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Simulation-Based Performance Analysis of Phosphoric Acid Fuel Cells: Polarization Behavior, Power Density, and Sensitivity to Operating Conditions

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تحليل أداء خلايا وقود حمض الفوسفوريك بالاعتماد على المحاكاة: سلوك الاستقطاب، كثافة القدرة، والحساسية لظروف التشغيل

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Abstract:
This study presents a comprehensive modeling and performance analysis of phosphoric acid fuel cells (PAFCs) using a hybrid simulation approach that integrates Aspen Plus for thermodynamic evaluation and Engineering Equation Solver (EES) for electrochemical kinetics. The primary objective is to generate polarization and power density curves while quantitatively isolating activation, ohmic, and concentration voltage losses. Furthermore, the parametric impacts of operating pressure and temperature on the net electrical power output are systematically investigated. The simulation results exhibit excellent agreement with established reference data, confirming that elevated operating pressures and temperatures—within operational material limits—substantially enhance reaction kinetics and mitigate ohmic losses, thereby boosting overall cell efficiency and peak power output. This validated model establishes a robust predictive framework for PAFC performance evaluation and its future integration with advanced waste heat recovery systems.

Keywords: Phosphoric acid fuel cell, PAFC, Aspen Plus, EES, Polarization curve, Voltage losses, Parametric analysis.

الملخص تقدم هذه الدراسة نمذجةً وتحليلاً شاملاً لأداء خلايا وقود حمض الفوسفوريك (PAFC) عبر منهجية محاكاة هجينة متطورة، تجمع بين برنامج Aspen Plus لمحاكاة الديناميكا الحرارية، وبرنامج EES لتحليل الحركية الكهروكيميائية. هدفت الدراسة إلى توليد منحنيات الاستقطاب وكثافة القدرة، مع إجراء تحليل كمي دقيق لخسائر الجهد بمختلف أنواعها (التنشيطية، الأومية، والتركيزية). علاوة على ذلك، تم استقصاء تأثير متغيرات ضغط التشغيل ودرجة الحرارة على إنتاج القدرة الكهربائية الصافية. وأظهرت النتائج تطابقاً ممتازاً مع البيانات المرجعية المعتمدة، مما يؤكد أن التشغيل عند ضغوط ودرجات حرارة مرتفعة —في حدود ما تسمح به المواد— يعزز من حركية التفاعل الكيميائي ويقلل الخسائر الأومية، الأمر الذي يؤدي بدوره إلى تحسين كفاءة الخلية ورفع ذروة قدرتها المتولدة. يمثل هذا النموذج إطاراً تنبؤياً رصيناً لتقييم أداء خلايا PAFC وتمهيداً لدمجها مستقبلاً مع أنظمة استرجاع الحرارة المفقودة.

الكلمات المفتاحية: خلايا وقود حمض الفوسفوريك، PAFC، برنامج Aspen Plus ، برنامجEES ، منحنى الاستقطاب، خسائر الجهد، التحليل البارامتري.

1. Introduction

Phosphoric Acid Fuel Cells (PAFC) represent a promising technology for clean energy generation, directly converting chemical energy into electricity through electrochemical reactions with high efficiency and minimal

