

Steady State Analysis and Control of PEM Fuel Cell Power Plant

Arhan Sayyed, Vaibhav Dev, Ashish Singh & Shikhar Mishra

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Abstract / Simulation experiments with the help of ever-fast computers are now widely used to understand the behavior of a model of a system. Even if the real system is worth to be worked on directly, simulations are cheaper, more feasible, and less time-demanding. So has its importance increased that can now be considered a discipline in itself. A great advantage of the simulation study is that it can be easily applied to models which are dangerous and/or money extensive to produce very good results. An electrochemical cell that derives the electrical power output when fed with fuel is called a fuel cell. Among different types, fuel cells containing polymer electrolytes (PEFCs) are preferred due to their high electrical efficiency and fuel energy performance. PEMFCs find their purpose generally for applications in portable fuel cells, stationary fuel cells, and also in transport. Steady-state analysis has always been vibrant in understanding models for design, control, process optimization, etc. The (V vs i) polarization curve and (P vs i) Power curve provides us with critical fundamental characteristics of the fuel cell: the Limiting Current (i_o) and Maxima of Power (P_o) and their variation with Temperature and Pressure provide us with important insights for the designing of an efficient PEM Fuel Cell Power Plant.

1. Introduction

The global energy demand is rising every year by 1.8 percent, growing to almost 50 percent by 2050. The need for a cleaner source of energy to meet the supply demands is expected to be fulfilled by fuel cells as they can be a cleaner energy source, which is required to address climate change, air pollution, and energy independence. An electrochemical cell that derives the electrical power output when fed with fuel is called as a fuel cell. The output from the cell is derived indefinitely when the fed hydrogen fuel is converted into electrical energy through electrochemical reactions in the electrode stack system of the fuel cell. The electrochemical reaction taking place is the reaction of hydrogen and oxygen giving water as the product.



Fig.1 Fuel Cell Basic Diagram

Among different types, fuel cells containing polymer electrolytes (PEFCs) are preferred due to their high electrical efficiency, power density, and durability. PEMFCs find their purpose generally for applications in portable fuel cells, stationary fuel cells, and also in transport. The construction of a Polymer Electrolyte Membrane fuel cell (PEMFC) consists of a polymer electrolyte membrane (for example, a perfluorinated sulfonic acid polymer) which conducts protons, which are the ionic charge carriers. PEM fuel cells operate in temperatures ranging from 323.15K to 373.15K, and pressure ranging from 1atm to 3 atm.

2. Applications of fuel cell technology

2.1. Transportation system:

Experiments with buses are being carried out around the world by powering them with hydrogen fuel cells in order to enhance the road transportation system. The trains operating with this technology emit low noise levels and function efficiently in various European countries. Hydrogen and fuel cells can find their applications in short-haul flights also. Hence, fuel cell technology has the ability to revolutionize the transportation system of the world.

2.2. Power Supply Systems:

Fuel cell technology has an enormous potential to meet the energy demands of the world as an efficient energy source for power supply systems facilitating commercial buildings and residential apartments. They are also being tested as Backup generators for data centers and as a source of portable power for various electronic devices in order to increase the effectiveness of the system.

3. Advantages of PEM Fuel cell

3.1. Remarkable performance

The PEMFC has the highest power density among all the fuel cells in the industry. These cells are able to operate in low temperatures, hence they start with less time and power input which makes them tremendously beneficial over other cells. Other parameters such as less weight, compact size, and high power density encourage to find its application at various industrial levels.

3.2. Stricter legislation

The industrial applications of PEMFC being environment friendly, it is preferred over other fuel cells. The goal of reducing carbon emissions and becoming carbon neutral is being strictly followed with rules and regulations over using technologies with low-carbon, and fuel cell technology can become viable by 2030 if hydrogen production and distribution are scaled-up.

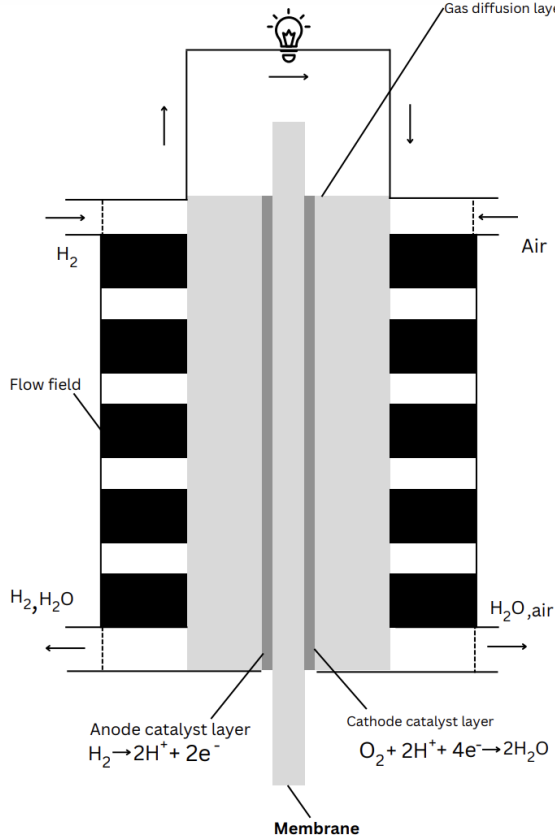


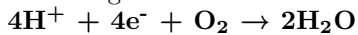
Fig.2 Internal Fuel Cell Diagram

4. Electrochemical reactions of fuel cell

The hydrogen stream is fed into the Electrode Assembly of the Membrane of the anode where it is split into protons and electrons catalytically, and the Oxidation part of the reaction (OHR) is given as:



The electrons generated are transported across the external circuit and the hydrogen ions (protons) generated are permeated to the cathode through the PEM, where the oxygen stream is combined with protons and electrons to generate water.



The electrons in the external circuit are used for power generation. The Operating Voltage or cell potential (V) is a function of Temperature (T), Pressure (P), and Current (i). The electrical power (P) generated by the fuel cell is the product of cell potential (V), and current (I) i.e ($P=V \cdot I$).

