MODELLING AND OPTIMIZATION OF A POLYMER ELECTROLYTE FUEL CELL

By

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ABSTRACT

The purpose of the research work is to investigate the performance of a Polymer Electrolyte Fuel cell under different operating parameters. The output voltage of a PEM fuel cell depends on various operating conditions involving complex chemical and electrical phenomena that are difficult to model.

This work focused on numerical simulation of a fuel cell electrochemical model under different readings of temperature, pressure and area of a cell. Genetic algorithm of MATLAB (version 7.8) was then used to optimize the fuel cell voltage and find the value of temperature, pressure and cell area under which maximum voltage can be obtained.

The thermo dynamical model of a fuel cell was then employed to optimize the relative humidity of output air which is a crucial measure of the water content in the fuel cell. The optimized values are used to establish limit operating temperature at the desired relative humidity under which the fuel cell can operate preserving suitable water content for its operation.

Finally a comparison is made of the obtained results which provide optimum operating conditions of fuel cell temperature, pressure, area and relative humidity.

The numerical simulation of both the models has been done using commercial software MATLAB (version 7.8) and the toolbox of Genetic Algorithm built in for the purpose has provided the optimized variables for both fuel cell voltage and relative humidity.

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LIST OF ABBREVIATIONS

Acell	Cell area (m^2)
Aactive	Active cell area (m^2)
CO_2 interface	Pressure of the oxygen gas at the surface of the catalyst at cathode (bar)
Enernst	Nernst voltage
F	Faradays constant
hf	Enthalpy of formation (KJ mol^{-1})
I	Load current (Amp)
I_L	Limiting current density (Amp/m^2)
ηact	Activation overvoltage (volts)
ηohmic	Ohmic overvoltage (volts)
ηconc	Concentration overvoltage (volts)
Pair	Air pressure (bars)
PH2 interface	Pressure of the hydrogen gas at the surface of the catalyst at cathode (bars)
PO2 interface	Pressure of the oxygen gas at the surface of the catalyst at cathode (bars)
Pcell	Fuel cell operating pressure (bar)
P win	Water partial pressure in input air (bars)
P sat in	Saturated vapor pressure in the input air (bars)
P sat out	Saturated vapor pressure in the output air (bars)
Pwgen	Water partial pressure generated by the chemical reaction (internal generation)
$P_{H20\ sat}$	Pressure of the hydrogen gas at the surface of the catalyst at cathode (bars)
R	Universal gas constant
RH_{out}	The relative humidity of output air (%)
RH_{in}	The relative humidity of input air (%)
$RH_{desired}$	The desired relative humidity of output air (%)

r_m	Specific resistivity of the membrane for the proton flow
t	Thickness of membrane (μm)
Tlimit	Limit operating pressure (bars)
Tcell	Fuel cell operating temperature (Kelvin)
Tin	Temperature of inlet air (^{0}C)
Tout	Temperature of outlet air (^{0}C)
x_{H20}	The molar fraction of water saturation in a gas stream for a given temperature
$x_{\text{other gases channel}}$	The molar fraction of other gases (apart from oxygen) in air stream
$x_{\text{in hum other gases}}$	The molar fraction of other gases (apart from oxygen) in the humidified stream at the inlet
$x_{\text{out hum other gases}}$	The molar fraction of other gases (apart from oxygen) in the humidified stream of air at the outlet
λair	Stoichiometry of gases

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Chapter 1

INTRODUCTION

Due to rising energy concerns and greenhouse emissions, great attention is being paid to fuel cell technology. As fuel cells create electricity chemically rather than by combustion they are also more efficient in extracting energy from a fuel.

A fuel cell is a device that converts the chemical energy of a fuel through a chemical reaction with oxygen or another oxidizing agent to electrical energy. Hydrogen is the most commonly used fuel but other hydrocarbons are often used. The fuel cell converts hydrogen and oxygen into water and in the process produces electricity.

A fuel cell consists of an electrolyte placed between two electrodes. Hydrogen enters the cell through anode (negative side) where the chemical reaction strips them of electrons. The hydrogen atoms are ionized and carry a positive electrical charge. The positively charged ‘protons’ diffuse through one side of the electrolyte and pass towards cathode. The electrons pass from the anode to cathode through an exterior circuit to provide electric power along the way. Oxygen enters the cathode (positive side) where hydrogen ions, protons, and electrons combine with oxygen ions to form water.

Polymer Electrolyte fuel cells or Proton Exchange membrane fuel cells are the most popular among the other types of fuel cells because of their efficient simple construction and operation. Significant developments have been carried out in PEM fuel cell technology but still they are not enough to replace the traditional stationary and mobile power sources. Some issues include water management, heat management, and catalytic activity. Therefore researchers are actively working out to address these concerns.

In this work focus is paid to optimize the fuel cell voltage through Genetic algorithm. The algorithm has also provided the operating conditions where the maximum point occurs. The membrane of the PEM fuel cell requires sufficient hydration so that protons ions are conducted efficiently. Too low water content in the membrane will cause it to dry hindering in the movement of protons across it while too much water will cause ‘flooding’ blocking the pores in electrode. Therefore a recommended gas stoichiometry and relative humidity of incoming air is required for the PEM fuel cell to maintain proper water content. The equations of thermo dynamical model used in this study have provided a range of these parameters and their effect on fuel cell performance.

The Genetic algorithm toolbox of MATLAB (version 7.8) has been found to be an effective tool for the optimization technique whereas parametric studies of fuel cell voltage under different operating conditions are also performed using simple programs written in MATLAB.

1.2 BASICS OF A POLYMER ELECTROLYTE FUEL CELL

Polymer Electrolyte Fuel Cells (PEM) work with a Polymer electrolyte in the form of thin permeable sheet ($\leq$50 µm). The PEMs are prime candidate for vehicle and other mobile applications of all sizes because of its compactness, quick startup, viability and low operating temperature range of 40 to 60 ^{0}C. The efficiency ranges from 40- 50 percent and cell outputs are generated from 50 to 250 KW. A PEMFC consists of a solid polymer membrane which is impermeable to gases but allows conduction of protons through it. The membrane which acts as the electrolyte is squeezed between two porous electrodes usually made up of carbon fiber, between the electrodes and membrane platinum particles are placed supported on carbon rods which speed up the reaction. The most commonly used membrane material used today is Nafion which is Polytetrafloroethylene chains known as Teflon. Sulphonic acid groups (HSO3) attach with the side chains of Teflon. The assembly of the gas diffusion layers (carbon cloth), catalyst layers and the membrane is called membrane electrode assembly (MEA).

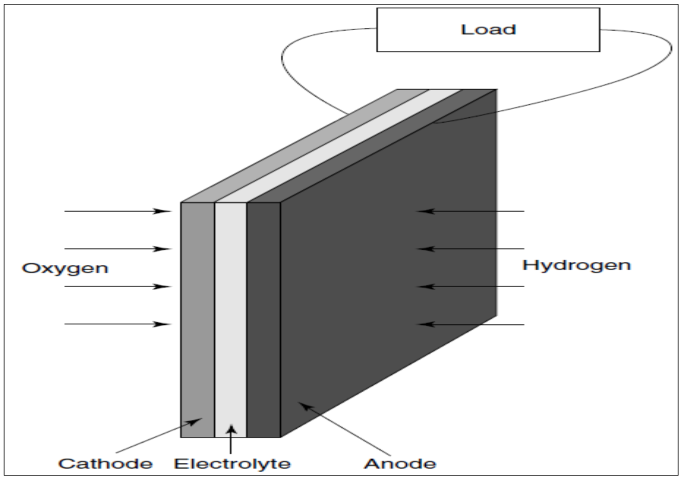


Fig 3.1: Basic construction of a PEM fuel cell [27]

A stream of hydrogen is delivered to the anode side (negative terminal) of the membrane electrode assembly. At the anode side it is catalytically split into protons and electrons. The oxidation reaction that takes place is

<u>At the anode:</u>

$$2H_2 \rightarrow 4H^+ + 4e-$$

This reaction also releases energy. The newly formed protons pass through the polymer electrolyte membrane to the cathode side while the electrons travel along an external load circuit also reach the cathode side of the membrane electrode assembly which creates voltage output by the fuel cell.

Air or in some cases pure oxygen is delivered to the cathode side (positive terminal) of the membrane electrode assembly where oxygen molecules react with H+ ions (protons) permeating from the membrane and electrons arrive from the external circuit to form water as a byproduct.

