



Effect of Optimum Mix of Operating and Design Parameters on Proton Exchange Membrane Fuel Cell Performance

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(Received 11 April, 2012, Accepted 12 May, 2012)

ABSTRACT : A program for calculating the effect of optimum mix of operating conditions including environmental (like temperature, pressure, stoichiometry of the gases) and design parameter (area of the cell) on the performance of a PEM fuel cell is developed in this research work. The load current, terminal voltage and power density etc are estimated at different conditions. The program finds out most suitable fit of design parameters with given environmental and electrical conditions by the application of Genetic Algorithm. The mathematical model of the fuel cell is developed on the basis of semi - empirical fuel cell stack model and associated with balance of plant (BOP) model. The program also generated characteristic graphs of fuel cell according to feasible parameters by using Graphical User Interface (GUI) in MATLAB. The application of this methodology results in a set of optimal mix of operating parameters with design parameters results large improvement in system performance with respect to slight variation in electrical conditions.

Keywords : Genetic Algorithm, Proton Exchange Membrane Fuel Cell, Performance of PEM Fuel Cell.

I. INTRODUCTION

For the increasing demand of clean and high density energy devices emerging fuel cells as a promising technology that may successfully supersede the combustion of fossil fuel as the dominant method of energy conversion. Among various type of fuel cell, PEM fuel cell is high energy efficient, has low pollutant emissions and quick startup as explained by the authors Shaoduan Ou *et al.* [1], Maher A.R.Sadiq *et al* [2], Arun Kumar *et al* [4] and Balaji Krishnamurthy *et al* [5]. PEM membrane fuel cell can be operated at low temperature (about 80°K) with high power density product and at same time without impact on the environment. PEM fuel cell has high startup system and shadow system performance [6]. The improvement in performance, reliability and durability as well as reduction in production cost remains critical prerequisite for the commercialization of PEM fuel cells. In PEM fuel cell, optimum mix of the operating parameters and design variable plays very important role for improving the performance.

Therefore it is necessary to study parametric effect on PEM fuel cell performance [2]. The physical and mathematical models are very important to study the performance of PEM fuel cell. The mathematical model is important tool in modeling [1], whereas the developments of physical models help the researchers in simulation process under practical parameters, which are necessary in PEM fuel cell modeling and optimization [2]. The maximum output power under different load voltage has been studied by the author in reference [3]. In this research work MATLAB codes has been developed by using genetic algorithm to find the

optimum structure of the stack for maximum output power. However the author [3] has not explained the effect of the area of the cell on the performance of PEM fuel cell with the change in operating parameters.

In this research work a program is developed to find the optimal area of the cell under different operating parameters such as temperature, pressure, stoichiometry of the reactant gases and area of the cell for improved performance. The optimal area of the fuel cell is configured by using genetic algorithms. In order to develop the design framework, the algorithm in both the analysis and programs are carefully selected in MATLAB 7.7. The code evaluation of the function depends on the simulation of the model which would measure solutions fitness. The present research work utilized the MATLAB programming language running on WINDOWS -XP platforms processors are 2.4GHz 32 Bit INTEL Pentium -4 with 4GB RAM.

II. MATHEMATICAL MODELING

Modeling of real - world applications has been seen a useful tool for decades which reduce the cost of development. In this research work the main interest is the development of fuel cell design, because it is not possible to accurately describe the behavior of the PEM fuel cell on the basis of mathematical model. The semi- empirical approach based on work by researchers at the Royal Military College (RMC) [7-10] is chosen in this research work. The RMC model is robust, flexible and is not steady - state but also has simplified transient aspects. The model has achieved an accuracy and adaptability that has allowed us to be

deemed functional for the current research. In this section, a mathematical and computational approach is presented for building a mathematical model of a PEM fuel cell stack. To simplify the analysis, the following assumptions are made and discussed by the authors [10-14].

- The present model is one dimensional.
- The gases distribution is ideal and uniform.
- The fuel is humidified and the oxidant is humidified air.
- The fuel cell works under 800C and the reaction product is liquid phase.
- Thermo dynamical properties are evaluated at the average stack temperature and temperature variations at the stack are neglected, overall average heat capacity of the stack is assumed to be constant.