environmental impact **[1]**. Characterized by their exceptional stability and reliability, (PAFC) are particularly well-suited for stationary power applications in the range of 100-400 kW **[2, 3]**. he performance of a fuel cell is fundamentally governed by its polarization curve, which delineates the relationship between current density and the generated cell voltage. The cell voltage is subject to three primary irreversible losses: activation overpotential, ohmic losses, and concentration overpotential **[4]**. Consequently, cell performance can be optimized by precisely controlling critical operating parameters, including operating pressure, temperature, gas composition, and current density **[1]**. (PAFC) operate at intermediate temperatures ranging from 150° to 210° C. This thermal regime facilitates the recovery of low-grade waste heat, thereby enhancing the overall system efficiency. Literature indicates that the net electrical efficiency of (PAFC) typically reaches 40–50%, with potential for further augmentation through the integration of waste heat recovery systems **[5, 6]**. In this context, the recent study by **[7]** serves as a pivotal reference. They simulated a hybrid system comprising a 300 kW (PAFC) coupled with an Organic Rankine Cycle (ORC) using (Aspen Plus) software. The present study builds directly upon this foundational work; it adopts the same system configuration to validate initial results before expanding the scope to include a more granular and rigorous analysis. Accordingly, this paper aims to provide a comprehensive performance analysis of the (PAFC) by investigating polarization and power density curves and quantifying the respective voltage losses. Furthermore, it conducts a detailed parametric study to evaluate the influence of operating pressure and temperature on electrical power output. This detailed characterization adds significant scientific and practical value to the understanding of system behavior under diverse operating conditions.

2. Mathematical Modeling of (PAFC)

Mathematical modeling is a fundamental tool for understanding the electrochemical behavior and performance characteristics of Phosphoric Acid Fuel Cells (PAFC). The model provides valuable insight into the processes that take place within the fuel cell system and helps predict the cell output voltage under various operating conditions. The mathematical modeling of an individual PAFC includes Nernst potential, activation loss, ohmic loss and concentration loss **[1]**. The overview is shown in **figure (1)** below.

Figure (1): Block diagram of an individual (PAFC).

The equation format of **figure (1)** can be expressed as below **[5,6,8]**

$$V_{cell}=E_{nernst}-V_{act}-V_{ohmic}-V_{conc}$$

Nernst Potential

The Nernst potential is the theoretical thermodynamic potential of a fuel cell under specific operating conditions, calculated based on the partial pressures of the reacting gases and the temperature. This potential represents the theoretical maximum potential that the cell can produce when no electric current is flowing **[1, 6,8]**.

$$E_{nernst}=E^0+\frac{R\,T}{n\,F}\ln\left(\frac{P_{H_2}P_{O2}^{0.5}}{P_{H2O}}\right)$$

Activation Loss:

Activation losses occur due to the need for activation energy to initiate electrochemical reactions at the electrodes (anode and cathode). These losses are significant at low current density values and depend on the reaction kinetics and electron transfer coefficient **[1]**.

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

Ohmic Loss:

Ohmic losses arise from the resistance to ion flow in the electrolyte and the resistance to electron flow across the electrodes and current collectors. These losses are directly proportional to the current density and depend on the ionic conductivity of the electrolyte **[1, 6, 8]**.

$$V_{ohmic}=R_{ohm}\,J$$

Concentration Loss:

Concentration losses occur due to the depletion of reactants at the electrode surface or the accumulation of products, leading to a decrease in the partial pressure of the reactants. These losses become significant at high current densities and approach the limiting current density **[1,6]**.

$$V_{conc}=\frac{R\,T}{\alpha\,nF}\ln\left(1-\frac{J}{J_L}\right)$$

3. Model Validation by Aspen Plus Software

To ensure the fidelity of the proposed mathematical model, a rigorous validation process was conducted prior to the parametric analysis of polarization and power curves. The system configuration was implemented

within the (Aspen Plus) simulation environment, replicating the topology and operating conditions of a benchmark study found in the literature **[7]**. A direct comparison between the simulation outputs and the reference data was performed to verify the model's accuracy. As demonstrated in **Table (1)**, the results exhibit a high degree of correlation, with minimal percentage deviation across key performance indicators, thereby confirming the reliability of the developed model for subsequent investigations.
Furthermore, **Figure (2)** illustrates the comprehensive process flow diagram (PFD) of the simulated (PAFC & ORC) system as constructed in (Aspen Plus). These schematic details the integration of electrochemical reactor blocks, heat exchangers, and stream connections, providing a visual representation of the mass and energy balance logic employed in this study. With the model successfully validated against established benchmarks, the framework is now deemed robust enough to proceed with a detailed sensitivity analysis of cell performance characteristics under varying operating conditions.

