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MODELING AND ANALYSIS OF PROTON EXCHANGE MEMBRANE (PEM) FUEL CELL

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ABSTRACT

The investigation of the modeling of Proton exchange Membrane Fuel cell is generally rely on the rudiments of the chemical reaction or other chemical equations which governs the behavior of fuel cell , But in this manuscript probes about likely numerical solutions of a fuel cell. This manuscript probes about maximum attainable potential upshot yielded by fuel cell by analyzing the Voltage - Current characteristics obtained from the simulative analysis of the fuel cell modeling of fuel cell done using Matlab for diverse operating condition and maximum harvestable latent output is evaluated at that juncture.

Keywords: proton exchange membrane fuel cell (PEMFC), chemical equations, potential output, matlab modeling V-I characteristics.

INTRODUCTION

Amid the Polymer Electrolyte Membrane fuel cell Proton Exchange Membrane Fuel cell is the most frequently used fuel cells. This sort of Fuel cells has the competence to operate in high power densities even at low temperature as result of that it reduces the whole volume, weight and cost of production. PEMFC has an immovable electrolyte membrane so there is straightforwardness in the progression of production and by this it trim downs corrosion which in turns shows likely way of lingering stack existence [1].

Alike to all other fuel cell PEM fuel cell also involves mainly three parts namely Anode, Cathode and Electrolyte also termed as the membrane. The PEM fuel cell has wide application in the province of automobiles and portable electronic appliances in earlier practice owing to the exploitation of platinum as catalyst the use of PEMs are truly constrained owing to the high cost of platinum however after the overture of Nafion the effective applications of PEMs are inflating again in present days [4]. Today PEMs have great expectations in the industrial worlds and the in the offing it can be utilized for the production of strewn power generation. It is potentially one of the most principal fuels for electrical energy production that is being probed in present being.
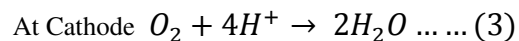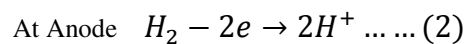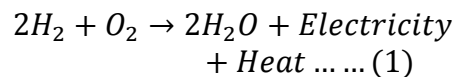
The polymer membrane

PEM is discovered by William Grubbs in the year of 1959, where he discovered that even devoid of the presence of solid membrane he found that it has the capability to transfer electrons and protons to the cathode which was taken care by Nafion and it is still on use till in present days. Nearly all commonly used membrane is Nafion which is the product of DuPont. This membrane is effectively a carbon chain which attached to it is fluoring atoms which are baptized as Teflon. Nafion allow up to 50% augment in dry weight. . This chattels result in five vital properties of the Nafion membrane, sturdily acidic, mechanically strong, Acidic very absorbvative and fine proton exchange conductors. The membrane permits the transfer of protons and the electrons posses peripheral path

for its travel these then convene in the cathode and thus as a spin - off of this reaction flanked by protons and oxygen in the cathode ware is formed. The PEM fuel cell likely has the possibilities to run even at the temperature less than 80 degree Celsius.

Introduction to PEMFC development of the modeling Fuel cell

Principal concept behind Fuel cell is conversion of chemical energy to mechanical energy by being indent with the converting oxygen and hydrogen directly in to electricity heat and water in an Electrochemical system process [2-3]. Hydrogen and oxygen incineration response as given in equation (1) and their apposite chemical reaction in both anode and cathode given in the equation (2) and (3) are the necessary essentials of PEM Fuel cell at the bottom.