At the cathode:

$$O_2 + 4e- + 4H^+ \rightarrow 2H_2$$

Hence the overall reaction is

$$2H_2 + O_2 \rightarrow 2H_2O$$

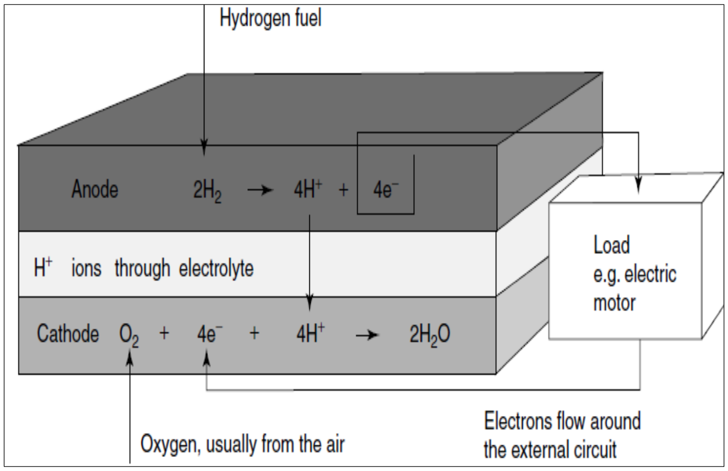


Fig 3.2: Simple operation of a PEM fuel cell [27]

1.3 EFFICIENCY AND LOSSES

1.3.1 Reversible Fuel cell voltage:

An important aspect of PEM fuel cells is the open circuit voltage and efficiency. If the fuel cell converts all of the chemical energy into electrical energy the open circuit voltage or the thermodynamic reversible cell potential of a PEM fuel cell at 25^0 C, 1 atmosphere is 1.23 volts if lower heating value of hydrogen is used.

$$E = -\Delta hf/2F \tag{3.1}$$

The potential corresponding to higher heating value or the thermo neutral potential is 1.48 volts.

This is the theoretical or maximum voltage of a PEM fuel cell but reductions are significant and the following voltage losses are encountered

1.3.2 Activation overvoltage:

These are the voltage losses that are caused because of the energy required to initiate the reaction. They occur because the chemical reaction initially does not begin due to which activation energy is required which insures the reaction tends towards the formation of electricity and water.

1.3.3 Concentration overvoltage:

These are the concentration losses or mass transport losses which occur as a result of reduction of the concentration of hydrogen and oxygen gases at the electrodes. They are caused due to mass transport concentration problems which are directly related to pressure issues.

1.3.4 Fuel crossover/Internal current loss:

These are the voltage losses which occur as a result of 'wasted fuel' that crosses directly through the electrolyte from the anode to the cathode without providing useful work or electrons through the external circuit. It can occur in two ways either fuel leaking through the electrode or electrons leaking through the electrode.

1.3.5 Ohmic Losses:

The Ohmic losses inside the fuel cell occur due to the resistance to the electron flow in bi polar plates and the resistance to the protons in membrane. They are caused due to resistances offered by electrode materials, electrolyte membrane and various interconnections between electrodes.

1.4 WATER MANAGEMENT, BACK DIFFUSION AND FLOODING OF MEMBRANE

Water management is one of the key issues in PEM fuel cells which depends on a number of factors and involves complex phenomenon. Since the membrane conduct protons across it the membrane needs to be hydrated for efficient conduction of ions. The conductivity of the electrolyte is higher when the membrane is fully saturated increasing the output voltage and efficiency of the fuel cell. But maintaining balanced water content in the cell is a challenge due to water production at the cathode and ‘water drag’. There are two components to water drag

1- Electro osmotic drag 2- Back diffusion

When the protons travel across the membrane from the anode to cathode they drag some water molecules with them. This phenomenon is known as ‘electro osmotic drag’. It is expressed as ratio of moles of water dragged per mole of proton transported or hydrogen utilized.

As the protons drag some water molecules, and since water is being produced at the cathode concentration of water at there is higher than the anode side. This concentration difference causes diffusion of water from the cathode side to the anode side which is known as ‘back diffusion of water’. If the amount of water exceeds the desired level then it will cause ‘flooding’ of the membrane blocking its pores and making conduction of ions and electrons difficult. Similarly if the transport rate of water due to electro osmotic drag is higher than by back diffusion of water the membrane will become dehydrated or dry out again causing inefficiency to conduct current.

The water produced at the cathode can be used to humidify the membrane but as mentioned before at high current densities water molecules are carried away by H^+ ions. The anode side of the membrane is most likely to be drier than the cathode side, due to at which high current densities the anode tends to be dried out faster even if the cathode is hydrated. Another issue is the drying of air at temperature greater than 60 ^{0}C. The air at this temperature dries out the electrode faster than water is produced by Hydrogen oxygen reaction.

A solution for these issues is to humidify the air, hydrogen or both before entering the fuel cell. Pressurizing the air prior to its entry is also an option but they are accompanied with the cost of compressor and humidifier as well. Therefore a combination of temperature, humidity, stoichiometry and pressure is required to maintain a suitable water production in the fuel cell as factors relative humidity, input temperature and saturated pressure are the most influential in maintaining balanced water content in the PEM fuel cell.

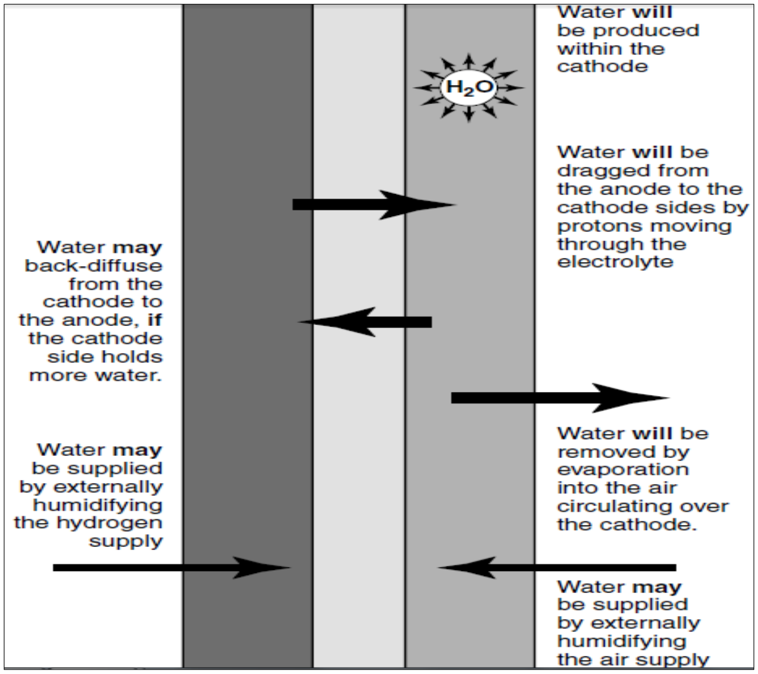


Fig 3.3: The different water movements in a PEM fuel cell [27]

Chapter 2

REVIEW OF PREVIOUS STUDIES

Substantial work has been carried out to optimize the PEM fuel cell voltage and power through different optimization algorithms using MATLAB. Efforts have been made to carry out analysis on PEM fuel cells to find out the optimum voltage, power density, efficiency and net power output at particular conditions of pressure and temperature. Some studies have also performed sensitivity analysis to indicate the factors that highly affect the PEM fuel cell performance. Several of them are mentioned below.

ZDong *et al* [1] performed a detailed optimization of the model named 'Generalized Steady State Electrochemical Model' to provide polarization curves and fuel cell efficiencies. The PEM fuel cell was modeled with the complete Balance of Plant (BOP) components namely compressor, humidifier and cooling system. They analyzed fuel cell voltage, efficiency, amount of heat rejected and net power of the stack using three algorithms of MATLAB; Sequential Quadratic Programming (SQP), Simulated Annealing (SA) and Genetic algorithm (GA). The chosen design variables were operating temperature, pressure and air stoichiometry.

ZDong *et al* [2] in continuation with the previous study carried out another optimization study on a model of low speed fuel cell hybrid electric vehicles, a fuel cell battery scooter. The PEM fuel cell is modeled as a whole system with the balance of plants. The fuel cell is considered in the form of a stack with 43 cells each having an active area of 96 cm^2 .

The work extended to optimize the net out power and exergetic efficiency using Sequential Quadratic Programming, Simulated Annealing and Genetic algorithm of MATLAB.

The optimization results obtained were then used to determine whether the low speed vehicle will be able to provide adequate power to follow the load cycle.

Narendar *et al* [3] performed mathematical modeling and optimization of a single PEM fuel cell. They evaluated the effects of temperature, pressure, gas stoichiometry, cell area and membrane thickness on fuel cell voltage. The optimum point where fuel cell showed maximum voltage was found using Genetic algorithm in MATLAB.

A Shokui Rad *et al* [4] optimized power density of a Ballard Mark V fuel cell system comprising of 35 cells using Hybrid optimization algorithm. The mathematical model however did not consider any balance of plant, heat or water management issues. The design variables considered were current density and temperature.