Table (1): Model Validation and Efficiency Benchmarking.

The study	HHV (KJ/mol)	m_{H2}(mol/s)	P_{elec} (KW)	Efficiency	Error (%)
[7]	286.630	2.61810	300.171	40%	
This Study	286.630	2.61810	300.129	39.9%	%0.00025

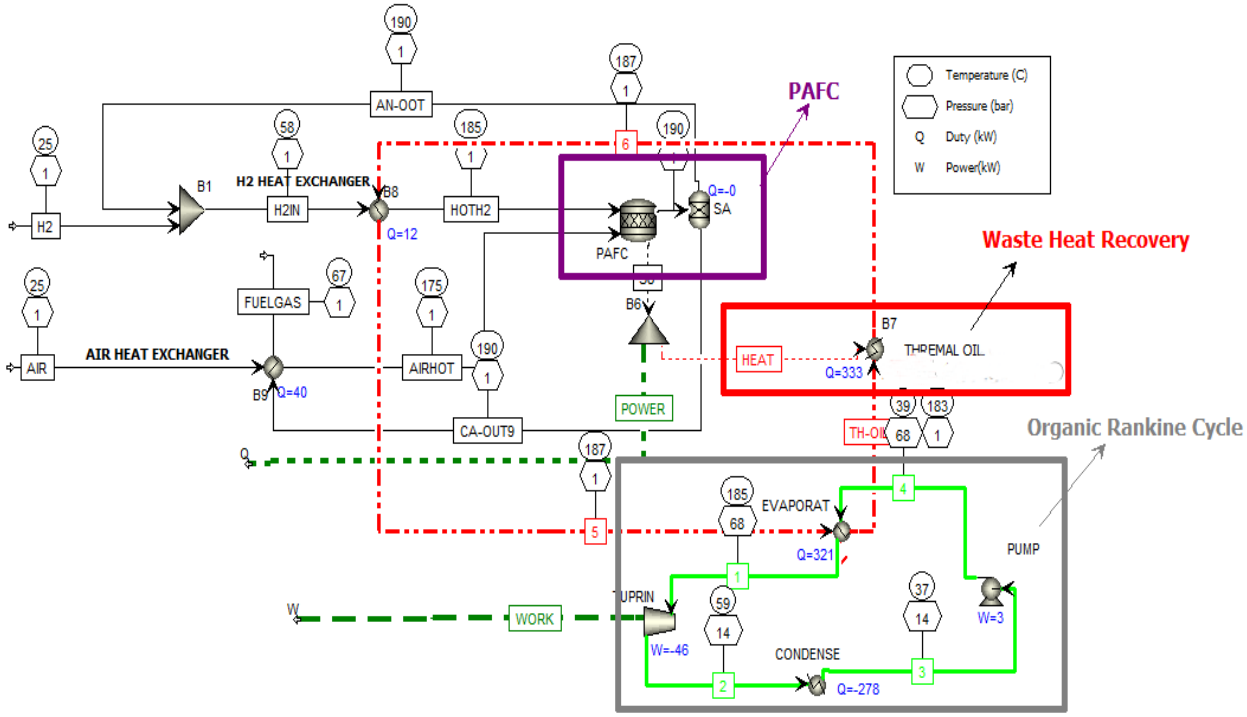

Figure (2): Aspen Plus simulation flowsheet of the studied and validated (PAFC & ORC) system.

4. Performance analysis of a phosphoric acid fuel cell (PAFC) using (EES) equation solving software:

A comprehensive study and performance analysis of the Phosphoric Acid Fuel Cell (PAFC) has been conducted using precise mathematical equations implemented in the Engineering Equation Solver (EES) software, based on the fundamental parameters outlined in **Table (2)** Subsequently, the equations presented above are employed to determine the actual operating voltage, quantify voltage losses, and generate the polarization and current density curves. This analytical approach facilitates a deeper understanding of the internal phenomena within the fuel cell, ultimately enabling the optimization of the overall system performance.
The **Table (2)** presents the input parameters entered into the (EES) software, followed by the voltage loss equations utilized to generate the study curves.