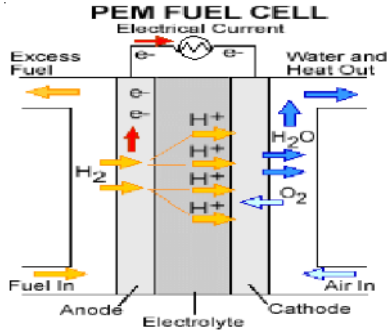


Fig. 1. Schematic diagram of PEM fuel cell.

A schematic diagram of a PEM fuel cell and its internal losses are shown in Fig. 1 and Fig. 2. For the details of the working of PEM fuel cell, the readers can refer to the references [13-15].

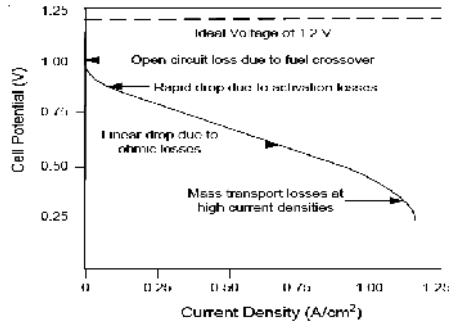


Fig. 2. Different voltage losses in PEM fuel cell.

There are different mathematical models in the literature which simulate the behavior of PEM fuel cell. Some are based on curve-fitting experiments [4] others are semi-empirical models that combine experimental data with parametric equations adjusted by comparison with cells physical variables like pressure and temperature [5]. In both cases, the activation over-potential, ohmic over-potential and concentration over-potential, which are crucial in describing the dynamical behavior of fuel cell.

Design Equations :

The cell voltage was defined as follows :

$$V_{cell} = E_{cell} - V_{act, cell} - V_{ohmic, cell} - V_{conc, cell} \quad \dots (1)$$

where $V_{act, cell}$, $V_{ohmic, cell}$ and $V_{conc, cell}$ are the activation loss, Ohmic resistance loss and concentration loss of the fuel cell as shown in Fig. 2. E_{cell} is actual open-circuit voltage of the fuel cell and is expressed as follows Maher *et al.* [2],

$$E_{cell} = 1.229 - 0.85 \times 10^{-3}(T_{cell} - 298.15) + 4.31 \times 10^{-5}T_{cell} [\ln(p_{H_2}) + 0.5\ln(p_{O_2})] \quad \dots (2)$$

The activation loss is often described through the Butler-Volmer equation,

$$V_{act, cell} = \left[\frac{RT_{cell}}{\alpha F} \ln \left(\frac{I_{density}}{I_a} \right) \right]_a + \left[\frac{RT_{cell}}{\alpha F} \ln \left(\frac{I_{density}}{I_a} \right) \right]_c \quad \dots (3)$$

The Ohmic over potential is expressed as,

$$V_{ohmic, cell} = I \times R \quad \dots (4)$$

where

$$R = \frac{t_m}{\lambda_m \times A_m} + \frac{t_e}{\lambda_e \times A_e} \quad \dots (5)$$

where t_e , t_m are the gas diffusion layer thickness and wet membrane thickness, λ_e , λ_m are the electrode ionic conductivity and the membrane ionic conductivity A_e , A_m , cross section of electrode and the cross sections of membrane respectively.