$$2H_2 + O_2 \rightarrow 2H_2O + Electricity + Heat \dots\dots(1)$$

At Anode $\quad H_2 - 2e \rightarrow 2H^+ \dots\dots(2)$

At Cathode $\quad O_2 + 4H^+ \rightarrow 2H_2O \dots\dots(3)$

Essential rudiment fuel cell diagram is depicted in Figure-1 [5] the figure depicts the composition of the PEM the vital rudiments which have to be considered for the opposite operational of the system within cathode and anode rods, Electrodes and membrane. Electrode primarily encompasses of gas diffusion layer and a catalyst layer [6]. Porous moderate hydrophobic structure equipped diffusion and catalyst layer. Hydrogen enters through the anode side and air is introduced through cathode side. Membrane present between anode and cathode exploited as electrolyte which stays indent to of transporting H+ from cathode and also perform reactant severance. Significant reaction as a product after the completion of these two reactions are given in the equation (1), (2) and (3).
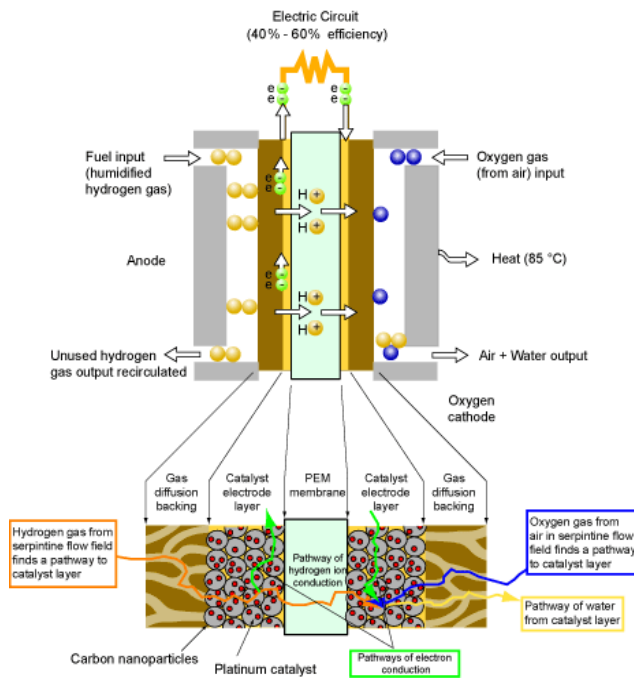
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Figure-1. Central fuel cell diagram.

Thermodynamics of Fuel cell

Thermodynamics is a conservation of energy in a given electrochemical system. Thermodynamics edicts reigns the changes in all such systems which are typically based on experience. These edicts can envisage the changes that occur in the organization but still they cannot envisage the preciseness to the rate and the changes that can happen [7 - 9].

A. First law of Thermodynamics

Edicts of conservation of energy termed as first law of thermodynamics elucidates that 'Energy neither be created nor be destroyed but it can be transformed from one from to another form ' explicates that the total energy available in the system does not varies but the form in which it present or available can vary, mathematically signified as equation (4).

$$dE = Q - W \dots \dots (4)$$

Known energy of the system symbolized as E, Heat input to the system symbolized as Q and work done is symbolized as W. likely like open system fuel cell too allows both mass and energy flows through its boundaries. For an open system energy variations can be expressed as in equation (5).

$$\Delta E = \Delta U + \Delta KE + \Delta PE + \Delta(PV) \dots \dots (5)$$

Known Internal energy of the system symbolized as Q, KE symbolized Kinetic Energy and PE symbolized as Potential energy available in the system, Where PV is the Pressure - Volume work done on the fluid. Summation of Internal energy with work done of the system termed as enthalpy is given in the equation (6).

$$H = U + PV \dots \dots (6)$$

The variation in energy of open system is observed form equation (5) and (6) and written in equation (7).

$$\Delta H = Q - W \dots \dots (7)$$

Effective application of First law of thermodynamics in Fuel cell

Simple Incineration response happens in fuel cell is described in equation (8)

$$Fuel + Oxidant = Product \dots \dots (8)$$

Above equation portrays an electrochemical reaction which involves the electron transportation from one electrode to other. Electrons transported in numbers rely on the stoishiometyr of the fuel being oxidized as here in this case fuel cell it is hydrogen. Equivalent amount of Electrical energy bestowed by chemical change of an transported electrons explicated in equation (9).

$$F = Ae \dots \dots (9)$$

Known Faraday's constant which is equivalent to 96493 coulombs is given by 'F', charge of an electron equivalent to 1.6×10^{-19} C symbolized as 'e' and Avagadro's number equivalent to 6.023×10^{23} is symbolized as A thus from the above discussion we can conclude that the quantity of electric energy that occurs given in (9)

$$Electricity = NF \dots \dots (10)$$

Known sum of electrons transported in terms of numbers symbolized as N and the electrical work done in the reaction due to the transfer of the electron is given in equation (11)

$$W = -NFE \dots \dots (11)$$

Known Potential difference between the two electrodes (Cell voltage). Negative sign in equation (11) has no significance but it just indicates the work is being done in the system now putting equation (11) in equation (7) we have.

$$\Delta H = Q - NFE \dots \dots (12)$$

B. Second law of Thermodynamics

First edicts of thermodynamics stated only about the law of conservation of total energy and it has no information about direction of the follow of energy transfer and we know that heat transfer happens naturally only from hot body to cold body. Thus the shortcomings of the first edicts are rectified in second law of

thermodynamics and it is elucidated as "The total entropy of the system cannot be decrease other than by increasing the entropy of some other system" Entropy is the measure of disorderliness of the system. Entropy is the measure of the upheaval of the system.