Table (2): Inputs and Simulation Results of (PAFC) [1][6][7]

Parameter	Unit	Value
Temperature	T_{cell}	463.2 [K]
Gas Constant	R	8.31441 [J/mol *k]

Faraday	F	96484.56 [C/mol]
Represents the reference potential at T_{cell}	E^0	1.089[V]
Partial pressure of hydrogen	P_{H2}	0.98692[Atm]
Partial pressure of oxygen	P_{O2}	0.20448[Atm]
Partial pressure of vapor	P_{H2O}	0.01085[Atm]
Number of electrons participating in the reaction	n	2[e]
Electron transfer coefficient	α	0.5
Current density	J	0.35 [A/cm^2]
Internal resistance	R_{OHM}	0.3[Ω]
Limiting current density	J_L	0.6 [A/cm^2]
Exchange current density	J_0	0.01[A/cm^2]
Fuel cell efficiency	$_{Cell}\eta$	40%
Hydrogen utilization	$_{H2}\lambda$	0.8
oxygen utilization	$_{O2}\lambda$	0.7

5. Result and discussion

This section presents a focused analysis of the Phosphoric Acid Fuel Cell (PAFC) performance, centered on the generation and interpretation of its polarization and power density curves. By quantifying activation, ohmic, and concentration losses, we evaluate the cell's electrochemical behavior under varying operating pressures and temperatures. These results establish a critical baseline for understanding the system's efficiency limits and optimal operational window.

5.1. Phosphoric acid fuel cell polarization curve

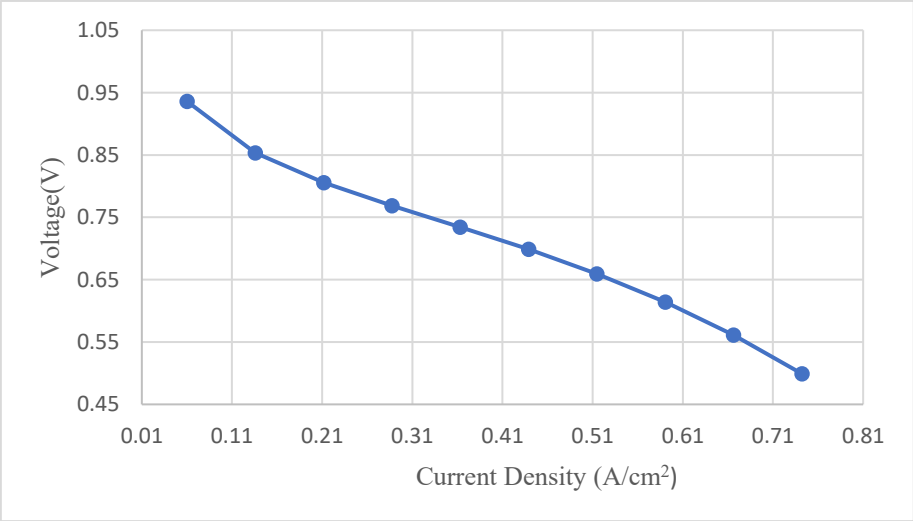

Figure (3): Polarization curve for a (PAFC) phosphoric acid fuel cell.

Figure (3) illustrates the polarization curve of the Phosphoric Acid Fuel Cell (PAFC). The voltage begins at a high value of approximately 0.94 V at near-zero current densities, then declines progressively as the current

density increases, reaching approximately 0.5 V at a high current density of about 0.75 A/cm². This voltage drop is not an anomaly; rather, it is the inherent consequence of the electrochemical and physical losses occurring within the cell during operation, a phenomenon that will be further elucidated in the subsequent curve depicted in **Figure (4**) Furthermore, as highlighted by Dr. Hassan Abdul-Zahra **[9]** in his academic lectures, these cells typically operate within a voltage range of 600–800 mV at current densities ranging from 100 to 400 mA/cm².

