

Modelling and Simulation of Hydrogen Fuel Cells

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ABSTRACT: This paper reviews fuel cell technology status and some of its challenges worldwide. In the view of technological developments vehicle and component manufactures ,transport providers ,the energy industry , and even householders are seriously looking at alternative energy sources and fuels especially hydrogen and hydrogen powered fuel cells. Fuel cells have emerged as an important technology in various non-linear loads in industrial, commercial and residential sectors. A mathematical model of hydrogen fuel cell is described with control parameters. A hydrogen fuel cell design is simulated using MATLAB/SIMULINK and the results are discussed.

INDEX TERMS: Fuel, hydrogen, parameters, simulation

I. INTRODUCTION

The benefits of hydrogen fuel cells are wide ranging because of their low noise and high power quality. Fuel cell systems are ideal for use in hospitals or IT centre or mobile applications. They offer high efficiencies which are independent of size. The potential effects of climate change are irreversible and very serious. The transition from current energy infrastructure to a clean and secure energy infrastructure based on hydrogen and other alternative fuels will take decades as the difficult challenges posed by technological and economic barriers. A sustainable high quality of life demands clean, safe, reliable energy system at affordable prices. Fuel cells lead the way in clean and efficient energy conversions. They are powering innovations in a wide range of products, ranging from very small portable devices such as mobile phones, laptops and in applications like cars, delivery vehicles, buses and ships. Energy demands at present are met by thermal, hydro-electric, nuclear and solar power plants. Unfortunately efficiency is very low (20%) and environmental pollution is very high due to the production of greenhouse gases like carbon dioxide, carbon monoxide etc. These gases will increase atmospheric temperature and causes the reduction of ozone layer. Hydroelectric power plants demand source and space whereas nuclear power plants demands fuel reuse and disposal to a safe place.

Fuel cells have been called as the “microchip of the hydrogen age,” this clean renewable energy source is seen as alternative to fossil fuel used in running world’s economy. Drivers, limitations, and opportunities in the fuel cell market in India have been discussed [1]. Technical feasibility study in applying air cooling as an alternative for closed cathode stack designs is reported using a down-scaled 3-cell stack assembly [2]. A fuel cell (FC) maximum power point tracking (MPPT) with fuel flow optimization is presented is to extract the maximum power from a FC at different fuel flow rates and to protect the FC from over-current and voltage collapse across terminals. The system is composed of a tracker with a buck converter able to change the output impedance of the FC and therefore its power [3]. A brief review and comparison of polymer electrolyte fuel cells (PEFCs) and solid oxide fuel cells (SOFCs) with significant scientific challenges are discussed [4].The primary transportation alternatives which hold the greatest potential for averting societal threats are evaluated [5].The fuel cell cars turned out to be the most promising to meet future environmental demands. In addition to an efficient process to produce the mechanical energy, recuperation of energy is a potential step to increase mileage of passenger cars [6]. The design and manufacturing alternatives for Proton Exchange Membrane (PEM) fuel cells are described and analyzed within the context of vehicle applications [7].

Fuel cell technology is recently becoming one of the most interesting fields for the car companies to invest in. This interest is because of their high efficiency and zero environmental pollution. Polymer electrolyte membrane fuel cells (PEMFC) are the most appropriate type of fuel cells for use in vehicles due to their low performance temperature and high power density [8]. Environmental, sustainability issues and the role of hydrogen and fuel cell technologies have emerged as potential solutions to these issues. The commercialization plans in various industrialized countries (USA, Canada, Japan, etc.) have started identifying the most likely early markets for hydrogen as an energy carrier and fuel cell as energy producing device [9]. Intelligent Energy has

developed a proprietary fuel cell stack, cooled via evaporation rather than by use of separate cooling channels.

As a case study, a conventional London Taxi black cab is discussed [10]. With fuel cell/battery, city buses the output power of the fuel cell is controlled by a D.C. converter and the output ports of the converter and the output ports of the converter and the battery are connected in parallel to supply power for the electric motor. A closed-loop control algorithm is necessary to eliminate the errors between the output and target power of the fuel cell system [11]. The potential for Solid-Oxide Fuel Cells (SOFC) to provide electrical generation on-board commercial aircraft has been described [12]. The impact of the edge cooling is studied via a mathematical model of the three-dimensional two-phase flow and the associated conservation equations of mass, momentum, species, energy, and charge. The model includes the stack, ambient, fan, and fins used for cooling [13]. The design and balance-of-plant of a novel anaerobic digestion (AD) biogas solid oxide fuel cell (SOFC) plant is assessed. Biogas from waste-water treatment plant is the fuel feeding the SOFC system. Simultaneous multi-generation of electricity, heat and a fuel (algae) via exhaust carbon recycling is accomplished in the proposed plant configuration [14]. A dynamic MATLAB Simulink model of a H3-350 Reformed Methanol Fuel Cell (RMFC) standalone battery charger produced by Serenergy is developed on the basis of theoretical and empirical methods. The advantage of RMFC systems is that they use liquid methanol as a fuel instead of gaseous hydrogen, which is difficult and energy consuming to store and transport [15]