The concentration over-potential can be described by the following expression :

$$V_{conc, cell} = \frac{RT_{cell}}{nF} \ln \left(\frac{I_{Limiting}}{I_{Limiting} - I_{density}} \right) \quad \dots (6)$$

To calculate the fuel cell output voltage, the effective partial pressures of H_2 and O_2 need to be determined. In a gas mixture consisting of N species, the diffusion of component i through the porous electrodes can be described by the Stefan-Maxwell formulation [11];

$$\nabla x_i = \frac{RT}{P} \sum_{j=1}^a \frac{x_i N_j - x_j N_i}{D_{ij}} \quad \dots (7)$$

The diffusion of water at anode can be described by the following expression :

$$\frac{dx_{H_2O}}{dx} = \frac{RT_{cell}}{P_a} \left(\frac{x_{H_2O} N_{H_2} - x_{H_2} N_{H_2O}}{D_{H_2O, H_2}} \right) \quad \dots (8)$$

The molar flux of H_2 can be estimated by using following equation [17];

$$N_{H_2O} = \frac{I_{density}}{2F} \quad \dots (9)$$

The diffusion of water at cathode can be calculated by using following expression :

$$\begin{aligned} \frac{dx_{H_2O}}{dx} &= \frac{RT_{cell}}{P_c} \left(\frac{x_{O_2} N_{H_2O} - x_{H_2O} N_{O_2}}{D_{H_2O,O_2}} \right) \\ &= \frac{RT_{cell}}{P_c} \left(\frac{-x_{H_2O} N_{O_2}}{D_{H_2O,O_2}} \right) \end{aligned} \quad \dots (10)$$

where the molar fraction of water at anode is expressed as;

$$X_{H_2O}^a = x_{H_2O}^{chanel} \exp \left(\frac{RT_{cell} I_{density}}{2FP_{H_2} D_{H_2O,H_2}} \right) \quad \dots (11)$$

$$P_{H_2} = \frac{P_{H_2O}}{x_{H_2O}^a (1 - x_{H_2O}^a)} \quad \dots (12)$$

$$P_{H_2O} = 0.5 P_{H_2O}^{sat} \left[\frac{1}{x_{H_2O}^{chanel} \exp \left(\frac{RT_{cell} I_{density} I_a}{2FP_a D_{H_2O,H_2}} \right)} \right] \quad \dots (13)$$

$$\begin{aligned} \ln(P_{H_2O}^{sat}) &= 70.434642 - \frac{7362.6981}{T_{cell}} + \\ &69521 \times 10^{-7} \times T_{cell} - 9 \times \ln T_{cell} \end{aligned} \quad \dots (14)$$

The effective molar fraction of water at the cathode catalyze interface is defined as;

$$x_{H_2O}^c = x_{H_2O}^{chanel} \exp \left(\frac{RT_{cell} I_{density} I_c}{2FP_{H_2} D_{H_2O,O_2}} \right) \quad \dots (15)$$

The partial pressure of oxygen at cathode can be calculated by using following expression [11];

$$P_{O_2} = P_{cell} \left[1 - x_{H_2O}^{sat} - x_{H_2O}^c \exp \left(\frac{0.291 I_{density}}{T_{cell}^{0.332}} \right) \right] \quad \dots (16)$$

where

$$x_{H_2O}^{sat} = \frac{P_{H_2O}^{sat}}{P_{cell}} \quad \dots (17)$$

Therefore, the output voltage of PEM fuel cell is defined as:

$$V_{out} = N_{cell} \times V_{cell} \quad \dots (18)$$

Hence the power density of the PEM fuel cell can be calculated by using the following equation;

$$P_{density} = I_{density} \times V_{cell} \quad \dots (19)$$

III. GENETIC ALGORITHM

In the present research work, the design and analysis tool incorporates one - dimensional semi empirical PEM fuel cell model with a genetic based optimization algorithm. Genetic algorithm is more accurate to solve inherently complex optimization problems as modification of all designed parameters is achieved simultaneously. This technique is accepted [20, 21, 22] and is being used throughout the world for similar studies.

A simple genetic algorithm is an iterative procedure, which maintains constant size population P of candidate solutions. During each iterative step (generation) three genetic operators (reproduction, crossover and mutation) are performing to generate new populations (offspring), and the chromosome of new populations is evaluated via the value of fitness which is related to cost function. Based on these genetic operators and evaluations, the better new populations of candidate solution are formed.