5. PEM fuel cell power plant

A fuel supply system, a humidifier water heater, a humidifier pump, a coolant pump, a stack of fuel cells, re-circulating blowers, gas heaters, inlet and outlet valves of the solenoid, mass flow rate controllers, humidifiers, and a control system make up a fuel cell power plant. The subsystems of the PEM fuel cell power component are:

5.1. Electrode system and Hydrogen Storage:

The electrode stack system is used to stack electrode materials into specific lengths and stacks the positive electrode, negative electrode, and separator alternately in layers. High-pressure tanks (350-700 bar or 5000-10,000 psi) are required for the storage of gaseous hydrogen, whereas liquid hydrogen needs freezing temperatures to prevent it from reversing its state and becoming a gas. Hydrogen can also be stored by adsorption and absorption processes, either on the surface of solid materials (as in surface adsorption) or inside of them (internal absorption).

5.2. Water Management System:

The water balance in the fuel cell stack is the primary problem with PEMFCs. By flooding the electrodes and obstructing diffusion to the catalyst sites, more water might cause problems. The cathode reaction and the humidification of the reactant gases cause water to form in the cell. Either the gas diffusion backing will move it to the flow channel, or heaters will evaporate it.

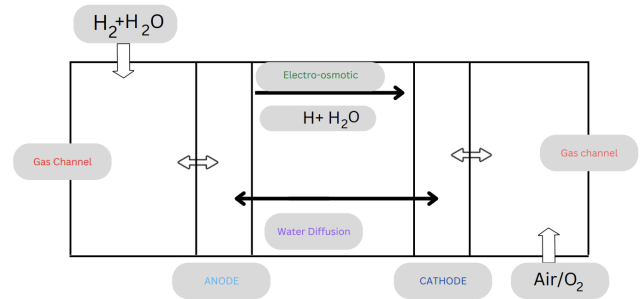


Fig.3 Water Management system of PEMFC

5.3. Gas Humidification System:

The electrical conductivity of the membrane electrolyte in the cell is ensured by humidifying the incoming reactant gases. To extract electricity from the fuel cell stack, humidification is required. The humidification unit comprises of controllers, membrane-based shell and tube-type humidifiers, thermocouples, and a hot water pump with a range of 7-10V, and 22-24V water heating coils. The gases used in the PEM fuel cell need to be humidified. Otherwise, conductivity declines, and more electricity is converted to heat before it exits the membrane.

5.4. Gas heating system:

The gas heating system is used to raise the temperature of the humidified gas by 2-3 degrees Celsius and lower the relative humidity of gases in order to prevent condensation caused by loss of heat in the gas tube lining from the humidifier to stack, which may cause flooding of water and obstruction of the flow of gas in bipolar plate channels.

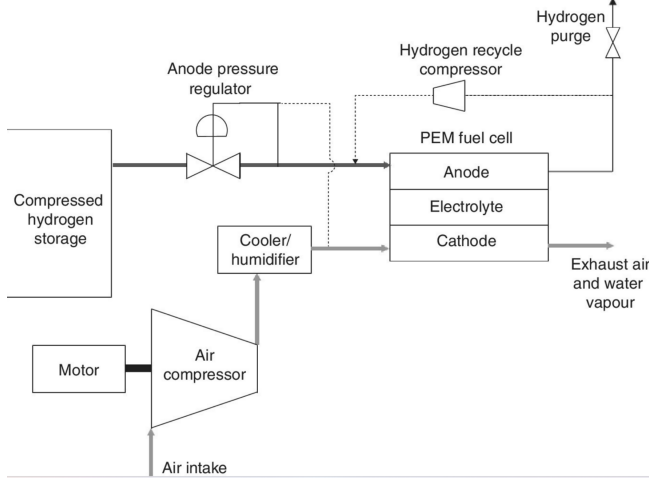


Fig.4 An Example of PEMFC Power Plant

6. Problem Formulation

6.1. Polarization curve and Power curve Equation:

The electrical power(P) generated by the fuel cell, as already said, is the multiplication product of cell potential(V) and current(I): $P=VI$. Kinetic and transport restrictions inside the cell place a limit on the actual current that the PEMFC can produce. Studying the link between operating voltage and current produced by the fuel cell is crucial for maximizing the power output of the cell. At the equilibrium potential, the fuel cell's maximum free energy is attained. As a consequence, the polarization curve illustrating the steady state potential-current(V vs I) relationship can be used to describe the fuel cell performance. Here, the actual operating voltage(V), is given by:

$$V = (E_{\text{thermo}}) - (V_{\text{act}}) - (V_{\text{ohm}}) - (V_{\text{conc}}) \quad (i)$$

We synthesize the above equation after combining the effects of the losses that recurred in the fuel cell system.

6.2. Open Circuit Voltage(E_{thermo}):

Gibb's free energy of formation, which is dependent on the temperature and pressure of the reactants, is the free energy of the fuel cell. One mole of H_2 molecules consumed in the process produces a total charge release in the hydrogen fuel cell that is equal to: $(-2)N_A \cdot e = (-2) \cdot F$ Coulombs/mol

If E_{thermo} is the open circuit voltage, to drive these electrons around the electrical circuit, the electrical work done is given by,

$$\text{Electrical work} = (\text{Charge}) \cdot (\text{Voltage}) = (-2)F \cdot E_{\text{thermo}}$$

Hence, we consider the equation: $E_{\text{thermo}} = \Delta G/2F$

The Gibbs Function(G) is defined in terms of temperature(T), pressure(P), enthalpy(H), and entropy(S), such that: $G = H - TS$.

Thermodynamically, The Gibbs energy change is formulated as follows:

$$dG = dH - TdS - SdT$$

Using the 1st & 2nd laws of thermodynamics as follows:

$$dV = TdS - PdV,$$

$$dH = dU + PdV + VdP$$

On putting these values in the Gibbs Energy Change equation, then we get:

$$dG = VdP - SdT$$

Using the ideal gas equation to calculate Volume(V), $V=nRT/P$, where n = Number of moles of gas. On substituting $n=1$, we get the following integral equation:

$$\int dG = \int (RT/P) \cdot dP - \int SdT$$

Here, the first term on the RHS is the constant temperature contribution to ΔG and the second term is the constant pressure contribution to ΔG .

On integrating the equation, we get:

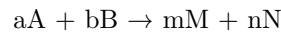
$$G = G^\circ + RT \cdot \ln(P/P_o) - S(T-T_o)$$

Here, (T)= Temperature of the chemical reaction, (T_o) = Reference Temperature and G° = Reference Gibb's Free Energy.

For an ideal gas, the ratio of the partial pressure of the gas over the standard pressure is the activity of gas, $a_i = P_i/P_o$.