A Rezazadeh *et al* [5] proposed a control system based on Particle Swarm optimization whose results were compared with another controller based on Genetic algorithm. An electrical equivalent circuit of a PEM fuel cell is modeled and the goal is to adjust the stack voltage of 32 cells with the variation of load current. The proposed controller also found out the optimal hydrogen and oxygen partial pressures for maintaining the desired stack voltage.

Another optimization study of PEM fuel cell using Particle Swarm optimization was performed by M Sedighizadeh *et al* [6]. They have identified the optimum values of empirical constants, membrane constant and resistance contacts which are then compared with the reference results by Genetic algorithm.

Xin Li *et al* [7] used Hybrid Particle Swarm optimization to perform the optimization of the modeling parameters of the fuel cell. Sensitivity analysis was first done to classify the parameters as insensitive, highly sensitive and sensitive parameters according to their influence.

The sensitive and highly sensitive parameters are optimized after which voltage current curves are obtained on these parameters. The results showed improvements between normal curves of unoptimized values and those of optimized values.

Multi objective optimization of a PEM fuel cell is conducted by Suha *et al* [8] for maximizing the power output, energy and exergy efficiencies also minimizing the emissions and cost generation. The fuel cell was modeled in the form a stack consisting of 97 cells each having an area of 900 cm^2 effective area. The multi objective optimization was executed using Genetic algorithm and the objective parameters were produced work, energy efficiency, exergy efficiency and the cost of work produced.

MT Outerio *et al* [9] has investigated a method for parameter extraction of a fuel cell dynamical model using Simulated Annealing (SA) in SIMULINK. They validated their results with an experimental setup of NEXA fuel cell of Ballard’s Power system. The SIMULINK model simulates for optimization and compares it with experimental data to calculate the objective function. After simulation the parameters extracted by SA are used to characterize the fuel cell performance. The study has in detail investigated the temperature effects on stack voltage.

Vincenzo Di Dio *et al* [10] developed a mathematical dynamical model of a PEMFC coupled with an automotive synchronous electrical power drive in MATLAB. They also modeled in the form a stack consisting 35 cells each having an active area of 232 cm^2 . They studied the behavior of the stack feeding the electric motor on which a load cycle for disabled people was being applied through curves of stack voltage, power output and efficiency.

J.M Correa *et al* [11] used an effective tool ‘Multi Parametric Sensitivity Analysis’ on a 500 W BCS PEMFC stack with 32 cells. The study aimed at defining the effect of all parameters on a dynamic PEMFC model. The analysis classified them into three categories ‘insensitive’, ‘sensitive’ and ‘highly insensitive’. The dynamical response of the stack was analyzed by studying the effects of capacitance on stack voltage, load current and dynamic voltage with respect to time.

An optimal PEMFC system design with functional performance as well as production costs was investigated by D.Xue and Z. Dong [12]. They performed a joint optimization to improve functional performance while minimizing cost on a bus powered by Ballard's Mark V fuel cells. 24 Ballard fuel stacks were integrated into a 120 KW electric engine. The balance of plants consisting of compressor, water pump, heat exchanger and cooling modules was also considered.

R. Seyezhai and B.L Mathur [13] modeled the static and dynamic models of a PEMFC and studied the steady state as well as transient response of the fuel cell in MATLAB/ SIMULINK. The static model was used to analyze the output voltage of the fuel cell under different operating conditions of anode pressure, cathode pressure and temperature. The dynamic response of the fuel cell model over short and long time periods was also studied.

Foyou Chen *et al* [14] established a lumped parameter model of PEMFC to optimize the fuel cell power and obtain the optimized operational parameters of cathode and anode pressure, stoichiometry, and stack temperature. The polarization curves of voltage and power were compared with those obtained from unoptimized parameters.

M.ELSayed Youssef *et al* [15] also developed a lumped model of PEMFCs taken account into the electrochemical model of fuel cell with the gas flow considerations. It was then used to study the effects of input temperature, pressure, stoichiometric ratio, membrane thickness and gas diffusion layer on fuel cell voltage.

Another optimization study performed by Mojtaba Tafaoli *et al* [16] applied Genetic algorithm on a quasi two dimensional isothermal model to simulate flow behavior in channels and membrane electrode assembly. The MATLAB optimization code was executed to obtain power densities at different cell temperature, cathode and anode pressures. The results were validated with the help of experimental setup of 25 cm^2 active PEMFC.

Piwen Li *et al* [17] performed a comprehensive analysis and optimization of current collecting systems in a PEMFC. The dimensions of current collection ribs were optimized to get a maximized power density in a fuel cell. They analyzed both 2D and 3D current collecting systems in the gas delivery field of PEMFCs. The fuel cell voltage and power densities were evaluated at different diameters of current collector which were then validated from experimental curves.

Frano Barbir *et al* [18] designed and optimized a PEMFC system for backup power applications. Their study focused on a Regenerative Fuel cell system which operates alternatively as an electrolyzer and a fuel cell. The paper focused on the option of using two seperate stacks for each purpose. The effect of operating pressure on compression power, humidification, active cell area and aspects of water management were studied.

Luis A. M Riascos and David D. Pereira [19] introduced a control technique for maintaining the limit operating temperature of PEMFC. The tests on PEMFC were performed considering two conditions; PEM fuel cells without extra humidification and with extra humidification. They studied in detail the effects of temperature and humidity of the input air and devised a control technique for the humidifier to maintain the humidity of output air.

Luis A.M Riascos *et al* [20] also modeled a control system to ensure that the airflow rate and temperature are within prescribed limits during operation. The new control technique based on the controlling the relative humidity was established, the PEM fuel cell was modeled in MATLAB and the controller was developed in LAB VIEW.

Luis A.M Riascos *et al* [21] further continued their work and similarly modeled a control strategy on the fuel cell model for optimal operating temperature. They considered the desired relative humidity and minimum air stoichiometry as given conditions which adjust the limit operating temperature.

A.A Kulikovsky [22] studied in details the effect of stoichiometric ratio on the performance of PEMFC. The study aimed to rationalize the effect of stoichiometric ratio on cell performance curve and voltage loss due to oxygen transport across the backing layer. He also performed a fitting procedure of the performance curve using genetic algorithm.

V.Perez Herranz *et al* [23] developed a test bench to monitor a 3KW PEMFC fuel stack consisting of 36 cells each having an active area of 200 cm^2. They studied the steady state response of the fuel cell under different pressure feed gas and air stoichiometry by monitoring the voltage of each individual cell in the stack.

The effect of stoichiometry on dynamic behavior of a PEMFC was investigated by Sunhoe Kim *et al* [24]. They studied the transient response by observing the undershoot and over shoot behavior of the fuel cell system with different initial and final stoichiometry.

Lin Wang *et al* [25] experimentally studied the effects of different operating parameters on the performance of PEMFC using pure hydrogen on the anode and cathode. They also developed a single 3D model and compared the modeling results with experimental data. The effects of temperature, operating pressure and anode humidification on cell voltage were analyzed using a PEM fuel cell with an active surface area of 51.84 cm^2 .

Catlin Glenn [26] in his work combined the computational fluid dynamics and genetic algorithm techniques to optimize the flow channels of a PEM fuel cell model. He optimized the net power density of the fuel cell by optimizing the geometric parameters of serpentine flow channels of a fuel cell. The optimization was performed using Genetic algorithm and the parameters obtained by it were applied on a CFD model using FLUENT to analyze its performance.

Chapter 3

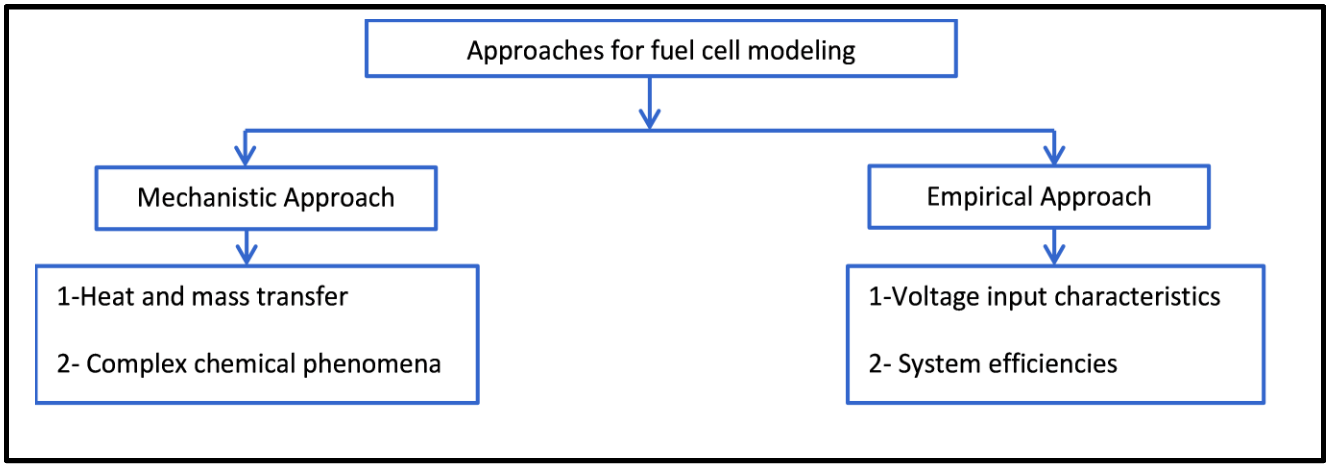
PEM FUEL CELL MODELING

Mathematical models of fuel cells are needed to analyze their performance and for their efficient design. These models help in simulating the process and phenomenon involved in a fuel cell without the need of conducting costly and time consuming experiments. Two major approaches for modeling fuel cells are applied.

