open - circuit voltage, and η_{act} , η_{ohmic} , and η_{conc} are the activation, ohmic, and concentration overpotentials, respectively.

3.2. Governing Equations

3.2.1. Reversible Voltage (Nernst Potential)

The reversible potential of the PEMFC is determined from:

$$E_r(T_{rif}, P_{rif}) = \frac{-\Delta G}{nF} = \frac{237340}{2 \cdot 96485} = 1.229 \quad (V) \quad (2)$$

Where ΔG ($J \text{ mol}^{-1}$) is the Gibbs free energy change of the electrochemical reaction, $n = 2$ is the number of exchanged electrons, and F ($C \text{ mol}^{-1}$) is the Faraday constant.

The open – circuit voltage is obtained using the Nernst equation:

$$E_{Nernst} = E_r(T_{rif}, P_{rif}) - \frac{\Delta S}{nF}(T - T_{rif}) + \frac{RT}{nF} \ln \left(\frac{p_{H_2} p_{O_2}^{0.5}}{p_{H_2O}} \right) \quad (V) \quad (3)$$

Where: ΔS ($J \text{ mol}^{-1} \text{ K}^{-1}$) is the entropy change, T (K) is the operating temperature, T_{rif} (K) is the reference temperature, p_{H_2} , p_{O_2} , p_{H_2O} (atm) are the partial pressures of hydrogen, oxygen, and water vapor, and R ($J \text{ mol}^{-1} \text{ K}^{-1}$) is the ideal gas constant.

This relation reflects the effects of temperature and reactant gas pressures on the open-circuit voltage.

3.2.2. Activation Losses

Activation losses are governed by the electrochemical reaction kinetics at both the anode and cathode. Based on the Tafel equation:

$$\eta_{\text{act}} = \eta_{\text{act,c}} + \eta_{\text{act,a}} = \frac{RT}{\alpha_c F} \ln \left(\frac{i + i_{\text{loss}}}{i_{0,c}} \right) + \frac{RT}{\alpha_a F} \ln \left(\frac{i + i_{\text{loss}}}{i_{0,a}} \right) \quad (V) \quad (4)$$

Where i (A cm^{-2}) is the cell current density, i_{loss} (A cm^{-2}) represents the internal current loss accounting for fuel crossover and parasitic electrochemical effects, $i_{0,a}$ and $i_{0,c}$ (A cm^{-2}) are the exchange current densities of the anode and cathode, and α_a and α_c are the charge – transfer coefficients (typically ranging from 0.5 to 1).

3.2.3. Ohmic Losses

Ohmic losses consist of proton conduction losses in the membrane and electronic resistance in bipolar plates and interconnects. The total ohmic drop is:

$$\eta_{\text{ohmic}} = I(R_m + r) \quad (V) \quad (5)$$

Where I (A) represent the operating current of the fuel cell, R_m (Ω) is the membrane resistance and r are the resistance of other components such as bipolar plates and current collectors. The value of R_m (Ω) depends on the water content in the membrane:

$$\lambda = 0.043 + 17.81a_m - 39.95a_m^2 + 36.0a_m^3 \quad (6)$$

$$R_m = \frac{t_m}{A_{\text{cell}} (0.00514\lambda - 0.00326) \exp \left[1268 \left(\frac{1}{T} - \frac{1}{303} \right) \right]} \quad (\Omega) \quad (7)$$

Where t_m (μm) is the membrane thickness, A_{cell} (cm^2) is the active area of the cell, and a_m (0 – 1) is the average water activity between the anode and cathode.

3.2.4. Concentration Losses

Concentration (mass – transport) losses occur at high current densities when reactant diffusion becomes rate – limiting:

$$\eta_{\text{conc}} = \frac{RT}{nF} \ln \left(\frac{i_L}{i_L - i} \right) \quad (V) \quad (8)$$

The limiting current density i_L is defined by:

$$i_L = nFh_m \left[(C_{\text{in}} - C_{\text{out}}) / \ln \left(\frac{C_{\text{in}}}{C_{\text{out}}} \right) \right] \quad (\text{Acm}^{-2}) \quad (9)$$

Where h_m (m s^{-1}) is the mass transport coefficient at the cathode, and C_{in} , C_{out} (mol m^{-3}) are inlet and outlet oxygen concentrations. The model also uses a correction factor $K = 15$ to match the polarization curve in the high current density region:

$$\eta_{\text{conc}}^* = K\eta_{\text{conc}} \quad (V) \quad (10)$$

3.3. Simulation Parameters

The model employs the parameters summarized in Table 1, including electrochemical constants, gas partial pressures, membrane properties, limiting – current parameters, and operating temperature range. Key parameters such as $i_{0,a}$, $i_{0,c}$, t_m , p_{H_2} , p_{O_2} , and temperature T are varied to evaluate their effects on the PEMFC polarization characteristics.