II. MATHEMATICAL MODEL

The simplified model of a fuel cell stack operating at nominal conditions of temperature and pressure is as shown in Fig (1). The parameters of the equivalent circuit can be modified based on the polarization curve as shown in Fig (2). The inputs are the value of the voltage at no load, as well as the nominal and the maximum operating points, for the parameters to be calculated. A diode is used to prevent the flow of negative current into the stack.

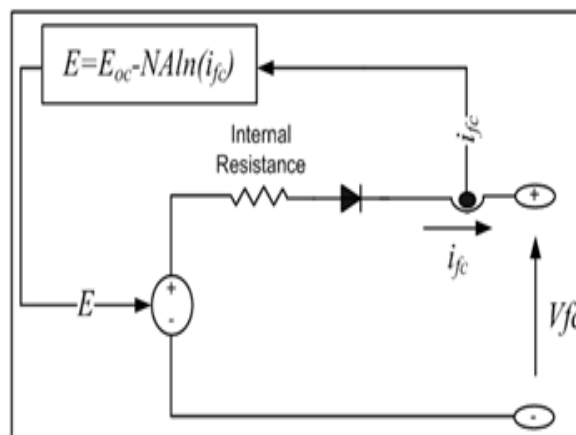


Fig-1: Equivalent circuit of fuel cell stack

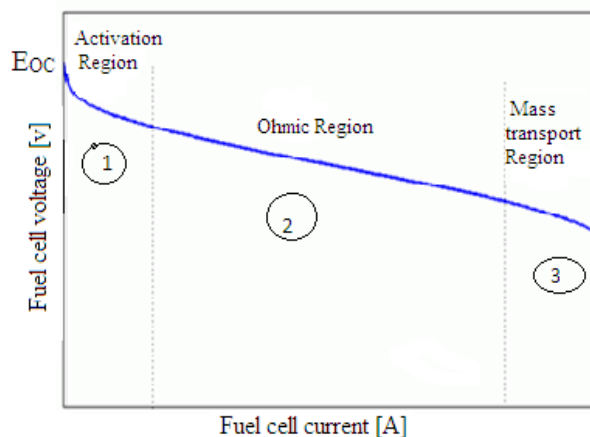


Fig-2: Polarization curve

The polarization curve in Fig (2) consists of three regions:

2.1 Region 1

The first region represents the activation voltage drop due to the slowness of the chemical reactions taking place at electrode surfaces. Depending on the temperature and operating pressure, type of electrode, and catalyst used, this region is more or less wide.

2.2 Region 2

The second region represents the resistive losses due the internal resistance of the fuel cell stack.

2.3 Region 3

Finally, the third region represents the mass transport losses resulting from the change in concentration of reactants as the fuel is used.

DETAILED MODEL

The detailed model represents a hydrogen fuel cell stack when the parameters such as pressures, temperature, compositions, and flow rates of fuel and air vary. These variations affect the open circuit voltage as well as the Tafel slope. The equivalent circuit and the simplified model are as shown in Fig 3.

The open circuit voltage and the Tafel slope are modified as follows:

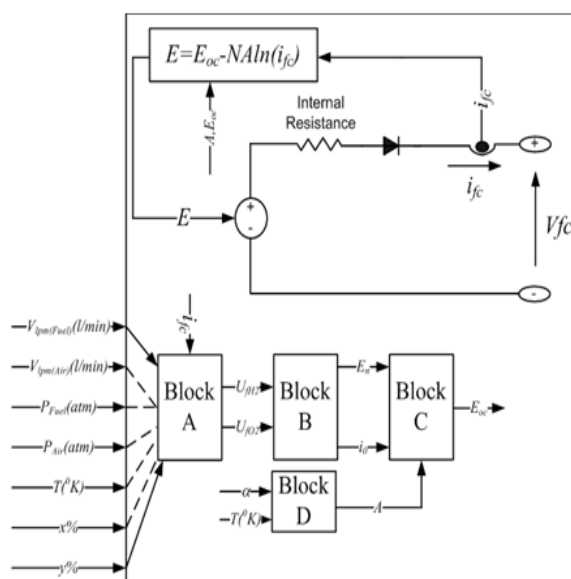


Fig-3: Simplified model of the fuel cell stack

$$(1)$$

$$A(2)$$

Where,

E_{OC} = Open circuit voltage (v)