3.1 APPROACHES FOR FUEL CELL MODELING

3.1.1 First Approach

The first approach is the use of 'mechanistic models' which deal with simulation of heat, mass transfer and electrochemical phenomena in fuel cells. These models simultaneously involve multi-phase, multi-component, temperature gradients and multi-dimensional mass transfer with complex electrochemical reactions. They are mostly applied by using computational fluid dynamics.



3.1.2 Second approach

The second approach is the use of 'models based on empirical and semi empirical equations' which are applied to predict the effect of different input parameters on the voltage current characteristics of the fuel cell without examining in depth the physical and electrochemical phenomena involved in the chemical reaction. Empirical models are further classified according to the analysis they are used to perform on fuel cells [9]. The fuel cell models are broadly divided into dynamic models and steady state models. [28]

3.2 TYPES OF FUEL CELL MODELS

3.2.1 Dynamic models

In dynamic models the two major dynamic properties; fuel/air flow and temperature change according to any variations or disturbances on surrounding operating conditions and step load changes. They are mostly used to observe the transient behavior of a fuel cell.

3.2.2 Large signal models

They involve the transient behavior of the fuel cell by evaluating phenomena known as 'charge double layer'. The model assumes a time constant in the form of charge layer capacitance due to anode and cathode contact interface with the membrane.

3.2.3 Small signal models

These models assume another charge layer capacitance which dominates a portion of the frequency domain. Impedance is also added for the adsorption and electrode electrolyte reactions which produce another time constant.

3.2.4 Steady state model

These models are especially used for characterizing the time independent output of the fuel cell and take into account the steady state behavior of a fuel cell by analyzing the anode and cathode kinetics. The activation overvoltage, concentration and ohmic losses are considered to produce polarization curves and system efficiencies.

3.3 MODELS USED IN THE PRESENT STUDY

Two types of steady state models are employed here to observe the output and water content of the fuel cell separately.

3.3.1 Electrochemical model of a Polymer electrolyte fuel cell

A fuel cell model which characterizes the fuel cell voltage of the fuel cell is called an electrochemical model. The model implemented in this work for the optimization of fuel cell voltage is based on the ‘Generalized steady state zero dimensional, semi empirical and static model’.[1]-[21] It involves the steady state relations of irreversible voltage losses, electrode pressures and current density and helps us to predict the polarization curve of the fuel cell at different operating conditions.

3.3.2 Thermo dynamical model of a Polymer electrolyte fuel cell

The calculations of relative humidity and limit operating temperature of a fuel cell form the thermo dynamical of a fuel cell. It essentially analyzes the water management of a PEM fuel cell by studying the effects of inlet humidity and saturated pressure on the output relative humidity of the fuel cell. The rate of water production and air usage can also be evaluated. [21]

Chapter4

GENETIC ALGORITHM

Genetic algorithm is a part of Evolutionary algorithms (EA) and is a method for solving optimization problems and works on the ideas of natural evolution and genetics. It repeatedly modifies a population of individual solutions and at each step it selects individual at random from the current population to be parents and produces children from them for the next generation. Over successive generations the solution evolves or moves towards the optimum solution. Genetic algorithm (GA) is based on the Darwin's theory of evolution which states 'survival of the fittest'.

4.1 Operation of a genetic algorithm

Optimization is a process which involves finding the best or optimal solution of a function while satisfying all the constraints of the function to be optimized. The genetic algorithm searches the optimal solution by mimicking the natural processes of **Selection, Crossover and Mutation** as they are analogous in our DNA**.** The algorithm begins with a random set of population which is a set of individuals from the search space and evaluates them according to their fitness value which represents a possible solution for the objective function.

Single objective optimization $\min f(x)_{i=n} = f(x)$

Multi objective optimization $\min F(x) = (f_1(x), f_2(x), f_3(x) \ldots .. f(n))$

Each individual can be represented in the form of a finite length of vector which can be coded as binary digits. The closer the individual is with the optimal solution the more chances it has to survive for the next generation. GA forms a population of size (N) by selecting its chromosomes (n) which contain the solution in the form of genes. The genes can be Boolean, floating points, integers or a combination of these.

Genetic algorithm uses two most important parameter crossover and mutation to form new population. Crossover operator produces new children by combining the vector entries of the parents. While the mutation operator produces new offspring by randomly making changes to the genes or applying mutations to the parents.

4.2 Main working parameters of the Genetic algorithm

4.2.1- Selection

The selection function evaluates the individuals according to their fitness values of the objective function. They are also known as Reproduction operators which select chromosomes to be parents to crossover and produce new children. The selection functions are

- Roulette wheel selection - Gauss selection - Rank selection – Tournament selection

The Roulette wheel works by dividing a circle into N sectors where N is the number of individuals of a population. The individual is selected according to the probability (P) which is proportional to its fitness value to the sum of all the fitness values of individuals in the generation.

$$Pi = Fi/\sum_{k=1}^{n} Fk$$

Where Pi= Probability of ith string, n=population size F_k = Fitness for kth string in the population.

The Rank selection is a better option which sorts individuals according to their fitness function and assigns them a rank with rank 1 as the best individual, rank 2 for the second best and so on. The probability for the selection of an individual is given by the relation where β is a user defined function

$$Pi = \beta(1-\beta)^{rank-1}$$

4.2.2 Crossover

Crossover is the first step in the recombination process by which genes of the parents are selected and recombined to form children with new chromosomes. It takes the best characteristics (genes) from the parents according to the probability of the operator and creates a new offspring.

The most widely used crossover operators are

– Scattered crossover   –Two point   –Arithmetic   –Heuristic

4.3.2.1 Scattered Crossover

In the scattered crossover corresponding genes of a parent are recombined to form genes of children by the following relation

Genes in population N- Parent genes $P_1= [a_1, b_1]$ $P_2= [a_2, b_2]$

Genes in population N+1- Child genes $C_1= [a_1, b_2]$ $C_2= [a_2, b_1]$

4.3.2.2 Two point crossover

The two point crossover select two random crossover points in the parents and interchanges the chromosomes from the selected points to produce a new offspring.

Genes in population N- Parent genes $P_1= a_1\ a_2a_3\ b_1b_2b_3$ $P_2= a_4\ a_5\ a_6\ b_4b_5b_6$

Genes in population N+1- Child genes $C_1= a_1\ \mathbf{a_5}\ \mathbf{a_6}\ b_1b_2b_3$ $C_2= a_4\ \mathbf{a_2}\ \mathbf{a_3}\ b_4\ b_5b_6$

4.3.2.3 Arithmetic operator

It crosses the genes of the parents to form offspring according to the equation

Genes in population N- Parent genes $P_1= [a_1\ a_2\ a_3]$ $P_2= [a_4\ a_5\ a_6]$

Genes in population N+1- Child genes $C_1= k \times [a_1\ a_2\ a_3] + (1-k) \times [a_4\ a_5\ a_6]$

$C_2= (1-k)\ [a_1\ a_2\ a_3] + a \times [a_4\ a_5\ a_6]$

Where k= random weighting factor

4.3.2.4 Heuristic operator

It evaluates the parents according to their fitness values and produces the offspring according to the following relation

Genes in population N+1- Child genes C_1= Best parent +r x (Best parent – Worst parent)

C_2= Best parent

Where r is a factor which is a random number between 0 and 1.

4.2.3 Mutation

Mutation is an important genetic operator which is performed after crossover takes place, it maintains a diversity in the population as the algorithm evolves by creating new generations. Mutation makes random alterations in the gene of a chromosome which produce new gene values for the next population. These new values help the genetic algorithm to move towards a diverse solution otherwise the solution will be stagnated to a local point in the search space.