Table 1. Simulation Parameters

Parameter	Value	Unit
$i_{0,c}$	10^{-4}	$A\ cm^{-2}$
$i_{0,a}$	10^{-3}	$A\ cm^{-2}$
α_a, α_c	0.5	
I_{loss}	0.003	$A\ cm^{-2}$
t_m	178	μm
A_{cell}	50	Cm^2
r	0.002	Ω
a_m	0.6	
T	303.15 – 363.15	K
p_{H_2}	0.2 – 1.0	atm
p_{O_2}	0.05 – 1.0	atm
p_{H_2O}	0.047	atm
h_m	0.001	$m\ s^{-1}$
C_{in}	40	$mol\ m^{-3}$
C_{out}	5	$mol\ m^{-3}$

Source: Amphlett et al. (1996); Springer et al. (1991); Wang and Chen (2001)

4. Results and Discussion

4.1. Results

Figure 1 presents the PEMFC simulation model developed in the MATLAB – Simulink environment. This model enables evaluation of the effects of various operating parameters on the polarization ($I - V$) characteristics of a single fuel cell. The results are analyzed through four investigation groups: the influence of temperature, hydrogen partial pressure, oxygen partial pressure, and membrane thickness.

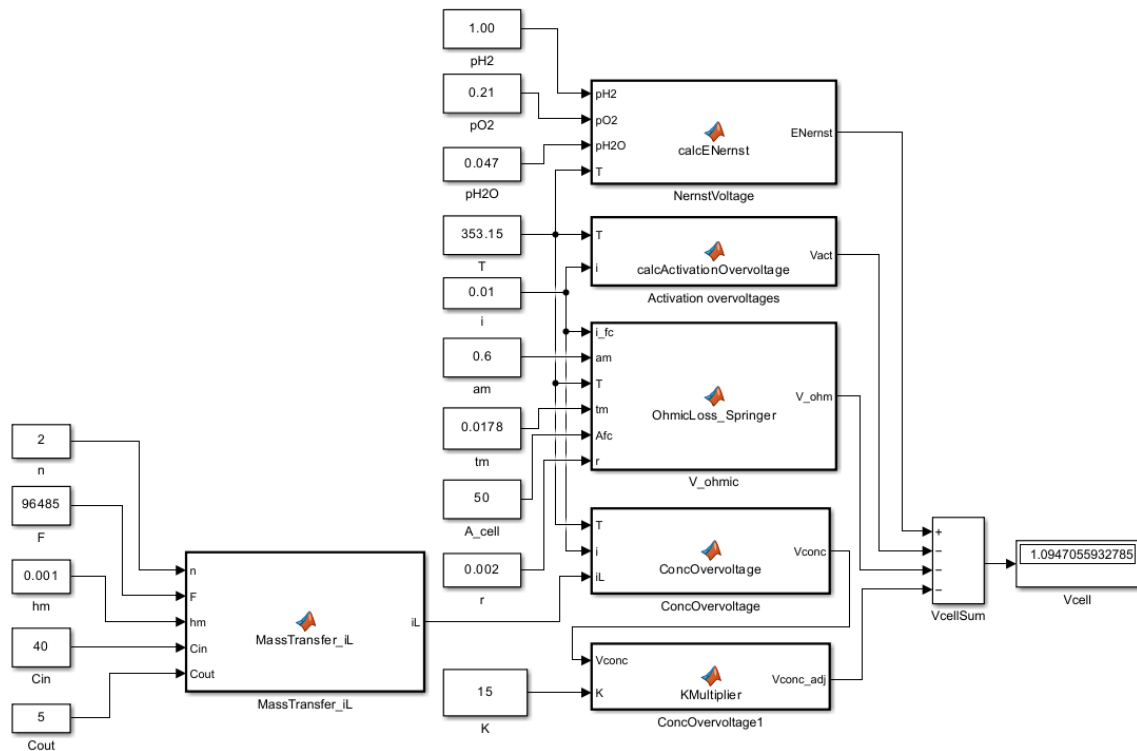


Figure 1. Simulink model of a single PEMFC

Source: Author, 2025

4.1.1. Effect of Temperature

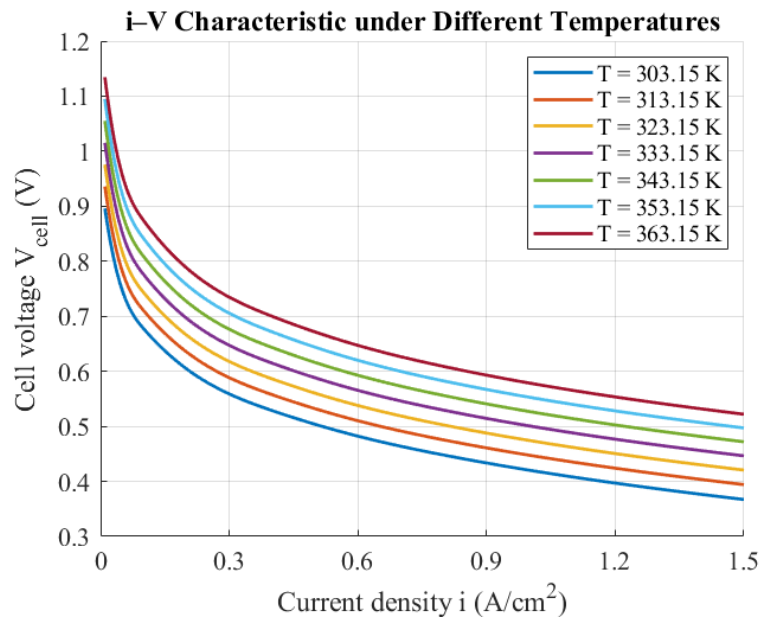


Figure 2. Polarization curves at different operating temperatures.

Source: Author, 2025

Figure 2 illustrates the polarization curves of the PEMFC at temperatures ranging from 303.15 K to 363.15 K, while keeping other parameters constant. As temperature increases:

- The open – circuit voltage increases slightly due to the rise in the Nernst potential,