A = Tafel slope

R = 8.3145 J/ (mol K)

F = 96485 A s/mol

z = Number of moving electrons

= Nernst voltage, which is the thermodynamics voltage of the cells and depends on the temperatures and partial pressures of reactants and products inside the stack

= Exchange current, which is the current resulting from the continual backward and forward flow of electrons from and to the electrolyte at no load. It depends also on the temperatures and partial pressures of reactants inside the stack.

= Charge transfer coefficient, which depends on the type of electrodes and catalysts used

T = Temperature of operation (K)

For a given Air and Fuel flow rate, the Nominal rate of conversion of hydrogen and oxygen is given by:

$$U_{fH_2} = \frac{6000RTNi_{fc}}{zFP_{fuel}V_{lpm}(fuel)} \quad (3)$$

$$U_{fO_2} = \frac{6000RTNi_{fc}}{2zFP_{air}V_{lpm}(air)} \quad (4)$$

Where,

Nominal rate of conversion of hydrogen

= Nominal rate of conversion of oxygen

= Absolute pressure of fuel (atm)

= supply pressure of air (atm)

= Fuel flow rate (l/min)

= Air flow rate (l/min)

x = Percentage of hydrogen in the fuel (%)

y = Percentage of oxygen in the oxidant (%)

The Nernst voltage for a given exchange current density (i_0) for a partial pressure of hydrogen () and oxygen () inside the stack is given by :

$$E_n = \left\{ \begin{array}{l} 1.229 + (T - 298) \frac{-44.43}{zF} + \frac{RT}{zF} \\ 1.229 + (T - 298) \frac{-44.43}{zF} + \frac{RT}{zF} \end{array} \right\} \quad (5)$$

$$i_0 = \frac{zFk(P_{H_2} + P_{O_2})}{Rh} e^{\frac{\Delta G}{RT}} \quad (6)$$

E_n = Nernst voltage

i_0 = Exchange current

= Partial pressure of hydrogen inside the stack

= Partial pressure of oxygen inside the stack

= Partial pressure of water vapor inside the stack

k = Boltzmann's constant = 1.38×10^{-23} J/ K

h = Planck's constant = 6.626×10^{-34} J s

G = Size of the activation barrier which depends on the type of electrode and catalyst used

The partial pressures , and are determined in steady state as follows:

$$(7)$$

$$(8)$$

$$(9)$$

Where,

W = Percentage of water vapor in the oxidant (%)

Block C and D calculate the new values of the open circuit voltage (E_{OC}) and Tafel slope, respectively.

The material parameters η , G are calculated based on the polarization curve at nominal conditions of operation along with some additional parameters, such as the low heating value (LHV) efficiency of the stack, composition of fuel and air, supply pressures and temperatures, etc. They can be easily obtained from the manufacturer's data sheet.

The nominal rates of conversion of gases are calculated as follows:

$$U_{fH_2} = \frac{\eta_{nom} \Delta h^0(H_2O(gas))N}{zFV_{nom}} \quad (10)$$

$$U_{fO_2} = \frac{6000RT_{nom}NI_{nom}}{2zFP_{air}V_{ipm}(air)_{nom} \times 0.21} \quad (11)$$

Where,

η = Nominal LHV efficiency of the stack (%)

Δh^0 = Standard enthalpy of formation (J/mol)

N = Nominal voltage (V)

I_{nom} = Nominal current (A)

V_{nom} = Nominal air flow rate (l/min)

P_{air} = Nominal absolute air supply pressure (Pa)

T_{nom} = Nominal operating temperature (k)

III. EXTRACTION OF PARAMETERS FROM DATASHEET

This example uses the Ned Stack PS6 data sheet from Ned Stack as shown in Appendix-A