Here, P_i = Partial pressure of the gas (i),
 P_o = Standard pressure = 1 atm.

For a chemical reaction,



The Gibbs free energy of formation ΔG_f of the reaction is equal to the difference between that of products and the reactants.

$$\Delta G_f = m \cdot (G_M) + n \cdot (G_N) - a \cdot (G_A) - b \cdot (G_B)$$

On putting $G = G^\circ + RT \cdot \ln(P/P_o) - S(T-T_o)$, we get:

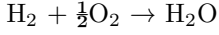
$$\Delta G^\circ = m \cdot (G_M)_o + n \cdot (G_N)_o - a \cdot (G_A)_o - b \cdot (G_B)_o$$

$$\Delta S^\circ = m \cdot (S_M)_o + n \cdot (S_N)_o - a \cdot (S_A)_o - b \cdot (S_B)_o$$

We get, (ΔG° , ΔS° for reaction)

$$G = G^\circ + RT \cdot \ln([a_M]m \cdot [a_N]n / [a_A]a \cdot [a_B]b) - S^\circ(T - T_o)$$

Applying this equation to hydrogen fuel cell reaction, we get:



$$\Delta G = \Delta G^\circ + RT \cdot \ln([a_{H_2O}] / [a_{H_2}] \cdot [a_{O_2}]^{0.5}) - \Delta S^\circ(T - T_o)$$

Because the fuel cell's end product is liquid, then $[a_{H_2O}]$ can be assumed as unity, $[a_{H_2O}] = 1$

$$\Delta G = -nF \cdot (E_{cell}), n=2$$

For temperature $T_o = 298.15K$, $\Delta G^\circ = -2F \cdot (E)_o$,

On putting ΔG and ΔG° values in the equation, we get:

$$E_{cell} = E_o + RT/2F \ln([P_{H_2}] \cdot [P_{O_2}]^{0.5}) + \Delta S^\circ/2F(T - T_o)$$

Here we have, $\Delta G^\circ = -237kJ/mol$, $(E)_o = 1.228V$, and $\Delta H_o = -241.83kJ/mol$. Also, $\Delta S^\circ = (\Delta H^\circ - \Delta G^\circ)/T_o$ and $E_{thermo} = E_{cell}$. Hence, $\Delta S^\circ = 163.8 J/molK$.

On putting all the values in the equation, we get:

$$E_{thermo} = 1.22 - 0.85 \cdot (10)^{-3}(T - 298.15) + 4.3086 \cdot (10)^{-5}T(\ln[P_{H_2}] + 0.5\ln[P_{O_2}]) \quad (ii)$$

Here, T is in Kelvin and P_{H_2}, P_{O_2} are in atm.

6.3. Activation losses(V_{act}):

The voltage needed to overcome the electrochemical reaction's activation energy on the catalytic surface gives rise to activation voltage loss. The cause of the activation loss is the reaction kinetics at the surface of the electrodes and activation overvoltage occurs at the cathode and is the most important cause of voltage drop and irreversibility. The activation overvoltage is related to the current density described by the Tafel equation, which is approximated by:

$$V_{act} = RT/2F \ln(i/i_o) \quad (\text{for } i \text{ greater than } i_o)$$

where i_o = Exchange current density

When this activation voltage is calculated experimentally to check its variation with temperature and current, we get:

$$V_{act} = \varepsilon_1 + \varepsilon_2 + \varepsilon_3 \cdot (T) \ln[O_2] + \varepsilon_4 \cdot T \ln(i)$$

where $[O_2] = ([P_{O_2}] \cdot \exp(498/T) / (5.08) \cdot 10^6)$ and $[P_{O_2}]$ is in Pascal.

$$\varepsilon_1 = -0.9514$$

$$\varepsilon_2 = +0.00312$$

$$\varepsilon_3 = -0.000187$$

$$\varepsilon_4 = +(7.4) \cdot 10^{-5}$$

On substituting the values and rearranging the equation to the requisite nature, we get:

$$V_{act} = -0.9514 + 0.00312T + (7.4) \cdot 10^{-5} \ln(i) - 0.000187 \cdot (T) \ln([0.21P] \cdot \exp(498/T) / (50.8)) \quad (iii)$$

6.4. Ohmic Losses(V_{ohm}):

The Ohmic loss is due to the flow of electrons and protons in the electrode and electrolyte respectively. The drop experienced by the voltage due to the ohmic losses is proportional to the current density, as follows: (V_{ohm}) = $i \cdot (R_{ohm})$, where r is the resistance, (the total internal resistance) and I , the current. The ohmic resistance is the ratio of membrane thickness t_m and membrane conductivity k_m , given as:

$$(R_{ohm}) = t_m / k_m$$

The membrane conductivity is the function of membrane water content λ_m , and Fuel cell temperature(T) in the form of:

$$k_m = (b_{11} \cdot \lambda_m - b_{12}) \exp(b_2 \cdot (1/303 - 1/T))$$

where, $\lambda_m = 0.063$, $b_{11} = 0.05139$, $b_{12} = 0.00326$, $b_2 = 1268$ and $t_m = 0.01275 \text{ cm}$ (Nafion 115).

On putting the values, the equation simplifies to:

$$V_{ohm} = K \cdot i \cdot \exp(-1/303 - 1/T), \text{ where } K = 0.033 \quad (iv)$$

6.5. Concentration losses(V_{conc}):

The high current density loss is the cause of the concentration overvoltage. The concentration loss term is usually ignored in the various models, because of higher order and less contribution to the overall value under moderate conditions. However, if the current density is high, this term can't be neglected.

The concentration loss is caused as a result when the concentration of the fuel and the oxidant gases are reduced at the active membrane surface (in the region of the electrode), as the oxygen is extracted. The extent of this reduction in concentration depends on the current from the fuel cell, and on physical factors.

Similarly, if hydrogen is supplied to the anode of a fuel cell, the current drawn from the cell consumes hydrogen and there will be a pressure drop which will result in a reduction in voltage.