Concept of entropy and reversible process of the system

A system endures reversible changes as even when it passes from initial to final state it relics in equilibrium with the milieu. An entropy created by irreversible process created in reversible process to by reducing the temperature gradient from finite to infinite temperature divergence [10]. Entropy is described by the equation (13).

$$\Delta S = \left(\frac{\Delta Q}{T}\right)_{rev} \dots \dots (13)$$

Where Measure of the entropy of the system is symbolized as S, frictional heat loss or heat transfer is symbolized as Q and temperature of the system is symbolized as T, Entropy is also a reversible process, therefore the mathematical expression can be expressed as (14)

$$\Delta S_{Total} = \Delta S_{System} + \Delta S_{Surrounding}$$
$$\geq 0 \dots \dots (14)$$

Effective application of the second law of thermodynamics and Gibbs free energy

In the equation (12) substitute Q=TΔS as it is obtained from the fuel cell entropy equation i.e.

$$\Delta H = T\Delta S - NFE \dots \dots (15)$$

Equation can be rewritten in differential form as

$$\Delta H = Tds - FEdN \dots \dots (16)$$

Work done is maximum and it is given by Gibbs free energy (G) as it is a reversible process.
$$\Delta G = -FEdN \dots \dots (17)$$

Substituting equation (17) in (16) we have

$$\Delta G = \Delta H - T\Delta S \dots \dots (18)$$

From the perception of the above equation it can be said that the change in enthalpy and entropy of the system at constant temperature can leverage the development of free energy as free energy is mainly due to the existence of the independent mass in the internal of the system so from this we can rewrite the equation as
$$\Delta U = \Delta Q - \Delta W \dots \dots (19)$$

$$\Delta U = T\Delta S - P\Delta V + \sum \mu i \Delta ni \dots \dots (20)$$

Where chemical potential is independent masses denoted as μ_i and in is the amount of masses present in the internal of the fuel cell that carries the free energy. The product of these is done which shows the work done of the masses and the summation is to include all the masses.

Circuit modeling of PEM Fuel cell

The Voltage - Current characteristics of a typical PEM fuel cell at normal air pressure and room temperature in fuel cell model losses are present which cause the cell potential to be lesser than its ideal voltage. The losses which are to be accounted in modeling of fuel cell are i) Activation loss ii) Concentration loss iii) Ohmic losses the voltage output of the fuel cell is given by Nernst equation as given in the equation (4).

$$E = N\left[\dot{E} - \left(\frac{RT}{nF}\right)\ln\left\{\pi\left(P_p^{vp}/P_r^{vr}\right)\right\} - L\right] \dots (21)$$

Losses contributions to PEM fuel cell are

Activation losses which can reduced maximizing catalyst area of contact activity inside the cell system, Ohmic losses are due to instead of passing through the load some electrons passes through the load and loss concentration raises due to decrease in concentration of reactant in electrode.

Proton exchange membrane Fuel cell modeling

Performance under a wide range of the fuel cell under any operating condition has to predicated by the designed model fuel cell, In fuel cell assumption taken are 1. Ideal gas properties 2.Negligibel ohmic potential drops 3.Incompressibel flow 4. Laminar flow 5.Catalyst layers and diffusion gas layers are considered to be isotropic

RESULTS AND DISCUSSIONS

Simulation analysis of modeling of Fuel cell dynamics based on chemical rudiments.

The chemical - Mechanism model for the output voltage of a single cell can be defined by the following expression.

$$V_{FC} = [E_{NERNST} - V_{ACT} - V_{OHMIC} - V_{CONC}] \dots (22)$$

Ideal output voltage ENernst

Electrochemical thermodynamic potential of the cell and it represents its reversible voltage which is an ideal output voltage represented by E_{Nernst}. E Nernst can be calculated by a modified version of the account the changes in the temperature with respect to the standard reference temperature 25 degree Celsius using the standard reference temperature (SPT). Than we can equate

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$$E_{Nernst} = 1.229 * 10^{-3}(T - 298.15) + 4.31 * 10^{-5}\left[\ln(P_{h2}) + \frac{1}{2}\ln(P_{o2})\right] \dots (23)$$

Figure-2. Simulation result of the Nerns't equation versus the current input at constant temperature and pressure.

Figure-3. Simulation of the voltage versus current curve for 500Wats fuel cell used in the study of PEMFC.