- Activation losses decrease significantly,
- The operating voltage at the same current density becomes higher.

These results indicate that higher temperature enhances the electrochemical reaction kinetics and improves the overall fuel cell performance.

4.1.2. Effect of Oxygen Partial Pressure (p_{O_2})

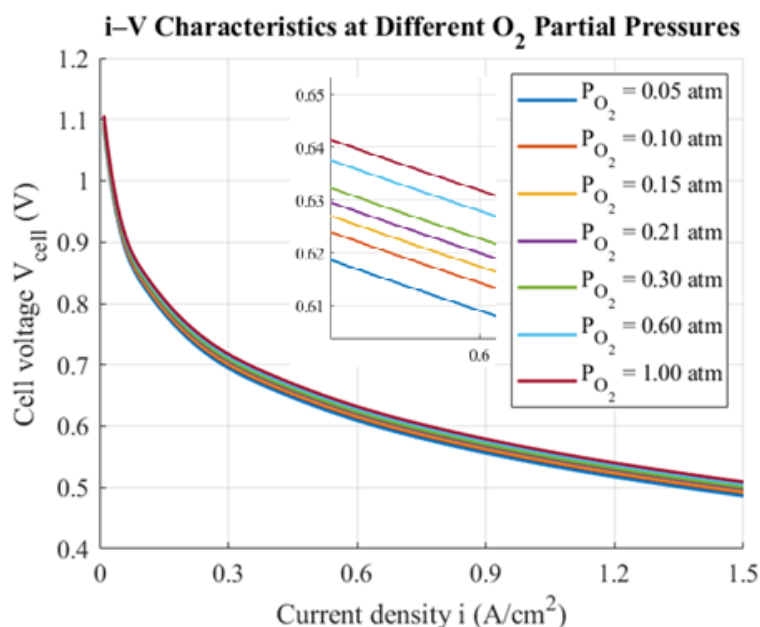


Figure 3. Polarization curves corresponding to various oxygen partial pressures (p_{O_2})

Source: Author, 2025

Figure 3 shows the polarization curves when the oxygen partial pressure is varied from 0.05 to 1.0 atm. As p_{O_2} increases:

- The output voltage increases,
- Cathode activation losses decrease,
- The polarization curve shifts upward, indicating improved performance.

However, the rate of improvement becomes less pronounced at higher pressures as the reaction approaches near-optimal conditions.

4.1.3. Effect of Hydrogen Partial Pressure (p_{H_2})

Figure 4 presents the changes in polarization characteristics when the hydrogen partial pressure is varied between 0.20 to 1.0 atm. The results indicate that:

- Increasing p_{H_2} enhances the electrochemical potential according to the Nernst equation,
- At high current densities, the voltage remains higher compared with low – pressure conditions.

This confirms that maintaining sufficiently high hydrogen pressure is essential for stable fuel supply and efficient energy conversion.