Hence, $V_{conc} = m \cdot \exp(ni)$, where $m = (4.15) \cdot 10^{-10} V$ and $n = 8 \cdot 10^{-2} \text{ cm/mA}$. On substituting these values, we get the equation as follows:

$$V_{conc} = ((4.15) \cdot 10^{-10}) \exp(n = 8 \cdot 10^{-2} \cdot i) \quad (v)$$

6.6. Equation Formulation:

As we have formulated the equations of all the components of the operating Voltage(V), the substitution of these equations will provide the Polarization curve and Power Curve Equation. After substituting the equations (ii), (iii), (iv), and (v) in equation (i), we get:

$$V = 1.22 - 0.85 \cdot (10)^{-3} \cdot (T-298.15) + 4.3086 \cdot (10)^{-5} \cdot T \cdot (\ln[P_{H_2}] + (0.5) \cdot \ln[P_{O_2}]) - (-0.9514 + 0.00312 \cdot T - 0.000187 \cdot (T) \cdot \ln([P_{O_2}] \cdot \exp(498/T)/50.8) + (7.4) \cdot 10^{-5} \cdot T \ln(i)) - 0.033i \cdot (\exp(-1268(1/303-1/T))) - ((4.15) \cdot 10^{-10}) \cdot \exp(8 \cdot 10^{-2} \cdot i))$$

Here, Temperature(T) is in Kelvin and Pressure $[P_{H_2}]$, $[P_{O_2}]$ are in atm. Generally, the operating temperature of the fuel cell lies between 50°C to 100°C and the pressure of Hydrogen and Air lies between 1 atm to 3 atm. Considering the mechanical operation of the fuel cell, we take $[P_{H_2}] = [P_{air}] = P(\text{atm})$. From this, we specifically consider $[P_{O_2}] = 0.21P$. (Generally, the air contains 21 mol% O_2 approximately.) On substituting the values of $[P_{H_2}]$ and $[P_{O_2}]$, we get the Polarization curve equation:

$$V = 1.22 - 0.85 \cdot (10)^{-3} \cdot (T-298.15) + 4.3086 \cdot (10)^{-5} \cdot T \cdot (\ln[P] + (0.5) \cdot \ln[0.21P]) - (-0.9514 + 0.00312 \cdot T - 0.000187 \cdot (T) \cdot \ln([0.21P] \cdot \exp(498/T)/50.8) + (7.4) \cdot 10^{-5} \cdot T \ln(i)) - 0.033i \cdot (\exp(-1268(1/303-1/T))) - ((4.15) \cdot 10^{-10}) \cdot \exp(8 \cdot 10^{-2} \cdot i))$$

We can derive the Power equation using the Polarization curve equation. This is because we know that the Power of the fuel can be calculated using the equation: $P = V \cdot i$, where $V =$ Cell potential, $i =$ Current. On substituting the Voltage equation, we get the Power Curve equation as follows:

$$P = 1.22 \cdot i - 0.85 \cdot (10)^{-3} \cdot i \cdot (T-298.15) + 4.3086 \cdot (10)^{-5} \cdot i \cdot T \cdot (\ln[P] + (0.5) \cdot \ln[0.21P]) - (-0.9514 \cdot i + 0.00312 \cdot i \cdot T - 0.000187 \cdot i \cdot (T) \cdot \ln([0.21P] \cdot \exp(498/T)/50.8) + (7.4) \cdot 10^{-5} \cdot i \cdot T \ln(i)) - 0.033(i^2) \cdot (\exp(-1268(1/303-1/T))) - ((4.15) \cdot 10^{-10}) \cdot i \cdot \exp(8 \cdot 10^{-2} \cdot i))$$

7. Numerical Analysis and Application of Polarization curve & Power curve equation

7.1. Steady State Analysis of PEM Fuel Cell

We know that the theoretical equation for Fuel Cell Voltage is a function of three input variables: Temperature(T), Pressure(P), and Current(i). So, Fuel Cell Voltage can be written in the form of $V = f(T, P, i)$.

$$V = 1.22 - 0.85 \cdot (10)^{-3} \cdot (T-298.15) + 4.3086 \cdot (10)^{-5} \cdot T \cdot (\ln[P_{H_2}] + (0.5) \cdot \ln[P_{O_2}]) - (-0.9514 + 0.00312 \cdot T - 0.000187 \cdot (T) \cdot \ln([P_{O_2}] \cdot \exp(498/T)/50.8) + (7.4) \cdot 10^{-5} \cdot T \ln(i)) - 0.033i \cdot (\exp(-1268(1/303-1/T))) - ((4.15) \cdot 10^{-10}) \cdot \exp(8 \cdot 10^{-2} \cdot i))$$

For steady-state analysis of the fuel cell reaction, it is considered that $T = 327.41K$, $[P_{H_2}] = 1 \text{ atm}$, and $[P_{O_2}] = 0.21 \text{ atm}$. On simplifying the equation based on these general parameters, we get:

$$V_{th} = 0.8820623 - 0.0305869 \cdot i - 0.024229 \cdot \ln(i) - 4.52 \cdot (10)^{-10} \cdot \exp(i)$$

The curve-fitting equation to the experimental data was derived by obtaining the coefficients of the equation from the graph of the reference paper with the help of DESMOS and Microsoft Excel. On substituting these values, we get:

$$V_{cf} = 0.79785 - 0.01712 \cdot i - 0.0601 \cdot \ln(i) - 3.168 \cdot (10)^{-5} \cdot (i^3)$$

On comparing the theoretical equation with the experimental data obtained at integral values, we see that the curve-fitting equation nearly fits completely with the experimental data, while the theoretical equation shows a symmetrical curve but takes a sharp change towards the higher values of current. The graphical analysis of the equations provides us with the variation between the nature of the curve between the theoretical, curve-fitting equation and the experimental data of the polarization curve.