5.2. Phosphoric acid fuel cell loss analysis curve

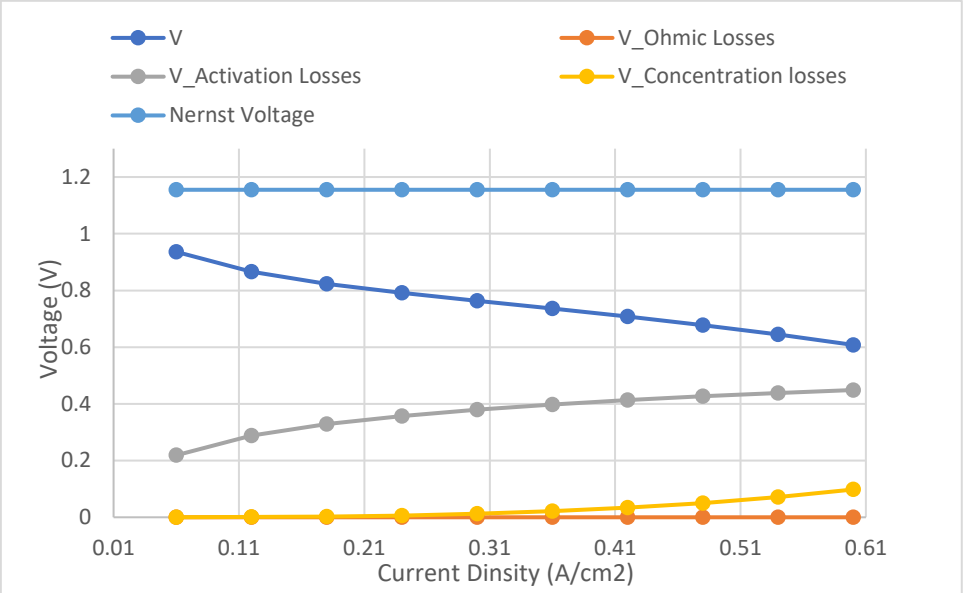

Figure (4): Phosphoric acid fuel cell effort loss curve.

The curve in Figure (4) illustrates the dynamic electrochemical behavior of the Phosphoric Acid Fuel Cell (PAFC) by depicting the gradual deviation of the actual operating voltage from the constant thermodynamic equilibrium voltage, known as the Nernst voltage. At low current densities, activation overpotential stemming from the sluggish kinetics of the electrochemical reactions on the catalyst surface dominates, resulting in an initial sharp drop in voltage. As the electrical load increases, ohmic losses progressively escalate due to the ionic resistance within the electrolyte and the electronic resistance in the external circuit, becoming the predominant factor in the intermediate operating region. Ultimately, concentration losses prevail as a result of the limited mass transport of reactants to the active reaction sites, causing a rapid decline in cell performance as the current density approaches its maximum limit. This progression reflects the complex interplay among thermodynamics, reaction kinetics, and mass transport in governing the energy conversion efficiency of the fuel cell.