The mutation operators are **– Flip bit** **– Boundary** **– Uniform** **– Gaussian**

4.2.4 Elitism

The elite count is an operator which significantly improves the performance of the genetic algorithm by retaining a suitable number of individuals with the best fitness value. These are the parents with the best fitness value in each generation. It is necessary for the genetic algorithm because the best chromosomes may be lost in while crossover and mutation of genes.

4.3 GA based optimization

The Genetic algorithm optimizes an objective function by either minimizing or maximizing the fitness value. The basic working principle for the optimization technique is explained below

1- Generates an initial population by selecting random individuals.

2- The solutions are evaluated according to their fitness function.

3- The algorithm checks them for termination whether the fitness limit has been achieved or not.

4- The operators of Reproduction, Crossover and Mutation are applied to produce a more diverse and genetically stronger population of new chromosomes namely children.

5- New generations are produced until the criteria for stopping is reached.

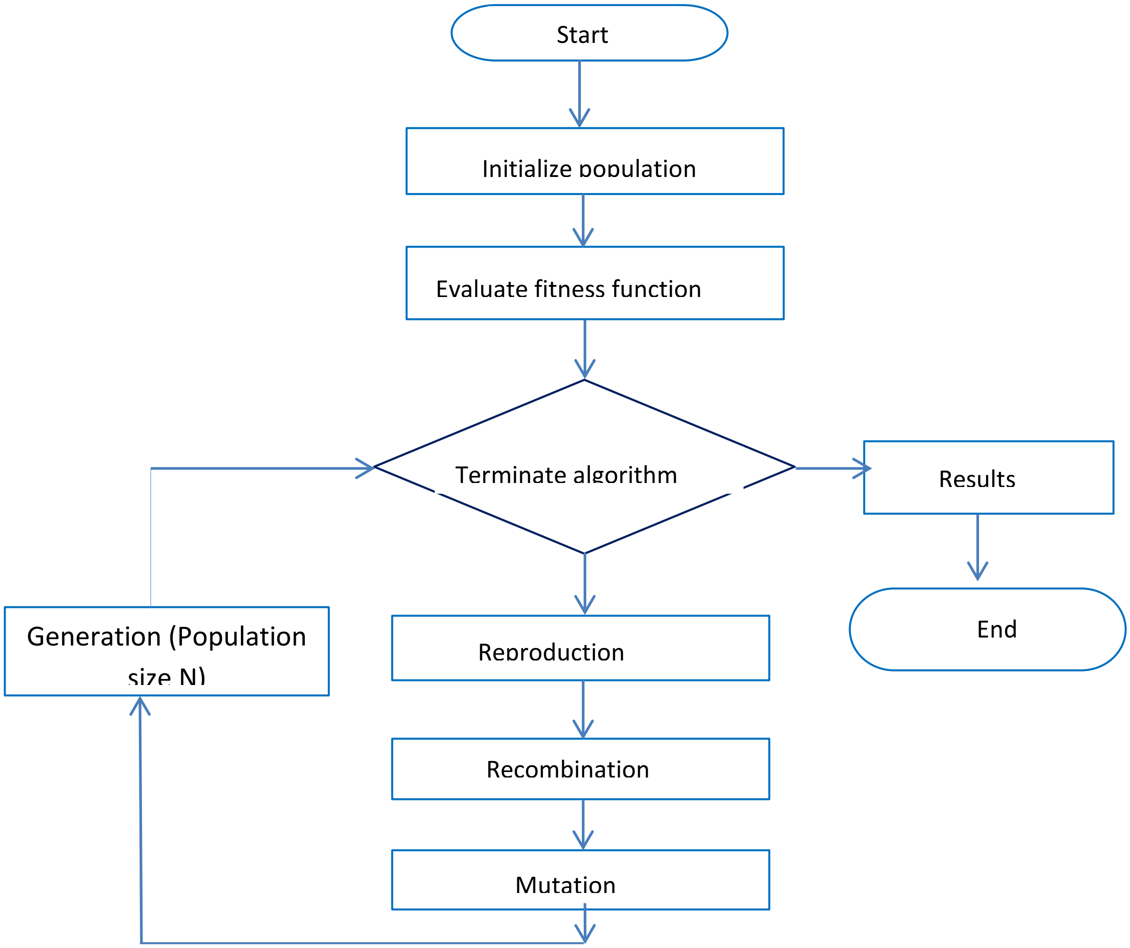


Fig 4.1 Working of the genetic algorithm

Chapter 5

SIMULATION AND OPTIMIZATION METHODOLY

5.1 METHODOLGY

A Polymer electrolyte fuel cell is modeled using two empirical models electro chemical model and thermo dynamical model. The effects of input parameters cell temperature, pressure, cell area, membrane thickness are studied on fuel cell voltage using the empirical equations [3]. The electro chemical model is then optimized by using Genetic algorithm toolbox of MATLAB (version 7.7). The thermo dynamical model [19] is used to establish limit operating temperature of a polymer electrolyte fuel cell and effects of air stoichiometry, air pressure and temperature on relative humidity are studied. The best operating conditions where balanced water content is achieved are found by optimizing air pressure, stoichiometry and inlet relative humidity. This model is used to study the effects of relative humidity on the water content of the PEM fuel cell. The results from both the models are compared to analyze the best operating conditions of the fuel cell on the basis of maximum cell voltage and output relative humidity.

The design variables chosen for the electro chemical model are temperature, pressure, cell area, membrane thickness, active area factor and number of cells with minimum and maximum limits as Xmin=[313,1.013,0.016,0.0015,0.56,1] and Xmax=[360,10.013,0.064,0.05,0.60,100] respectively.

Design variables for optimization of voltage: Temperature, Pressure, Cell area, Membrane thickness, Active area factor and number of cell

Limits: Xmin=[313,1.013,0.016,0.0015,0.56,1] Xmax=[360,10.013,0.064,0.05,0.60,100]

Design variables for optimization of relative humidity: Air pressure, Inlet air relative humidity and Stoichiometry.

Limits: Xmin= [1, 0.2, 1] Xmax= [8, 1, 10]

The Genetic algorithm toolbox maximizes the objective function

f (x) = -Vcell x ncell

f(x) =- RHout= - (Pwin+Pgen)/Psatout

The toolbox tries to find the minimum of the objective function therefore negative sign is included if a quantity needs to be maximized. The largest negative number then becomes the minimum value due to which the quantity of interest is maximized.

The Genetic optimization algorithm points out the maximum voltage and values of design variables where it is found. The design variables for thermo dynamical model are inlet humidity, air pressure and air stoichiometry. These design variables after parametric study and optimization using Genetic algorithm provide the optimum conditions for fuel cell performance at which it provides maximum voltage as well as the conditions of relative humidity and air stoichiometry where a balanced water content is achieved.

5.1.1 Assumptions

1) The reactant gas at cathode is assumed as air which is a mixture of nitrogen, oxygen and other gases.

2) The study has been done only on a fuel cell therefore neglecting the losses of current collecting plates, balance of plant, heat produced etc.

3) The pressure is assumed to be uniform, while partial pressures of gases and water molecules are considered.

4) The water is produced as a byproduct in the form of liquid.

5.2 EQUATIONS OF ELECTRO CHEMICAL MODEL

$$Vcell = Enernst + \eta act + \eta ohmic + \eta conc \tag{5.1}$$

$$\eta act = \beta 1 + \beta 2 Tcell + \beta 3 Tcell \ln(CO2\ interface) + \beta 4\ Tcell \ln(I) \tag{5.2}$$

$$CO2\ interface = \frac{PO2\ interface}{5.08 * 10^{6}\, e^{(-498/Tcell)}} \tag{5.3}$$

$$PO2\ interface = Pcell\, [\, 1 - xH2o - xother\ gaseschannel\ e^{(0.291 i/Tcell^{0.832})}\,] \tag{5.4}$$

$$xH2o^{sat} = \frac{PH20^{sat}}{Pcell} \tag{5.5}$$

$$ln\left(PH20^{sat}\right) = 70.43464 - \frac{7362.6981}{Tcell} + 0.0069 * Tcell - 9 * \ln(Tcell) \tag{5.6}$$

$$xchannel\ other\ gases = \frac{xin{,}hum\ other\ gases - xout{,}hum\ other\ gases}{ln\ (xin{,}humother\ gases\ /\ xout{,}hum\ other\ gases)} \tag{5.7}$$

$$xin, hum\ other\ gases = (1 - xH20\ ) * 0.79 \tag{5.8}$$

$$xout, hum\ other\ gases = \frac{1 - x\ H20^{sat}}{[1 + \left(\frac{\lambda air - 1}{\lambda air}\right) * \left(\frac{0.291}{0.79}\right)]} \tag{5.9}$$