Current (i)	Experimental Voltage(Vexp)	Theoretical Voltage(Vth)	Curve fitting Voltage(Vcf)	Relative Error(%) in Vth	Relative Error(%) in Vcf
1	0.780702157	0.851475399	0.78069832	9.065331851	0.000491535
2	0.722966838	0.804094234	0.721698414	11.22145466	0.175446953
3	0.682504363	0.763683314	0.679608041	11.89427577	0.424366708
4	0.642880518	0.726126149	0.644026189	12.94884952	0.178208948
5	0.609882	0.690132662	0.611562781	13.15839157	0.275591256
6	0.578914382	0.655128177	0.580602376	13.16495106	0.291579161
7	0.55002967	0.620806047	0.55019456	12.86773793	0.02997833
8	0.519236636	0.586982962	0.519695403	13.04729326	0.088354272
9	0.486524514	0.553539979	0.488622083	13.7743245	0.431133215
10	0.454659705	0.520394	0.456584636	14.45791095	0.423378445
11	0.423529	0.487480705	0.423250414	15.09972292	0.065777289
12	0.389662348	0.454739059	0.38832407	16.70079525	0.343445418
13	0.351306158	0.422086273	0.351535584	20.14770122	0.06530649
14	0.313991107	0.389359864	0.312632734	24.00346874	0.432614926
15	0.273176	0.356166391	0.271376183	30.37982521	0.658848906

Fig.5 Polarization curve analysis dataset

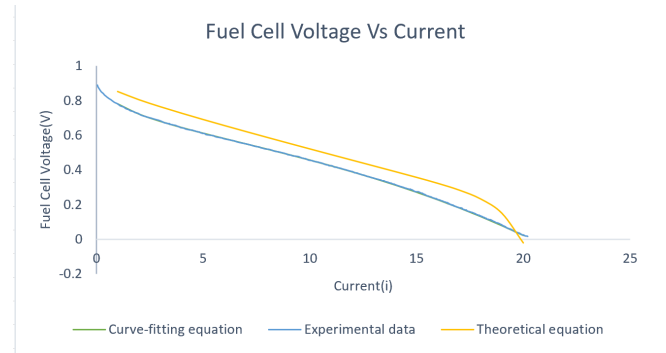


Fig.6 Polarization curve of Experimental Data, Theoretical and Curve-fitting Voltage with Current

On comparing the theoretical equation with experimental data, we see a relative error ranging between 5 percent to 30 percent, but while comparing the curve-fitting equation with the experimental data, we see a relative error of less than 1 percent. The significant error observed between experimental data and the theoretical equation is mainly because in the theoretical equation we have taken concentration loss to be an exponential function of current, while in the following conditions of experimentation, the concentration loss is contributing in the form of cubic function of current. The graphical analysis of experimental vs theoretical concentration losses shows us the origination of this error.

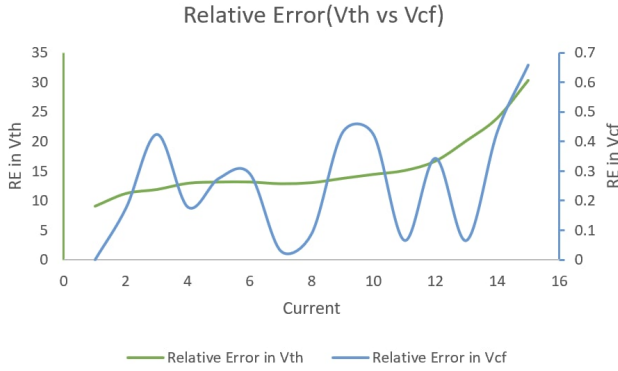


Fig.7 Error variation analysis of Polarization curve in Theoretical equation vs Curve fit equation with respect to experimental data

The graphical analysis of the concentration losses shows us that the exponential function varies similarly to the cubic function of current until a particular value of current is reached. After this value, the curve of the exponential function goes towards maximum deviation and then starts coming towards the cubic function.

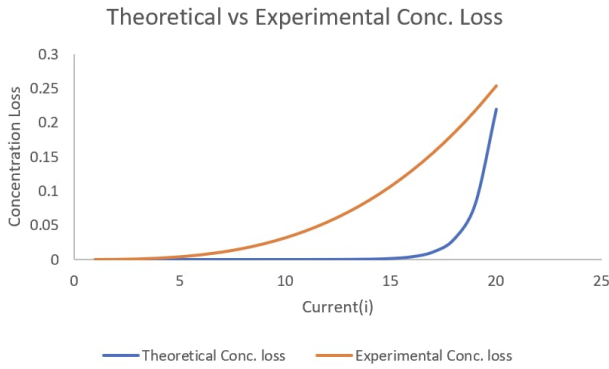


Fig.8 Variation of Concentration Losses with Current

Using the Polarization curve (V vs i), we can also derive the variation of Power (P) with current (i) ($P=iV$). On putting the values of V in the Power (P), we get the theoretical and curve-fitting equations, we get:

$$P_{th} = 0.8820623 \cdot i - 0.0305869 \cdot i^2 - 0.024229 \cdot \ln(i) - 4.52 \cdot (10)^{-10} \cdot i \exp(i)$$

$$P_{cf} = 0.79785 \cdot i - 0.01712 \cdot i^2 - 0.0601 \cdot \ln(i) - 3.168 \cdot (10)^{-5} \cdot (i^4)$$

On comparing the theoretical equation with the experimental data obtained at integral values, we see that the curve-fitting equation nearly fits completely with the experimental data, while the theoretical equation shows a symmetrical curve but takes a sharp change towards the higher values of current, similar to the Voltage variation of current. The graphical analysis of the equations provides us with the variation between the nature of the curve between the theoretical, curve-fitting equation and the experimental data as a curve with maxima at a particular current value within the domain of the input variable.

Current(i)	Experimental Power(Pexp)	Theoretical Power(Pth)	Curve fitting Power(Pcf)	Relative Error in Pth	Relative Error in Pcf
1	0.780702157	0.851475	0.780698	9.065332	0.000492
2	1.445933675	1.608188	1.443397	11.22145	0.175447
3	2.047513088	2.29105	2.038824	11.89428	0.424367
4	2.571522073	2.904505	2.576105	12.94885	0.178209
5	3.04941	3.450663	3.057814	13.15839	0.275591
6	3.473486293	3.930769	3.483614	13.16495	0.291579
7	3.850207692	4.345642	3.851362	12.86774	0.029978
8	4.153893085	4.695864	4.157563	13.04729	0.088354
9	4.378720627	4.98186	4.397599	13.77432	0.431133
10	4.546597047	5.20394	4.565846	14.45791	0.423378
11	4.658819	5.362288	4.655755	15.09972	0.065777
12	4.675948174	5.456869	4.659889	16.7008	0.343445
13	4.566980053	5.487122	4.569963	20.1477	0.065306
14	4.395875496	5.451038	4.376858	24.00347	0.432615
15	4.09764	5.342496	4.070643	30.37983	0.658849

Fig.9 Power curve analysis dataset

This equation provides the best representation of the variation of the energy produced per unit time in the fuel cell with respect to current (i). Here, again on comparing the theoretical equation with experimental data, we see a relative error ranging between 5% to 30%, but while comparing the curve-fitting equation with the experimental data, we see a relative error of less than 1%.