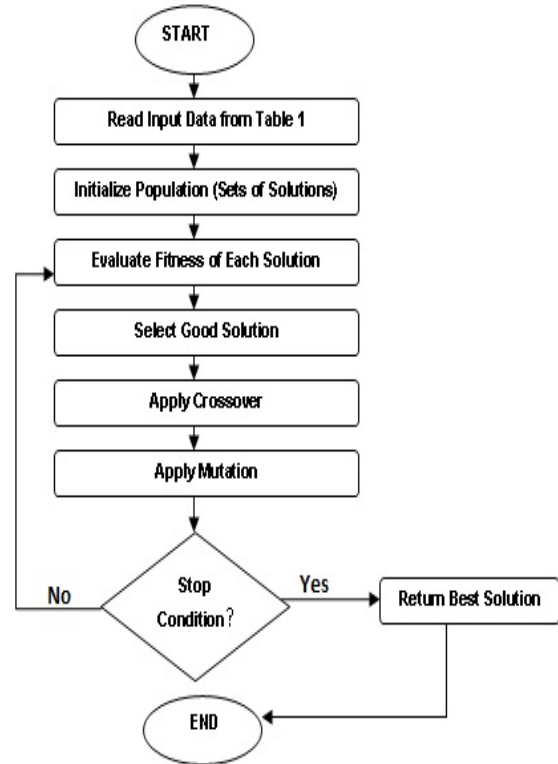


Fig. 3. Flow chart of genetic algorithm to obtain optimum point.

The flow chart to obtain the optimum point by using genetic algorithm has been discussed by the author [3] is given in fig.3. With the above description, a simple algorithm is given as follow [18];

- (i) Generate randomly a population of binary string.
- (ii) Calculate the fitness for each string in population.
- (iii) Create offspring string through reproduction, crossover and mutation operation.

- (iv) Evaluate the new string and calculate the fitness for each string (chromosome).
- (v) If the search goal is achieved, or an allowable generation is attained, return the best chromosome as the solution; otherwise go to step (iii).

The genetic algorithm consists of four main stages

- (a) Crossover
- (b) Mutation
- (c) Reproduction
- (d) Fitness

Table 1 : Design and operating parameters of the PEM Fuel Cell model.

Parameter	Value
Air stoichiometric flow ratio	2 - 8.5
Anode transfer coefficient (α_a)	0.5
Anode reference current density	$1.8 \times 10^{-3} \text{ A/m}^2$
Area of the cell (A_{cell})	16 cm^2 - 46 cm^2
Area of the membrane (A_m)	16 cm^2 - 46 cm^2
Cathode reference current density	2465.5 A/m^2
Cathode transfer coefficient (α_c)	1.0
Diffusion of hydrogen at anode ($D_{\text{H}_2\text{O}, \text{H}_2}$)	$1.0 \times 10^{-5} \times \epsilon^{1.5} \text{ m}^2/\text{s}$
Diffusion of oxygen at cathode ($D_{\text{H}_2\text{O}, \text{O}_2}$)	$1.0 \times 10^{-5} \times \epsilon^{1.5} \text{ m}^2/\text{s}$
Dry porosity of electrode (ϵ)	0.4
Electrode electronic conductivity (λ_e)	100S/m
Hydrogen reference mole fraction (x_{H_2})	0.84639
Membrane ionic conductivity (λ_m)	17.2 S/m
Oxygen reference mole fraction (x_{O_2})	0.17774
Pressure of the cell (P_{cell})	1.013 bar - 9.5 bar
Temperature of the cell (T_{cell})	298K-264K
Thickness of electrode (t_e)	$20 \times 10^{-2} \text{ m}$
Thickness of the membrane (t_m)	$50 \times 10^{-6} \text{ m}$
Width between anode channel to catalyst layer (l_a)	$10 \times 10^{-2} \text{ m}$
Width between cathode channel to catalyst layer (l_c)	$10 \times 10^{-2} \text{ m}$

IV. RESULT AND DISCUSSION

The values of design parameter and operating parameters details of PEM fuel cell are listed in table 1. The simulated results are validated with previously published results of Wang *et al.* [19] and the results were significantly improved. The computed polarization curve of PEM fuel cell model shows good agreement with previous published results of Wang *et al.* [19] as shown in Fig. 4.