$$\eta conc = \frac{RTcell}{2F} \ln(1 - \frac{I}{IL}) \tag{5.10}$$

$$\eta ohm = \eta ohm\ elect + \eta ohm\ protonic = i\ (\ Relectr + R\ protonic\ ) \tag{5.11}$$

$$R\ protonic = \frac{rm * t}{Aactive} \tag{5.12}$$

$$r\ m = \frac{181.6\ [1 + 0.03\ i + 0.062(\frac{Tcell}{303})^{2}\ i^{2.5}}{[\lambda\ membrane - 0.634 - 3i\ ]\ e^{3.25\ (Tcell - 303)/Tcell}} \tag{5.13}$$

$$Enernst =$$

$$1.229 - 0.85 * 10^{-3} (Tcell - 298.15) + 4.3085 * 10^{-5}\, Tcell(\ln(PH2interface)) + 0.5 \ln(PO2interface) \tag{5.14}$$

$$PH2\ interface = (0.5PH2O)[\frac{1}{(e^{1.653/Tcell}\ xH20\ channel^{1.334})} - 1\ ] \tag{5.15}$$

$$Aactive = Af * Acell \tag{5.16}$$

Table 5.1: Proposed electrochemical model

S.No	**Parameter**	**Meaning**	**Value**	**Unit**
1	Pcell	Fuel cell pressure	1.013 – 10	bars
2	Tcell	Fuel cell temperature	313 – 360	Kelvin
4	*i*	Current density	0.7	A/cm^2
5	I	Load current	200	Ampere
6	ncell	Number of cell	1-100	
6	λair	Air stoichiometry	7.5	
7	t	Membrane thickness	1.535-50	µm
8	λmembrane	Membrane constant	12	
9	A$_f$	Active area factor	0.56-0.60	
10	Acell	Area of cell	0.016-0.064	m^2
11	R	Universal gas constant	8.3145	J mol- 1K
12	F	Faradays constant	96485	C e^{-1}
13	β 1	Empirical coefficient	-0.954	
14	β 2	Empirical coefficient	-0.00312	
15	β 3	Empirical coefficient	0.000074	
16	β 4	Empirical coefficient	-0.000187	
17	I$_L$	Limiting current density	1.5	A/cm^2

The table presents the proposed electrochemical model and parameters used for the optimization of fuel cell voltage. Temperature, Pressure, Area, Membrane thickness, Active area factor and Number of cells are the design variables chosen for optimization.

Table 5.2: MATLAB Genetic algorithm toolbox settings

S.No	**Parameter**	**Value**
1	Objective function	Fuel cell voltage
2	Number of parameters	6
3	Number of generations	200
4	Population size	550
5	Crossover function	Scattered
6	Crossover fraction	0.8457
7	Selection function	Roulette
8	Mutation	Default
9	Time limit	Infinite
10	Migration	Default
11	Stall generations	100
13	Fitness limit	1.248

The above table shows the MATLAB settings for the Genetic algorithm toolbox, which governed the optimization procedure by the Genetic algorithm. The population size was set to be 550 and number of generations to be 200 so that best fitness limit is searched in a large search domain.

5.3 EQUATIONS OF THERMODYNAMICAL MODEL

$$Tlimit = 96.25 + 23.55\, ln \left[\frac{1}{RHdesired}\left(\frac{0.421.Pair}{\lambda\, air + 0.188}\right) + Pwin + 0.01751\right] \tag{5.18}$$

$$Pwin = (Psat\ in * RHin) \tag{5.19}$$

$$Psatin = -0.03089 + 0.02451 e^{(Tin/26.67)} \tag{5.20}$$

$$Psatout = -0.03089 + 0.02451 e^{\left(\frac{Tout}{26.67}\right)} \tag{5.21}$$

$$Pwgen = \frac{42.1*Pair}{\lambda-0.188} \tag{5.22}$$

$$\lambda = (\frac{42.1*\,Pair}{RHdesired\,*Psatout-Pwin}) - 0.188 \tag{5.23}$$

$$RHout = \frac{Pwin+Pwgen}{Psatout} \tag{5.24}$$

$$RHdes = \frac{[\left(\frac{42.1*Pair}{\lambda+0.188}\right)+Pwin]}{Psatout} \tag{5.25}$$

$$mw = 9.34 * 10^{-8} \quad (\frac{Power}{Cellvoltage}) \tag{5.26}$$

$$mwr = 0.622\left(\frac{Pw}{P-Pw}\right)ma \tag{5.27}$$

$$ma = 3.57 * 10^{-7} * \lambda * \frac{Power}{Vcell} \tag{5.28}$$

Table 5.3: Proposed thermo dynamical model

S.No	**Parameter**	**Meaning**	**Value**	**Unit**
1	RHin	Relative humidity of input air	20-100	%
2	λair	Air stoichiometry	2-10	
3	Tin	Inlet air temperature	30	^{0} C
4	Pair	Air pressure	1-8	bars
6	Tout	Outlet air temperature	60	^{0} C

Chapter 6

RESULTS AND DISCUSSION

6.1 NEED FOR GLOBAL OPTIMIZATION METHOD

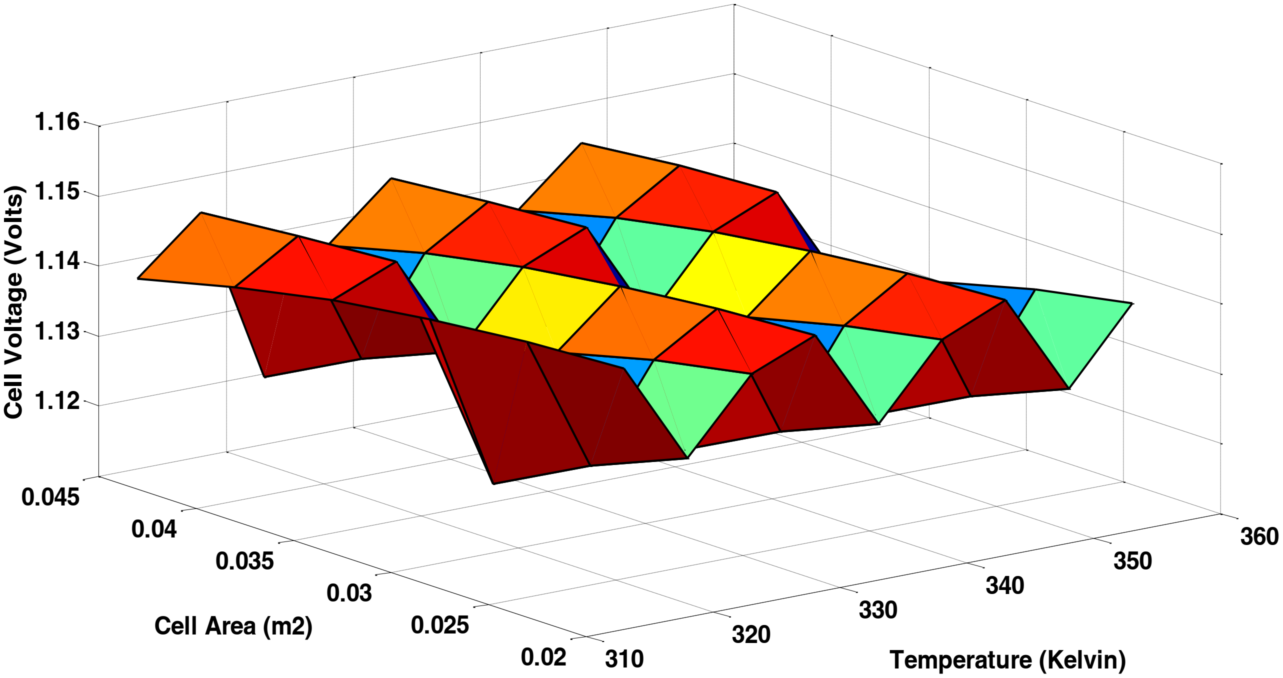


Fig 6.1: Function shape of fuel cell voltage at cell area and temperature

Fig 6.1 shows the need for global optimization method required for the electrochemical model as the fuel cell voltage which is the objective function to be maximized is complex and rapidly changes values at different points of different parameters. Here the shape of the function is analyzed at two parameters; cell area and temperature. Pressure, number of cells and membrane thickness are kept constant hence their combined effects cannot be analyzed in Fig

These local methods cannot be used for optimization strategies here as they will tend to move the optimum point towards local optima which will not explore the effect of all possible solutions at all parameters. The fitness landscape cannot be analyzed by traditional methods of search as they find the local optima of the function without taking into account all possible solutions.

Similarly Fig 6.2 shows here the function shape for voltage at cell area with pressure which is diverse at all combinations of these parameters.