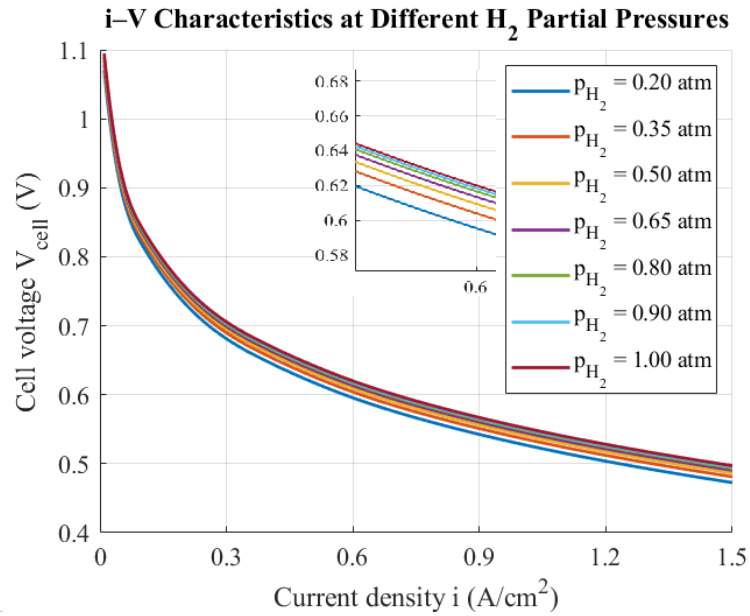


Figure 4. Polarization curves corresponding to various hydrogen partial pressures (p_{H₂})

Source: Author, 2025

4.1.4. Effect of Membrane Thickness

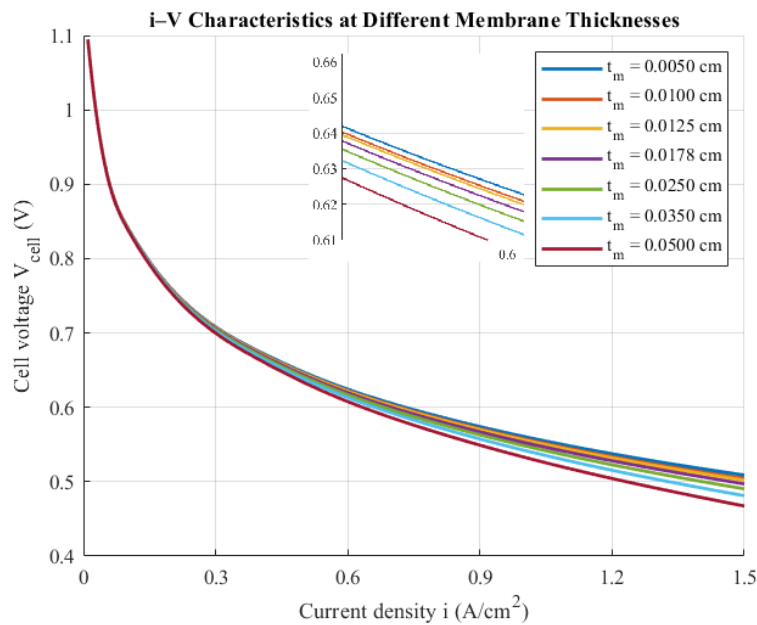


Figure 5. Polarization curves for different membrane thicknesses

Source: Author, 2025

Figure 5 illustrates the polarization curves corresponding to different membrane thicknesses.

Membrane thickness mainly affects the ohmic loss according to:

$$R_m = \frac{t_m}{\sigma_m A_{cell}} \quad (\Omega) \tag{11}$$

When membrane thickness increases from 0.005 to 0.05 mm:

- The cell voltage decreases noticeably at medium and high current densities,
- The slope of the polarization curve becomes steeper because of increased internal resistance.

These results demonstrate that using a thinner membrane or one with higher proton conductivity can reduce internal losses and enhance PEMFC performance.

4.2. Discussion

The simulation results demonstrate that operating temperature, reactant gas partial pressures, and membrane thickness influence PEMFC performance through distinct electrochemical mechanisms. Increasing the operating temperature leads to improved electrochemical reaction kinetics, thereby reducing activation overpotentials. As a result, the cell voltage increases predominantly in the low – and medium – current – density regions, which is consistent with classical PEMFC modeling results reported by Amphlett et al. (1995) and Rowe and Li (2001).