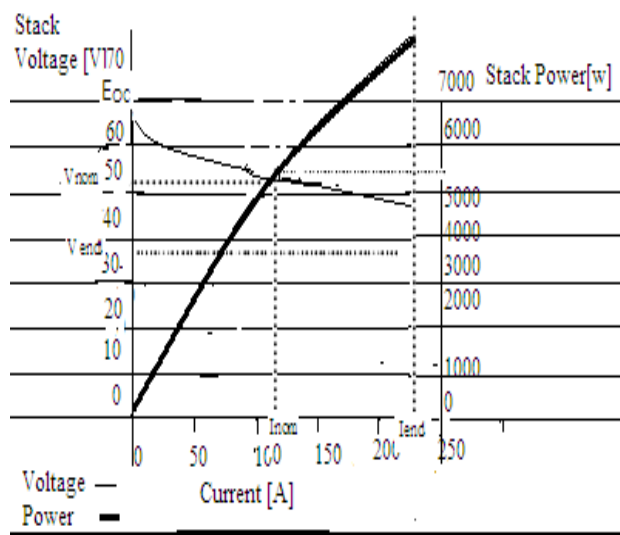


Fig-4: Ned stack PS6 curves from datasheet

The rated power of the stack is 5.5kW and the nominal voltage is 48 V. The following detailed parameters are deduced from the data sheet.

Open circuit voltage (Eoc) = 65 V

Nominal operating point [I nom, Vnom] = [133.3, 45]

Maximum operating point [I end, Vend] = [225, 37]

Nominal stack efficiency () = 55 %

Operating temperature = 65

Nominal supply pressure [Air] = [1.5 1]

If the pressure given is relative to the atmospheric pressure, add 1 bar to get the absolute pressure.

Nominal composition (%) [, , (Air)] = [99.999, 21, 1]

If air is used as oxidant, assume 21% of and 1% of O in case their percentages are not specified.

Number of cells:

Can be estimated from the formulas below:

$$N = \frac{2 \times 96485 \cdot V_{nom}}{241.83 \times 10^3 \cdot \eta_{nom}} \quad (12)$$

$$N = \frac{2 \times 96485.45}{241.83 \times 10^3 \cdot 0.55} = 65.28 = 65 \text{ cells}$$

Nominal air flow rate:

If the maximum air flow rate is given, the nominal flow rate can be calculated assuming constant oxygen utilization at any load. The current drawn by the cell is linearly dependent on air flow rate and the nominal flow rate is given by:

$$V_{lpm(air)nom} = \frac{I_{nom} \times V_{lpm(air)}}{I_{nom}} \quad (13)$$

In this case,

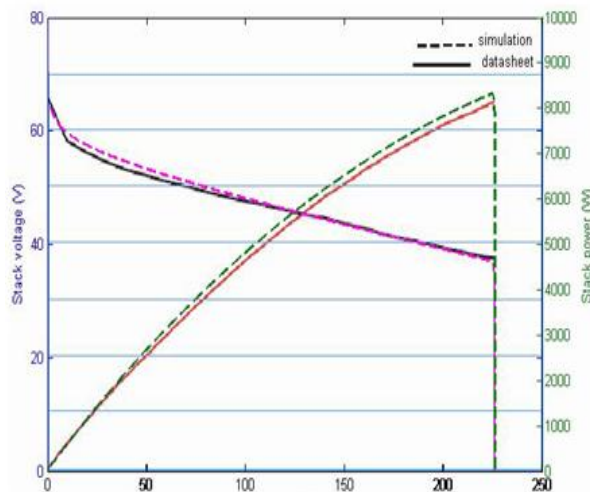
$$V_{lpm(air)nom} = \frac{133.3 \times 500}{225} = 297 \text{ litres/min}$$

Assume the rate of conversion of oxygen to be 50% (as it is usually the case for most fuel cell stacks) and the nominal air flow rates:

$$V_{lpm(air)nom} = \frac{6000RT_{nom}\Lambda}{2zFP_{air}n_{O_2}} \quad (14)$$

Fuel cell response time = 10 s

With the above parameters, the polarization curve of the stack operating at fixed nominal rate of conversion of gases is close to the data sheet curves as shown below. The orange dotted line shows the simulated stack voltage and green dotted line shows the simulated stack power.