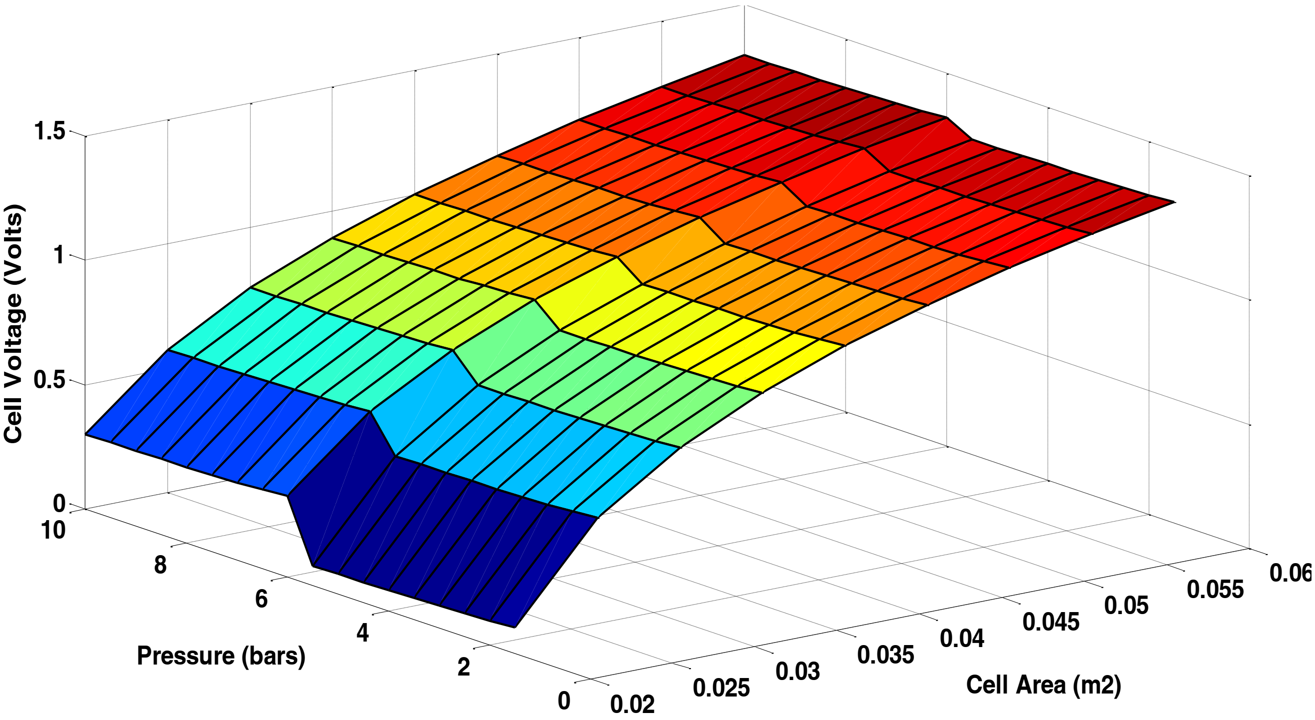


Fig 6.2: Function shape of fuel cell voltage at cell area and pressure

The objective function fuel cell voltage shows a different behavior at each parameter that is evident from Figures 6.1 and 6.2. The function shape is different showing a complex relationship between design variables and objective function.

Similarly Figures 6.3 and Figures 6.4 show a different performance of the fuel cell at cell area with the membrane thickness limit and temperature with pressure.