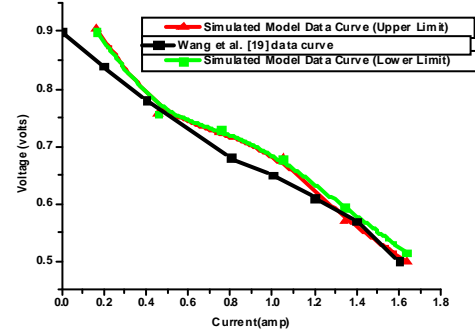


Fig. 4. Comparison of simulated model data of PEM fuel cell with Wang *et al.* [19] data.

A. Effect of operating temperature on PEM fuel cell performance

Fuel cell's voltage and output power at different temperature as a function of cell's current are shown in Fig. 5 and Fig. 6. The simulated results of the model are investigated between the temperatures 298 K to 358 K and other fuel cell's operating conditions as; fuel cell's operating pressure 3 bar, stoichiometry of the reactant gases 3, area of the cell 50 cm^2 , the membrane thickness is $3 \times 10^{-7} \text{ m}$, and the membrane humidity 100%.

It is observed from Fig. 5 the predicted cell voltage increases as we increase the temperature. The increase in cell voltage is due to the decrease in activation voltage with temperature.

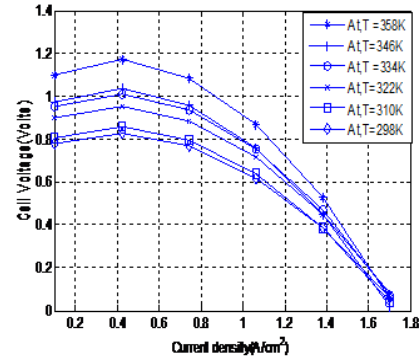


Fig. 5 Variation of voltage at with temperature.

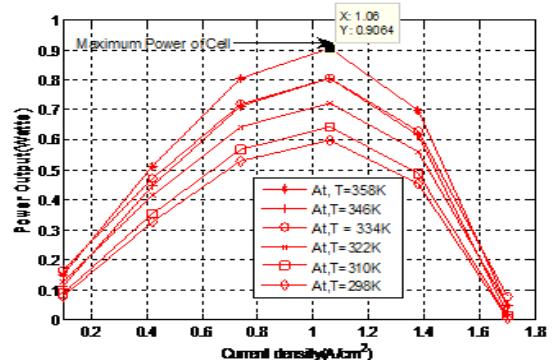


Fig. 6. Power curve at different temperature.

The results show that the activation overvoltage loss decreases about 0.0586 V in the temperature range of 50 K. The decrease in activation over voltage loss is because of the increase in exchange current density of the oxygen reduction reaction rapidly with temperature which enhances reaction kinetics. It is observed from the Fig. 6 maximum power of the fuel cell model is ~0.9064 watt at 1.06 amps. The results show that the highest rise in cell power output is about ~0.309 watt in the temperature range of 50 K at 1.7 amp. It is also observed from the results that the rise in power slightly shifted towards high current with increase in temperature.

B. Effect of operating pressure on PEM fuel cell performance

Pressure is one of effective basic operating parameter similar to the temperature which affects the performance of PEM fuel cell. The simulated results of the model are investigated between the pressures 1.01 bar to 9.5 bar and other operating conditions are; fuel cell's operating temperature 348K, stoichiometry of the reactant gases 3, area of the cell 50 cm², the membrane thickness is 3×10^{-7} m, and the membrane humidity 100%.

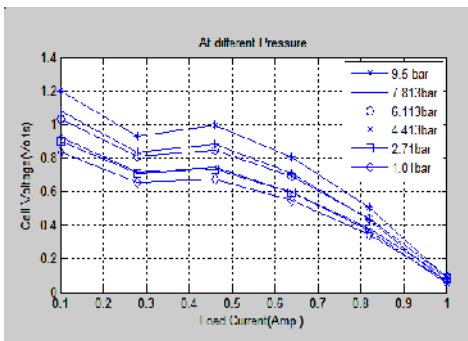


Fig. 7. Variation of voltage at with pressure.