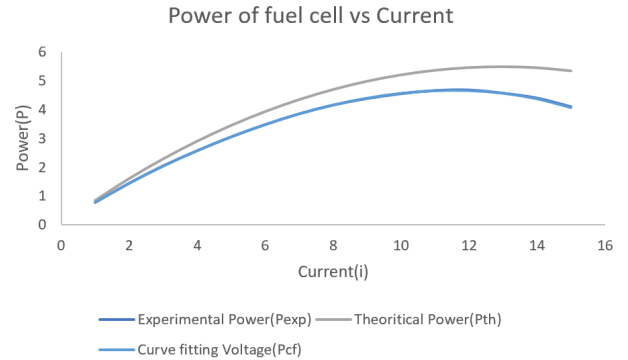


Fig.10 Power curve of Experimental Data, Theoretical and Curve-fitting Voltage with Current

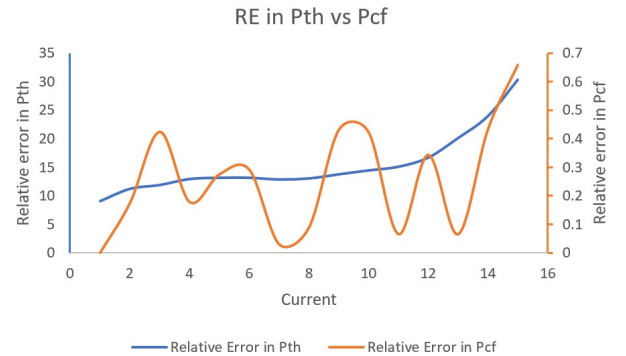


Fig.11 Error variation analysis of Power curve in Theoretical equation vs Curve fit equation with respect to experimental data

7.2. Contribution of Steady State Analysis to Polarization Curve and Power Curve

The Polarization curve(V vs i) and the Power curve(P vs i) give us information regarding two important fundamental points for the characteristics of the fuel cell i.e the Limiting Current point(i_o)(X-intercept value of the Polarization curve) and Power Maxima point(P_o)(Maxima of the Power curve). The characteristic study of the following points is essential for designing and articulating an efficient PEM Fuel Cell.

7.3. Shifting of Polarization Curve (V vs i) with Pressure and Temperature

7.3.1. Shifting of Polarization curve at Constant Temperature and Varying Pressure

We used the theoretical voltage equation to analyze the shifting of the Polarization curve by keeping the standard temperature of the fuel cell($T = 327.41$ K) in the equation and varying the pressure at three values of Pressure(P)= 1atm, 2atm, and 3atm and represented the curves in colors red, blue and green respectively using DESMOS. After the graphical analysis, we see that the Operating Voltage Curve shifts upwards as the pressure increases.

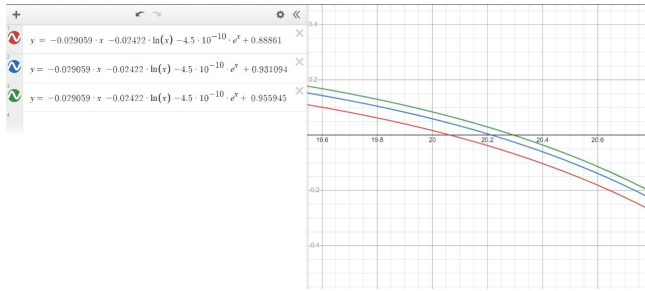


Fig.12 Variation of Polarization curve at constant temperature

7.3.2. Shifting of Polarization curve at Constant Pressure and Varying Temperature

We used the theoretical voltage equation to analyze the shifting of the Polarization curve by keeping the standard pressure of the fuel cell($P = 1$ atm) in the equation and varying the pressure at three values of Pressure(P)=50°C, 70°C, and 80°C, and represented the curves in colors red, blue and green respectively using DESMOS. After the graphical analysis, we see that the Operating Voltage Curve shifts upwards as the temperature increases.

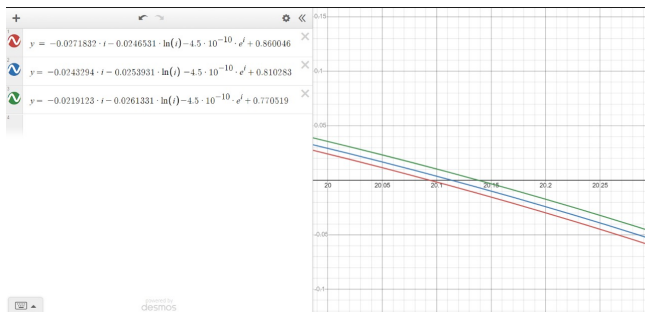


Fig.13 Variation of Polarization curve at constant pressure

7.4. Variation Of Limiting Current(i_o) with Temperature of Fuel Cell(T) using Newton-Raphson Method

The limiting current(i_o) is the value of the X-intercept of the Polarization curve i.e it is a root of the $V=f(i)$ function at a constant temperature. We know that the fuel cell operates from temperatures between 50°C to 100°C, and pressure ranging from 1atm to 3atm. The significance of the voltage losses can be explained with the help of the polarization curve diagram(below).

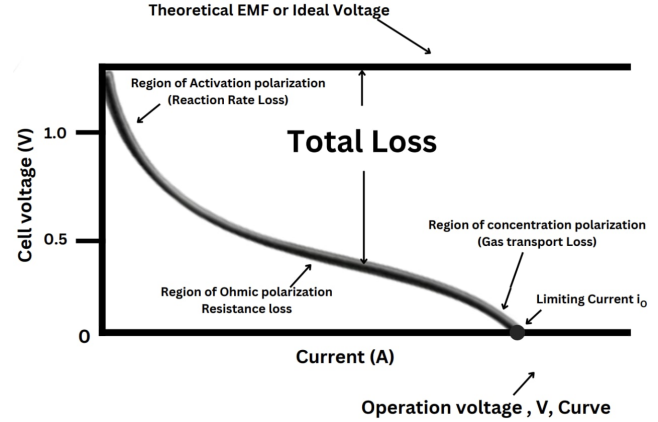


Fig.14 Significance of Voltage losses in Polarization Curve

In real-life experimentation analysis, the following current value is obtained when the Voltage loss is maximum i.e the voltage nearly tends to zero. The limiting current provides us with the boundary condition for the polarization curve in real-life experimentation analysis. Here, we studied the variation of Limiting Current(i_o) with the Temperature of the Fuel Cell(T) by finding the root of the equation using the Newton-Raphson Method with the help of a designed C++ program. The algorithm for the following code is as follows: The variation of voltage with current is as follows:

$$V = a \cdot i + b \cdot \ln(i) + d \cdot \exp(x) + c$$

Where a,b,c,d are temperature dependent parameters whose values are as follows:

$$\begin{aligned} a &= -0.033 \cdot (\exp(-1268(1/303-1/T))) \\ b &= (7.4) \cdot 10^{-5} T \\ c &= 1.22 - 0.85 \cdot 10^{-3} (T-298.15) + 4.3086 \cdot 10^{-5} T \cdot \ln[P] \\ &\quad + (0.5) \cdot 4.3086 \cdot 10^{-5} T \cdot \ln[0.21P] - (-0.9514 + 0.00312T \\ &\quad - 0.000187 \cdot (T) \ln([0.21P] \cdot \exp(498/T)/50.8)) \\ d &= (4.5) \cdot 10^{-10} \end{aligned}$$

Therefore, our final equation is:

$$\begin{aligned} V &= 1.22 - 0.85 \cdot (10)^{-3} \cdot (T-298.15) + 4.3086 \cdot (10)^{-5} \cdot T \cdot (\ln[P_{H_2}] + (0.5) \cdot \ln[P_{O_2}]) - (-0.9514 \\ &\quad + 0.00312 \cdot T - 0.000187 \cdot (T) \cdot \ln([P_{O_2}] \cdot \exp(498/T)/50.8) \\ &\quad + (7.4) \cdot 10^{-5} \cdot T \ln(i)) - 0.033 \cdot (\exp(-1268(1/303-1/T))) - \\ &\quad ((4.5) \cdot 10^{-10}) \cdot \exp(8 \cdot 10^{-2} \cdot i) \end{aligned}$$

The Newton-Raphson Method is used with Initial guess ϵ (0,89] to find values of i_o (Limiting Current) at a constant pressure of 1 atm for different temperatures. The algorithm is called "step-ladder".

Ladder 1: We have designed a code that gives us the root for the equation;

$$V = a \cdot i + b \cdot \ln(i) + d \cdot \exp(x) + c, \text{ for constant } a, b, c, d.$$

Ladder 2: Now we have defined functions $a(t)$,

$b(t)$, $c(t)$, and $d(t)$ which are functions of temperature, and we call them in our main function as a, b, c, d i.e.

$$V = a(T) \cdot i + b(T) \cdot \ln(i) + d(T) \cdot \exp(x) + c(T)$$

Ladder 3: Until ladder 2, our code is ready to give us the value of saturation current I_0 (the value where $V = 0$) for a particular temperature obtained by user input. Now we used a for loop to vary the temperature from 323K to 373K.

Output: Combining all 3 ladders we got a code that will provide us:

1. Values of a, b, c, d for different temperatures.
2. Value of Limiting current for different temperatures.

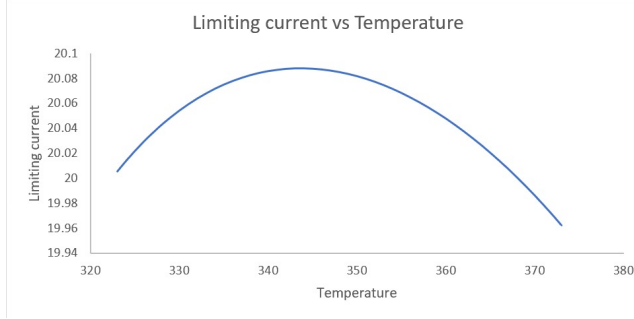


Fig.15 Variation of Limiting Current(i_0) with Temperature(T)

7.4.1. Excel Analysis for variation of Limiting Current(i_0) with Temperature(T):

Taking data from our code i.e. i_0 from temperature 323K to 373K, we used Excel to analyze the variation of limiting current with temperature.

Fuel Cell Temperature (K)	Current (A)	Fuel Cell Temperature (K)	Current (A)	Fuel Cell Temperature (K)	Current (A)	Fuel Cell Temperature (K)	Current (A)
323	20.0057	338	20.083	353	20.0749	368	20.0009
324	20.0143	339	20.0848	354	20.0719	369	19.9938
325	20.0223	340	20.0862	355	20.0686	370	19.9864
326	20.0298	341	20.0872	356	20.065	371	19.9787
327	20.0367	342	20.088	357	20.0612	372	19.9708
328	20.0432	343	20.0884	358	20.0571		
329	20.0491	344	20.0884	359	20.0527		
330	20.0546	345	20.0881	360	20.0481		
331	20.0596	346	20.0875	361	20.0431		
332	20.0642	347	20.0866	362	20.0379		
333	20.0683	348	20.0854	363	20.0324		
334	20.0721	349	20.0839	364	20.0267		
335	20.0754	350	20.0821	365	20.0206		
336	20.0783	351	20.08	366	20.0143		
337	20.0808	352	20.0776	367	20.0078		

Fig.16 Limiting Current(i_0) variation datasheet

From Graphical Analysis, we see that the Limiting current(i_0) increases from 323K to 343.5K, attains a maximum value of 20.884A, and then decreases from 343.5K to 373K. This shows us that the maximum value of Voltage loss for the following conditions of the PEM fuel cell will be obtained at 343.5K between the temperature range of 323K to 373K.

7.5. Variation Of Maxima of Power(P_o) with Temperature of Fuel Cell(T) using Newton-Raphson Method:

We know that, Power (P) = $V \cdot i$, where V =Voltage and i =current. On substituting the value the V in the equation, we get:

$$P = i^2 \cdot a(T) + b(T) \cdot i \cdot \ln(i) + d(T) \cdot i \cdot \exp(x) + i \cdot c(T)$$

Using the code (that we have shared in the file), we can get the maximum value of power for different temperatures, here we have shown our analysis for temperature 327.41K because the fuel cell used in the reference paper operates at the following considered temperature. At this operating temperature of the fuel cell, we get the values of $a(T)$, $b(T)$, $c(T)$, and $d(T)$ as follows:

$$\begin{aligned} a(T) &= -0.029059 \\ b(T) &= -0.0242283 \\ c(T) &= 0.882062 \\ d(T) &= -4.5 \cdot e^{-10} \end{aligned}$$

This gives us the value of current which gives the maximum value of power from the fuel cell. As per analysis from code, the value of current at which power is maximum is 13.9466 A, which we obtained by Newton-Raphson and calculated the real value using DESMOS, an error of 0.2% is observed in the value of current at Maxima of Power(P_o)=5.754W at 327.41K.