Among the investigated gas parameters, oxygen partial pressure exhibits the most significant impact on PEMFC performance. An increase in oxygen partial pressure enhances cathodic reaction kinetics and mitigates mass transport limitations, particularly under high current density operation. This behavior is clearly reflected in the upward shift of the polarization curves at high current densities and agrees well with the findings of Wang and Chen (2001), who emphasized the role of oxygen transport and liquid water effects in the cathode.

In contrast, variations in hydrogen partial pressure result in a comparatively modest improvement in cell voltage. This can be attributed to the fast hydrogen oxidation reaction at the anode, which is typically not rate – limiting under normal operating conditions. Consequently, increasing hydrogen partial pressure mainly affects the reversible cell voltage through the Nernst equation, with minimal influence on activation and concentration losses, as also observed in earlier mechanistic models (Bernardi & Verbrugge, 1991; Amphlett et al., 1995).

Membrane thickness directly affects ohmic losses by altering proton conduction resistance. Thicker membranes increase ionic resistance, leading to a more pronounced voltage drop at medium and high current densities. This trend is consistent with the membrane conductivity model proposed by Springer et al. (1991), which highlights the strong dependence of ohmic losses on membrane properties and hydration conditions. Although reducing membrane thickness improves voltage performance, practical considerations such as mechanical durability, gas crossover, and long – term stability must be considered in real PEMFC designs.

Overall, the MATLAB – Simulink model developed in this study successfully captures the fundamental electrochemical behavior of PEM fuel cells and reproduces performance trends that are consistent with established theoretical and experimental studies. The model therefore provides a reliable and efficient tool for parametric analysis, educational purposes, and preliminary optimization of PEMFC operating conditions.

5. Limitations and Future work

Although the developed MATLAB – Simulink model successfully captures key electrochemical behaviors of PEM fuel cells and provides insights into the effects of

temperature, reactant pressures, and membrane thickness, several limitations remain. The model has not yet been validated with experimental data, limiting the ability to confirm its real – world accuracy. In addition, water management, membrane hydration dynamics, and gas crossover were simplified and not modeled in detail. The model primarily focuses on steady - state performance without addressing transient behavior.

Future work should incorporate experimental validation, integrate more advanced sub – models for hydration and mass transport, and expand the model to analyze dynamic responses. Control strategies for temperature, humidity, and air supply should also be included to extend the applicability of the model for system – level design and optimization.

6. Conclusion

This study developed an electrochemical model and Simulink-based simulation framework to analyze the effects of key operating parameters – temperature, oxygen partial pressure, hydrogen partial pressure, and membrane thickness – on the voltage performance of PEM fuel cells. The results indicate that temperature has the strongest influence on cell voltage, followed by oxygen partial pressure, hydrogen partial pressure, and membrane thickness. Higher temperatures and reactant pressures improve reaction kinetics and mass transport, while thinner membranes reduce ohmic losses. These findings are consistent with established PEMFC operating principles and demonstrate the validity of the model. Overall, the study provides a practical foundation for optimizing PEMFC operation and supports further development of fuel – cell-based energy systems.

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Nomenclature

A nomenclature section is provided to summarize all symbols, parameters, and units used in the model.

Symbol	Description	Unit
V_{cell}	Cell voltage	V
E	Reversible cell voltage	V
E_0	Standard reversible voltage	V
η_{act}	Activation overpotential	V
$\eta_{act,a}$	Anode activation overpotential	V
$\eta_{act,c}$	Cathode activation overpotential	V
η_{ohm}	Ohmic overpotential	V

η_{con}	Concentration overpotential	V
i	Cell current density	A cm ⁻²
I_{loss}	Internal current loss	A cm ⁻²
I_{0a}	Anode exchange current density	A cm ⁻²
I_{0c}	Cathode exchange current density	A cm ⁻²
I_{lim}	Limiting current density	A cm ⁻²
R_m	Membrane resistance	Ω
t_m	Membrane thickness	μm
A_{cell}	Active cell area	cm ²
α_a	Anode charge-transfer coefficient	–
α_c	Cathode charge-transfer coefficient	–
λ	Membrane water content	–
T	Operating temperature	K
F	Faraday constant	C mol ⁻¹
R	Universal gas constant	J mol ⁻¹ K ⁻¹
p_{H_2}	Hydrogen partial pressure	atm
p_{O_2}	Oxygen partial pressure	atm
$p_{\text{H}_2\text{O}}$	Water vapor partial pressure	atm
r	Electronic resistance	Ω
h_m	Mass transfer coefficient	m s ⁻¹
C_{in}	Inlet oxygen concentration	mol m ⁻³
C_{out}	Outlet oxygen concentration	mol m ⁻³

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