5.3. The effect of current intensity and electrical power produced by fuel cells

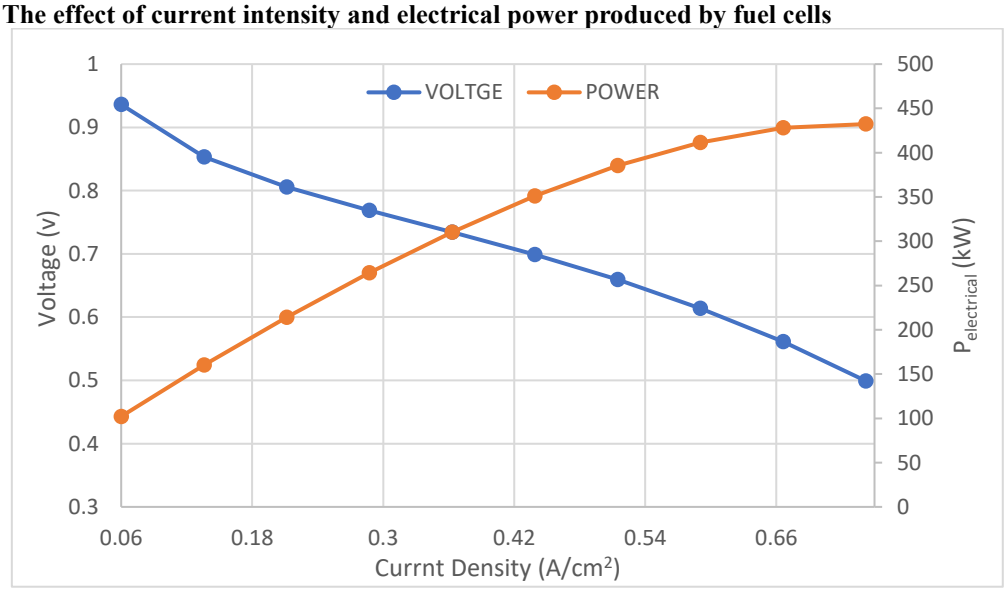

Figure (5): Polarization and electrical power curves of a phosphoric acid fuel cell (PAFC).

Figure (5) illustrates the relationship between current, cell voltage, and electrical power for the (PAFC), reflecting the cell's behavior under varying operating conditions. The blue curve, which depicts the voltage drop as the current increases, demonstrates the well-known physical phenomenon of voltage drop under load. This is a consequence of the internal losses incurred by the cell during operation, including activation losses resulting from sluggish electrochemical reactions at the electrode surfaces, ohmic losses caused by the electrical resistance of the cell materials, and concentration losses that emerge at high current densities due to reduced efficiency in gas transport to the reaction sites, as previously detailed in Figure (4) Conversely, the orange curve represents the electrical power output of the cell. It is a non-linear curve that gradually ascends with increasing current until it reaches its peak, after which it begins to gradually decline towards a saturation point at a current density of approximately 0.65–0.7 A/cm². It is strongly advised not to exceed this point in practical applications, as doing so leads to elevated temperatures, which accelerates the chemical degradation of materials, causes efficiency loss, and reduces the cell's lifespan. The peak of this curve, known as the Maximum Power Point (MPP), represents the optimal operating state of the cell, where the maximum utilization of the chemical energy stored in the fuel is achieved without unnecessary waste or loss. Regarding the specific operating point defined in this study, set at a voltage of 0.74 V and a current density of 0.35 A/cm², it is situated in the relatively stable region of the voltage curve. Here, the cell still maintains high energy conversion efficiency, even though the generated power, reaching approximately 300 kW, has not yet reached its theoretical peak. This indicates that the system was designed to operate within a safe and stable range, ensuring a longer lifespan for the components and minimizing thermal and electrochemical stress **[4]**.