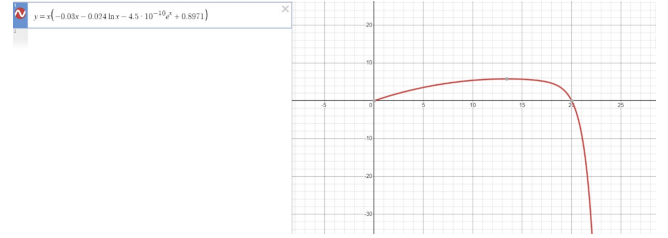


Fig.17 Maxima of Power(P_o) at 327.41K

On analyzing the variation of Maxima of Power(P_o) in the temperature range of 323K to 373K using Graphical Analysis, we get that the value of current at which the Maxima of Power is obtained decreases with temperature. In contrast, the value of the Maxima of Power(P_o) increases with temperature. The following result is obtained by applying Newton-Raphson Method on the derivative of the Power equation by modifying the code of the "step ladder" algorithm. The modified "step ladder" algorithm provides us the root of the derivative of the Power equation using Newton-Raphson Method and then provides us the value of Power by putting the value of the root in the Power equation.

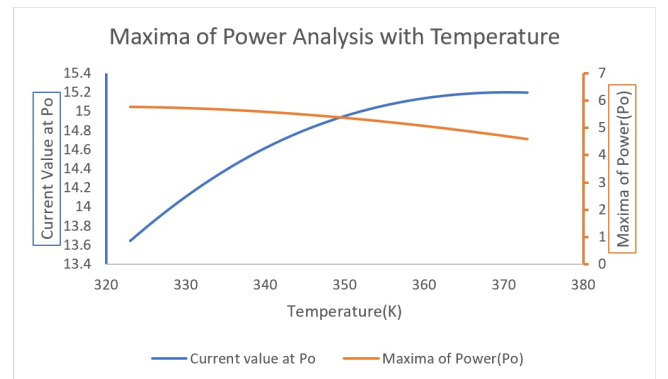


Fig.18 Variation of Maxima of Power(P_o) with Temperature(T)

7.5.1. Excel Analysis for variation of Maxima of Power(P_o) with Temperature(T):

Taking data from our code i.e. P_o and the current value at which P_o is reached from temperature 323K to 373K, we used Excel to analyze the variation of Maxima of Power(P_o) with temperature, along with the current associated to it. The output provided by the code provides us a datasheet, which on analysis provides us with the following variation of (P_o).

Temperature(T)	Current value at P_o	Maxima of Power(P_o)	Temperature(T)	Current value at P_o	Maxima of Power(P_o)
323	13.6449	5.77473	348	14.8977	5.42335
324	13.7162	5.77108	349	14.9255	5.39851
325	13.7858	5.76654	350	14.9518	5.37291
326	13.8537	5.76112	351	14.9766	5.34654
327	13.9199	5.75481	352	15	5.31942
328	13.9844	5.74762	353	15.0219	5.29156
329	14.0471	5.73955	354	15.0425	5.26297
330	14.108	5.7306	355	15.0616	5.23365
331	14.1671	5.72077	356	15.0795	5.20362
332	14.2244	5.71007	357	15.096	5.17289
333	14.2798	5.6985	358	15.1112	5.14146
334	14.3334	5.68606	359	15.1251	5.10935
335	14.3852	5.67275	360	15.1378	5.07657
336	14.4352	5.65858	361	15.1493	5.04313
337	14.4833	5.64356	362	15.1595	5.00903
338	14.5296	5.62768	363	15.1686	4.97429
339	14.5742	5.61096	364	15.1765	4.93892
340	14.6169	5.59339	365	15.1832	4.90293
341	14.6579	5.575	366	15.1888	4.86634
342	14.6972	5.55577	367	15.1933	4.82914
343	14.7347	5.53571	368	15.1966	4.79136
344	14.7706	5.51484	369	15.1989	4.753
345	14.8048	5.49317	370	15.2	4.71407
346	14.8373	5.47069	372	15.199	4.63457

Fig.19 Maxima of Power(P_o) variation datasheet

It is very important to consider the variation of all the characteristic concepts associated with the fuel cell i.e the Limiting current(i_o), the Maxima of Power(P_o), and the design & safety parameters, in order to design an efficient fuel cell at a given operating temperature.

8. Conclusion and Self Assessment

The paper starts with modelling the Proton Exchange Fuel Cell(PEMFC) power plant, by assuming the parameters and formulating the characteristic reactions of the electrochemical fuel cell. On the premise of the following electrochemical reactions, we derive the polarization curve(V vs i) and Power curve (P vs i) provide us with important fundamental characteristics of the fuel cell: the Limiting Current(i_o) and Maxima of Power(P_o) and their variation with Temperature and Pressure provide us with important insights for

the designing of an efficient PEM Fuel Cell Power Plant. The polarization curve provides us with the operating voltage analysis with the help of theoretical equation, curve-fitting equation, and experimental data. Then we derived the Power curve(P vs i), using the characteristic equations formulated for the polarization curve. Applying the knowledge of the polarization curve, we studied the variation of Limiting Current(i_o) with the Temperature(T) by finding the root of the equation using the Newton-Raphson Method with the help of a designed C++ program. Applying the knowledge of the Power Curve, we studied the variation of Maxima of Power(P_o) with Temperature(T) by finding the roots of the derivative of the Power curve using the Newton-Raphson Method with the help of a designed C++ program. The PEMFC power plant is designed using the following characteristic concepts: Systematic design of PEM power plant, Electrochemistry, Thermodynamics, Fuel cell fundamentals, Polarization curve, Power curve, and Newton-Raphson Method. We provided the derivation to the concepts using fundamental equations and related them with the experimental data along with the error analysis associated with it, and then provided substantial applications to the reference paper using the following concepts along with formulating their variation with the help of C++ code, Excel analysis, Origin labs, Diagrammatic Representations using Canva and DESMOS. Hence, we consider our term paper to be a (Level-2) paper.

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