Polarization loss activation

The slothfulness of the chemical reactions taking place inside the fuel cell as a portion of the voltage produce in the cell is the main cause for activation loss or used up during the driving time of the chemical reaction in transferring the protons and electrons from the anode to cathode and this voltage loss is highly nonlinear equation for activation polarization losses at STP given in the equation (24)

$$V_{act} = [-0.948 + (0.00286 + 0.002 * lnA + 4.3 * 10^{-5}\ln(C_{h2}))T + 7.6 * 10^{-5}Tln(Co2) - 1.93 * 10^{-4}T * \ln I_{FC}] \dots\dots (24)$$

Concentration of hydrogen in the catalytic inference of anode denoted as C_{h2} and concentration of oxygen in the catalytic interface of the cathode denoted as C_{O2} in (mol/cm^3) and the constant values refer to the parametric coefficients for the cell model and gain.

$$C_{O2} = \frac{P_{o2}}{\left(5.08 * 10^6 e^{-\frac{498}{t}}\right)}$$

$$C_{h2} = \frac{P_{h2}}{\left(5.08 * 10^6 e^{-\frac{498}{t}}\right)}$$
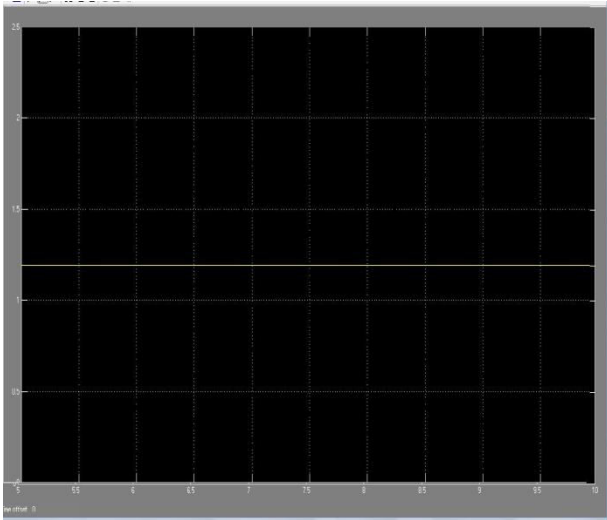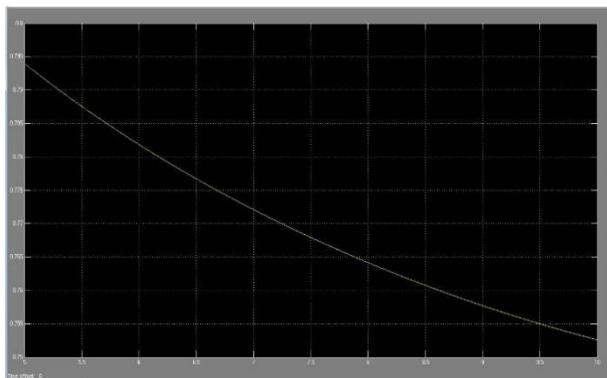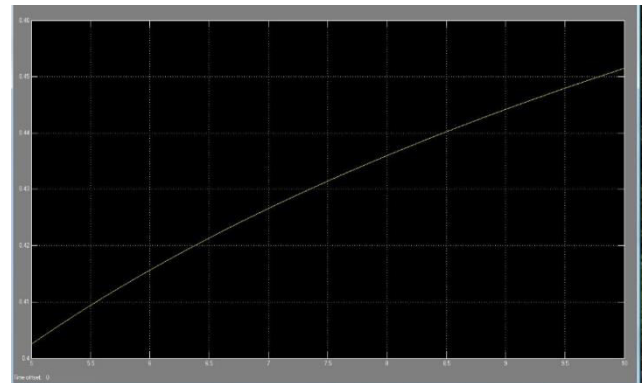
Operating current is symbolized as $I_{FC.}$

Figure-4. Simulation of the activation voltage versus Input current.

Ohmic polarization losses

Resistance of the collecting plates, carbon electrode and also resistance of transferring protons through the membrane are the main rationale for Ohmic polarization losses. Usually equivalent resistance can be formed as

$$R_M = \frac{P_M L}{A} \tag{25}$$

Losses due to the resistance to the transfer of protons through the membrane usually considered constant as Rc = 0.0003Ω so the ohmic polarization losses represented by the equation.
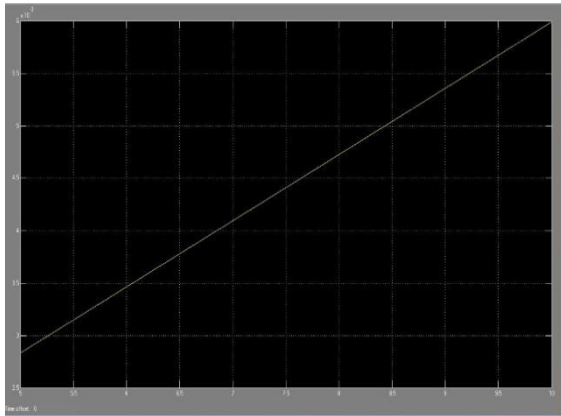
$$V_{ohmic} = I_{FC}(R_M + R_C) \dots (26)$$

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Figure-5. Simulation of the Ohmic voltage versus current of the Fuel cell.