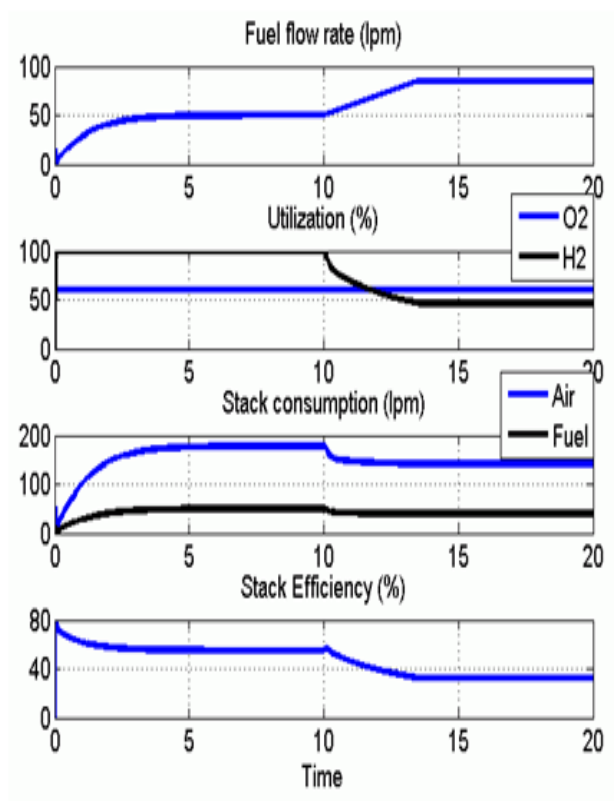


Fig-7: Simulation results showing fuel flow rate,

Utilization, stack consumption and efficiency

The DC bus voltage, which is very well regulated by the converter. The peak voltage of 122 V_{dc} at the beginning of the simulation is caused by the transient state of the voltage regulator.

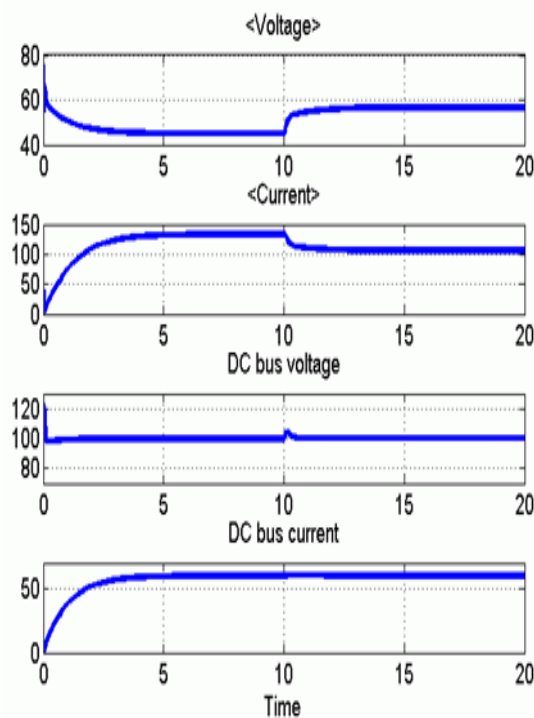


Fig-8: Simulation Results showing voltage, current, DC bus voltage and current

V. CONCLUSION

This paper has presented the mathematical model of a hydrogen fuel cell with different control parameters in matlab/Simulink environment. The simulated results show an increase of the Nernst voltage, so the fuel cell current will decrease. Therefore, the stack consumption and the efficiency will decrease. With this initial survey and analysis of hydrogen fuel cell, challenges of hydrogen fuel cell will be compared with other types of fuel cells for different linear and non-linear loads are the future scope of the work.

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APPENDIX-A

Type	6 K W fuel cell system	Ned stack PS6
Performance	Net Rated electrical peak power	7 KW (DC)
	Net Rated nominal power	5 KW (AC)
	Output voltage	60-30V (DC)
	Operating current range	0-225 A (DC)
	Typical beginning of life voltage range	42 V at Nominal
	Efficiency - LHV	55% [stack]/ 50% [system]
	Time from off model to idle	Within 3 Min

	Time from 10% to full power	Approx. 10 s
	Expected Life	20.000 h [stack]
	Maintenance Routine	2.000 h [system]
	Operational Ambient Temperature	-20 - +40°C
Fuel	H ₂ or Reformat	
	Purity	99.999% H ₂ or Reformat(<50ppm CO)
	Supply pressure	0.5-5 bar
	Stack operating pressure	ambient
	Maximum consumption	12.5 slpm/KW
Air delivery system	Flow rate	Max 500l/Min
	Supply Pressure	Ambient
Physical	Dimensions	400x600x1600 mm
	Mass	Approx. 80kg
Emissions	Water collected	75 l /min
	NO _x , SO _x	0
Cooling system requirements	Heat Rejection to coolant at maximum power	10 KW
	Maximum Ambient temperature	45°C
	FCPM Operating temperature	65°C
	Cooling Method	Radiator Fan