The operating pressure affects the many transport species which are vital for the fuel cell operation. The saturation pressure of water vapor depends only on the temperature and it remains constant for a variation of the inlet pressure. However, the output voltage and power of the cell are the function of input temperature and input pressure.

Fig. 7 and Fig. 8 depict output voltage and power curve for different pressure : 1.013, 2.7, 4.41, 6.1, 7.8 and 9.5 bar. The results show that output voltage increase about ~0.4248V in the pressure range of 10 bar at low current density. The increase in the output voltage of the fuel cell is due to the increase in partial pressure of the reactant gases which increases the rate of the reaction. The rationale is that more protons (H⁺ ions) are forced to move towards cathode for the completion of reaction which reduces the concentration overvoltage loss.

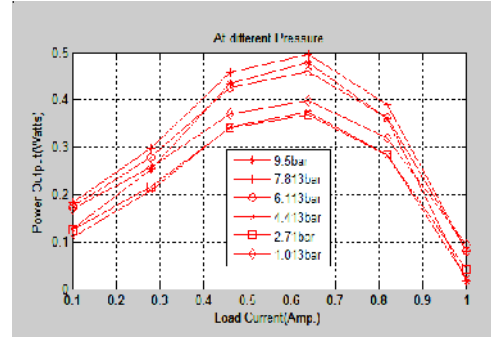


Fig. 8. Power curve at different pressure.

C. Effect of stoichiometry of the reactant gases on the performance of PEM fuel cell

The effect of the stoichiometry of the reactant gases on the performance of fuel cell is investigated in this simulation. The results are investigated between the stoichiometry ratio 2 to 8.5 and other operating conditions are; operating temperature 348 K, operating pressure 2.026 bar, area of the cell 50 cm², the membrane thickness is 3×10^{-7} m, and the membrane humidity 100%.

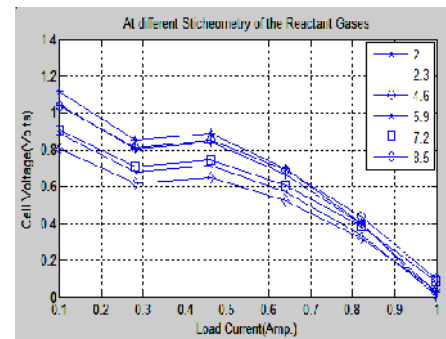


Fig. 9. Variation of voltage at with sticheimetry of reactant gases.

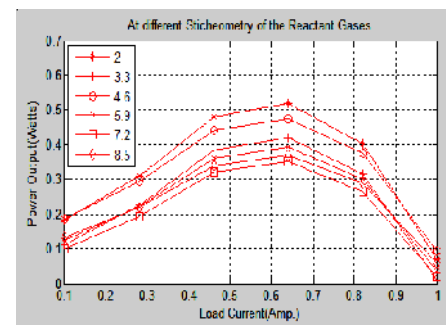


Fig. 10. Power curve at different sticheimetry of the reactant gases.

It is observed from the Fig. 9 and Fig. 10 that the performance of cell increases with the increase of stoichiometric ratio of the reactant gases. The results show that output voltage increases about 0.28 V at low current density in the range of 9 stoichiometry. This is owing to the fact that sufficient fuel is supplied to cell. It is also

observed from the fig. that the performance of cell is improved at high cathode gas stoichiometric ratio.

D. Effect of the cell area of the on the performance of PEM fuel cell

The simulated results of the model are investigated between the area of the cell from 16cm² to 46cm² and the other operating conditions are; operating temperature 310K, operating pressure 2 bar, stoichiometry of gases 3, the membrane thickness is 3×10^{-5} m and the membrane humidity 100%.