5.4. The effect of operating pressure on the rate of heat wasted from fuel cells

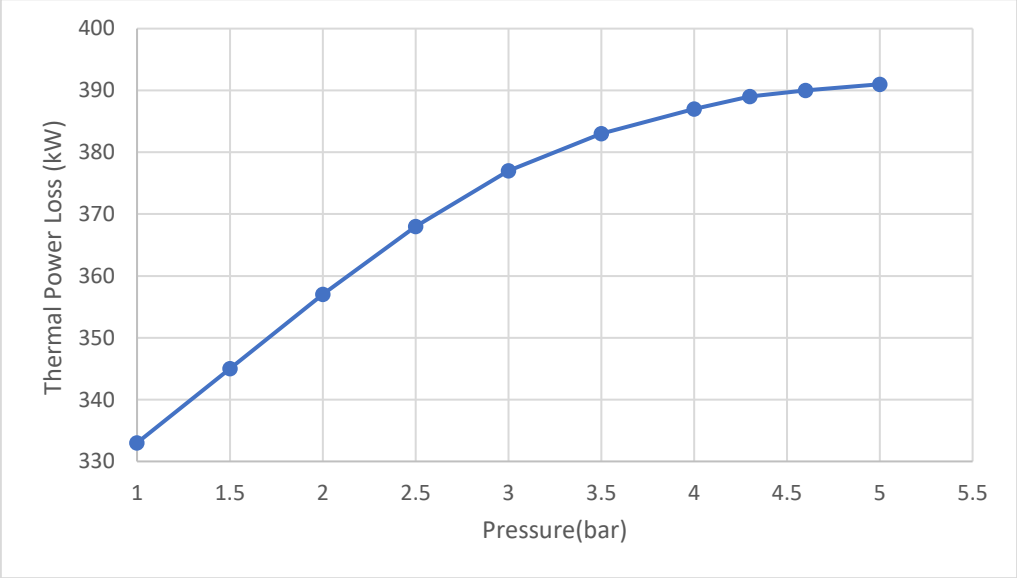

Figure (6): Impact curve of operating pressure on waste heat rate of (PAFC).

Figure (6) illustrates the relationship between operating pressure and the rate of waste heat rejection from the Phosphoric Acid Fuel Cell (PAFC). The curve exhibits distinct non-linear growth. In the initial pressure range from 1 to 3 bar, a sharp increase in the heat generation rate is observed as pressure rises. This behavior indicates that elevating the pressure increases the concentration of reactant gases (hydrogen and oxygen) on the electrode surfaces, thereby accelerating the electrochemical reaction rate. Consequently, thermal production resulting from activation and ohmic losses increases. Since this excess energy cannot be converted into electrical work, it is dissipated as waste heat, leading to a higher rate of heat rejection. Subsequently, in the pressure range from 3 to 4.5 bar, the curve begins to plateau. This transition indicates that the system is approaching a state of dynamic equilibrium driven by chemical saturation; despite the continued increase in pressure, the reactants cannot be transported to the active reaction sites with significantly greater efficiency. Finally, at pressures exceeding 4.5 bar, the curve becomes nearly horizontal, signifying that the waste heat rejection rate has reached a constant value. This plateau occurs because the available reaction sites become fully saturated, meaning there is no additional benefit to further increasing the operating pressure.