Concentration losses

Due to the concentration of the reactants at the surface of the electrode as fuel concentration losses arises is being used up the equation of the concentration loss given by equation

$$V_{Conc} = -B \ln \left(1 - \frac{J}{J_{MAX}} \right) \dots (27)$$

Jmax ranges from 500 to 1500mA/cm^2 and B(V) is the parametric coefficient which depends greatly on the cell and its operation state and J represents the actual current density of the cell expressed in (A/cm^2). By the summation of all losses along the Nernst equation we attain the required model for the fuel cell as given in the matlab/Simulink model simulation for the different voltage losses is obtained in the form of graphs.

Figure-6. Simulation of voltage concentration versus input current in the cell.

Double layer charging effect

Solid membrane which separates the electrodes acts as block for the flow of electrons and flow of H+ ions here the electrons takes the path through the anode to the cathode through the anode to the cathode through the external load and than reaches the cathode while the

protons pass through the electrolyte and reaches the cathode at the same time with the electrons. Due to this two charged layers of opposite polarity are formed across the boundary between the cathode and the porous membrane. These layers are referring to as the electrochemical double layer which can be store electrical energy and thus behave like a super conductor. The effect of this double layer capacitor is taken in the form of voltage drop across the activation and concentration resistance and it is given by VC and this voltage drop not affect the ohmic resistance in the cell. The equation is given by:

$$V_C = \left(1 - c \left(\frac{dvc}{dt} \right) (r_{act} + r_{conc}) \right) \dots (28)$$
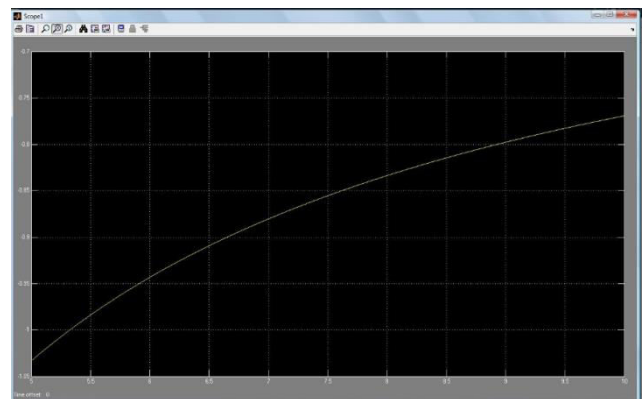

Figure-7. Simulation of double charge capacitor in the fuel cell i.e. capacitor voltage vs input current.

DISCUSSIONS

The fuel cell model of 500Watts can be characterized by performing small signal steady state and large signal measurement analysis. Modeling approach fully relies on these measurement results electrochemical phenomenon like temperature dependency charge double layer and

The fuel cell model of 500 W can be characterized by performing small signal steady state and large signal measurement analysis. The modeling approach fully relies on these measurement results, electrochemical phenomenon like temperature dependency charge double layer and adsorption effects are decisively covered with the current dependent element values. The power of PEM fuel cell depends on operating conditions such as flow, rates relative humidity and temperature of the gases. Mathematical modeling is very important for understanding this complexity. The models and results of other researchers is compared and evaluated. Results for the V - I characteristics of fuel cell shows the expected output voltage is dependent of the load current. Dynamic interaction effects with in a PEM fuel cell are significant and the detailed modeling for such transient effects is necessary. Using a simple procedure and data obtained from the literature it is possible to obtain a model for a fuel cell stack. The fuel cells are modelled by using

various mathematical equations. As well as base sense of these models was same more parameters were used in some of them for example neglected parameters of some mathematical model have been inspected in the dynamic model of fuel cell.

CONCLUSIONS

In this manuscript Dynamic behavior of a fuel cell which is a complex phenomenon which is modeled in mathematical equation including all loses which arises in PEM Fuel cell and simulated using mat lab / Simulink package. A PEM fuel cell has been modelled with this model exhaustively using more parameters. Dynamical structure of the model can be obtained to change the input parameters as required in this model the factors in the dynamic behavior of a PEM fuel cell are the reactant gases humidity change, various load changes and liquid water formation in cathode channel.

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