Fig. 11 and Fig. 12 depict the influence of the cell on the performance of PEM fuel cell model. It is observed that improvement in output power is about 0.3351 watt in the range of 34 cm² area of cell. The improvement in the performance of cell is because of the increase in rate of reaction in the cell with the area of cell. However, the increase in area of the cell could not improve similar performance as compared to variation in temperature, pressure, stoichiometry of the gases.

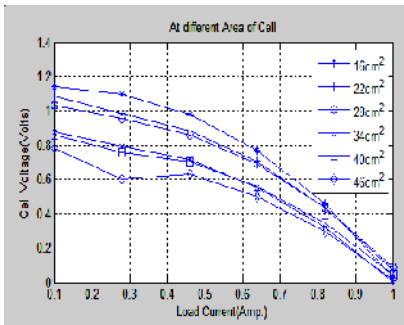


Fig. 11. Variation of voltage at with area of cell.

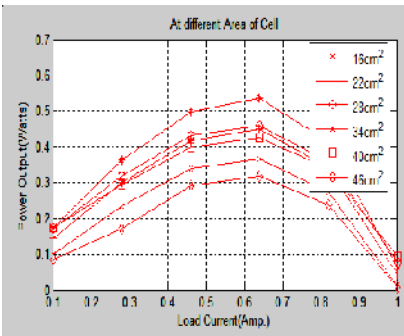


Fig. 12. Power curve at different area of the cell.

V. CONCLUSION

A semi empirical model of proton exchange membrane (PEM) fuel cell has been developed in the present research work. A highly non-linear set of algebraic equations are solved for computational modeling of the PEM fuel cell. The model is used to compute the effect of optimum mix of different range of operating parameters: pressures, stoichiometry of reactant gases, area of cell and temperatures

on the performance of fuel cell. The design and analysis tool incorporates one - dimensional semi empirical fuel cell model with a genetic based optimization algorithm. The main features of the design model are :

- A semi empirical model is designed to operate at optimum mix of different operating temperature, operating pressure, stoichiometry of gases and the area of the cell.
- The PEM fuel cell model is coupled to a genetic based optimization algorithm to predict the optimum point of operating and design parameters for improved performance as compared to the results of Wang *et al.* [19].

Genetic algorithm is more accurate to solve inherently complex optimization problems as modification of all designed parameters is achieved simultaneously. Over the past several years, operating parameters were kept as constant and their mutual variability was not investigated in fuel cell. This modeling limitation restricted the design to achieve improved performance in which simultaneous variation of many parameters have to be considered. Once all design parameters were considered in the design problem, the interdependence of the parameters could be clearly observed in the performance of the fuel cell. The results of present research work suggests that increase of operating temperature, operating pressure, stoichiometry of gases and area of cell are very much essential to achieve better performance of the fuel cell.

In order to develop the design framework, the algorithms in both the analysis and programs were carefully selected in MATLAB 7.7. Analysis and design programs were developed in-house in order to have full control of the solution process. To speed up convergence of the analysis, the genetic algorithm is used solve the nonlinear equations. This approach results in reduction of computational time.

Nomenclature

a, b	Constant terms in Tafel equation (Volts/Ke)
A_{cell}	Area of cell (m ²)
$D_{i,j}$	Effective binary diffusivity of $i-j$ pair (m ² /s)
E_{cell}	Reversible potential of each cell (Volts)
F	Faraday constant (96487 coloumb/mol)
I	Current (amperes)
$I_{density}$	Current density (A/m ²)
l_a	Width between anode channel to catalyst layer (meters)
l_b	Width between cathode channel to catalyst layer (meters)
M_i	Mole flow rate of species i (mole/s)
N_i	Superficial gas flux species i (mol/m ² .s)

N_{cell}	Number of cell in stack.
n_i	Moles of species i (mol)
P	Pressure (Pascal)
P_i	Partial pressure of species i (Pascal)
R	Gas constant, (8.3143J/mo.K)
T_{cell}	Temperature (K)
V_{cell}	Terminal voltage (Volts)
V_i	Voltage drop of type i (volts)
x_i	Mole fraction of species i
n	Number of electron participating.
α	Charge transfer coefficient.

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