5.5. The effect of operating temperature on the rate of heat wasted from fuel cells

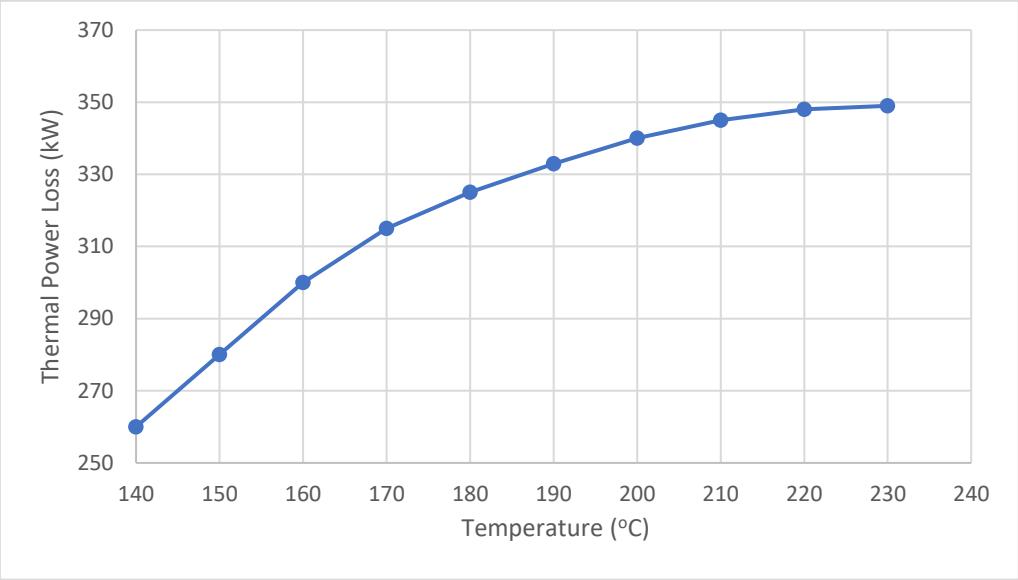

Figure (7): Curve showing the effect of operating temperature T (°C) of fuel cells (PAFC) on the rate of wasted heat.

Figure (7) illustrates the relationship between the operating temperature T (°C) and the rate of waste heat rejection for the Phosphoric Acid Fuel Cell (PAFC). The results reveal a non-linear relationship between temperature and the waste heat rejection rate. In the initial range from 140°to 180°C, the curve exhibits a quasi-linear increase. This is attributed to the fact that elevating the temperature accelerates the electrochemical reactions, thereby increasing the rate of heat generation driven by activation and ohmic losses. Furthermore, as the temperature rises, the electrical resistance of the phosphoric acid electrolyte decreases, facilitating electron conduction and reducing ohmic losses; however, this reduction in resistance leads to an increase in the electrical current, which consequently elevates the overall rate of waste heat rejection. Between 180° and 220°C, the curve begins to bend gradually, and the rate of increase in heat loss slows down. At 220°C, the heat rejection rate reaches 348 kW and then approximately stabilizes. This plateau occurs because the system approaches its operational limits; despite the continued rise in temperature, the reaction rate cannot increase significantly due to escalating concentration losses, which impede the efficient supply of reactant gases to the active sites. Beyond 220° C, adverse effects begin to manifest, most notably the evaporation of the phosphoric acid electrolyte. This leads to a decline in reaction efficiency and, consequently, a reduction in the rate of thermal waste. This behavior corroborates findings from previous studies, which establish that the optimal operating temperature range for (PAFC) lies between 150° and 220°C **[4,6,10]**.

6. Conclusions

This study concludes with a precise mathematical and performance analysis of the Phosphoric Acid Fuel Cell (PAFC) using (EES) software, providing deep insights into its electrochemical and thermodynamic dynamics. The polarization and power curve results demonstrate that the cell voltage decreases gradually from 0.94 V to 0.5 V as current density increases, governed by three primary loss mechanisms: activation, ohmic, and concentration losses. To ensure safe and stable operation, an optimal operating point was identified at 0.74 V and 0.35 A/cm² (yielding approximately 300 kW of power), with a strong recommendation not to exceed a current density of 0.7 A/cm² to prevent thermal stress and accelerate material degradation.

Thermally, the analysis revealed that increasing pressure and temperature leads to a non-linear rise in the waste heat rejection rate due to accelerated electrochemical reactions and reduced ohmic resistance. However, the system reaches a state of dynamic saturation at a pressure of 4.5 bar and a temperature of 220°C where waste heat peaks at 348 kW due to the dominance of concentration losses. Exceeding 220°C results in adverse effects, such as phosphoric acid evaporation and a subsequent drop in efficiency.

In conclusion, the primary novelty of this study lies in providing a practical, mathematically validated guideline for the optimal and sustainable operation of PAFC systems. By aligning seamlessly with established scientific literature, the findings confirm that precise control of electrical operating points (avoiding the saturation region), temperature 150°–220°C, and pressure up to 4.5 bar is essential for maximizing energy conversion efficiency, extending the cell's lifespan, and minimizing thermal and chemical losses.

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