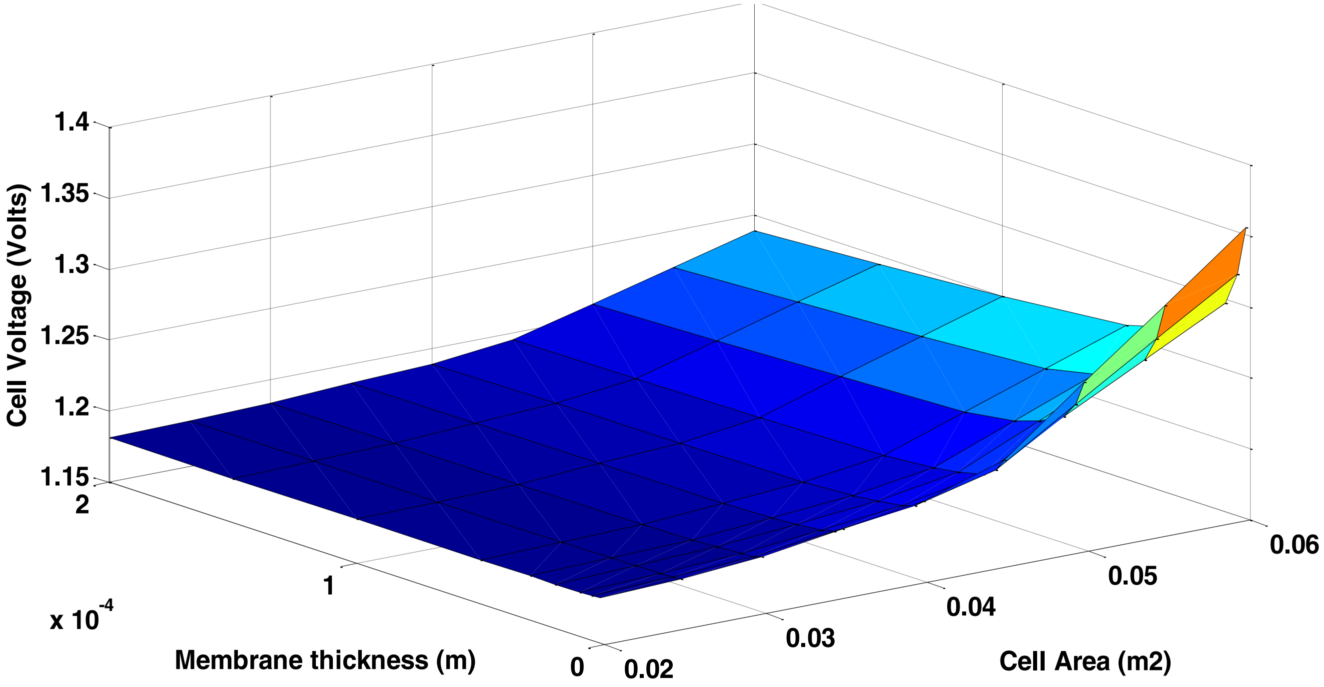


Fig 6.3: Function shape of fuel cell voltage at cell area and membrane thickness

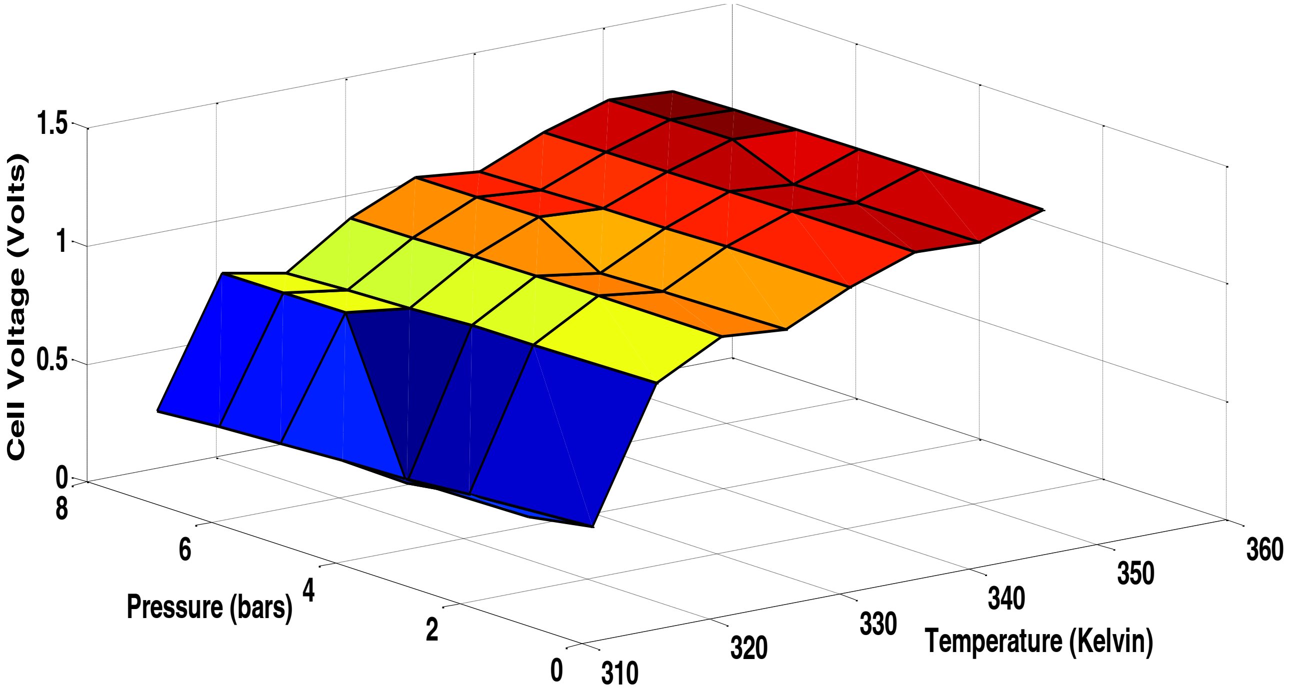


Fig 6.4: Function shape of fuel cell voltage at temperature and pressure

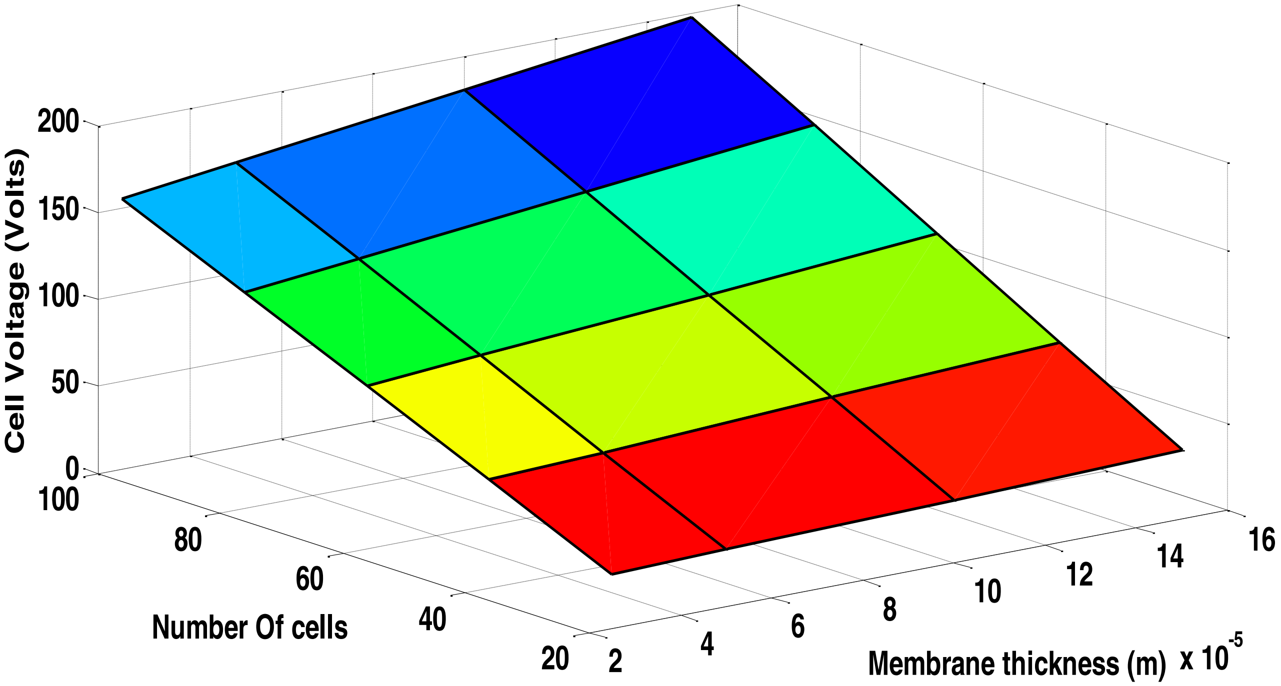


Fig 6.5: Function shape of fuel cell voltage at membrane thickness and number of cells

Fig 6.5 further asserts that since the fuel cell voltage is a complex function which depends on numerous operating conditions and the fuel cell's geometric parameters, a global method is needed to analyze and establish a global point where the whole domain of the function is optimized after the search of all possible solutions.

The behavior of voltage at the significant design variables of Cell pressure, temperature, area, membrane thickness, number of cells and active area factor is dissimilar and multifaceted. In addition the effect of these variables simultaneously cannot be established using traditional methods; therefore Genetic algorithm is used as the optimization technique to search the global solution for the function.

6.2 PARAMETRIC STUDY ON FUEL CELL VOLTAGE

A parametric study of the six design variables is performed here to study the effects of six design variables on Polymer electrolyte fuel cell.

6.2.1 Effect of operating pressure, temperature and cell area on fuel cell performance

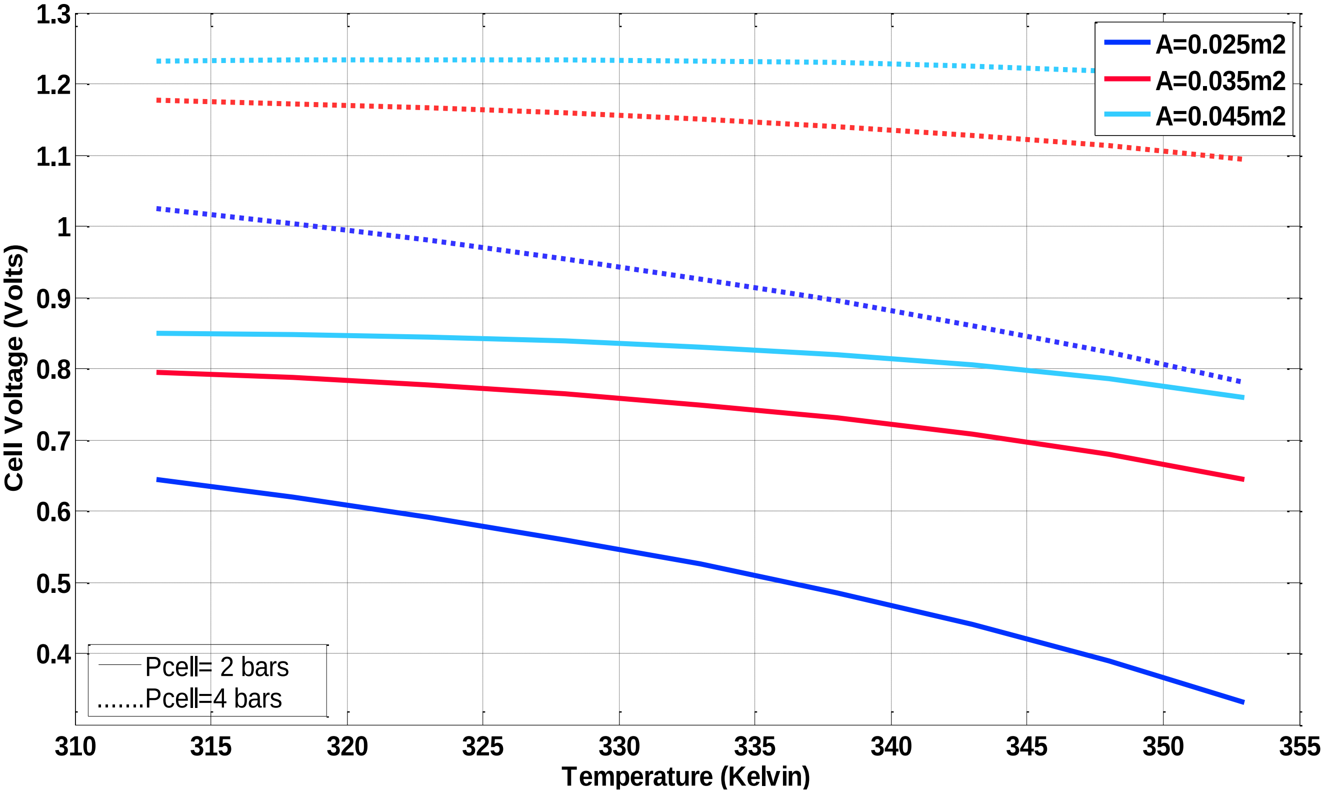


Fig 6.6: Cell voltage graph at variable pressure, temperature and area

Fig 6.6 shows the performance of a fuel cell increases with an increase in pressure and increase in area. The voltage increases from 0.6 volts to 1.23 volts as we increase the pressure from 2 bars to 4 bars. The increase in pressure increases the partial pressure of gases at the interface which thereby increases the activity of reaction as more protons (H^+) ions are available for reaction with oxygen molecules at the cathode. The voltage also rises with the increase in cell area since more surface area is available to the gas molecules for diffusion due to which higher activity of the reactants takes place at the cathode and anode sites. The increase in cell area also decreases the protonic resistance of the protons in the membrane due to which electrochemical reaction proceeds quickly.

6.2.2 Effect of membrane thickness, number of cells and area factor on fuel cell performance

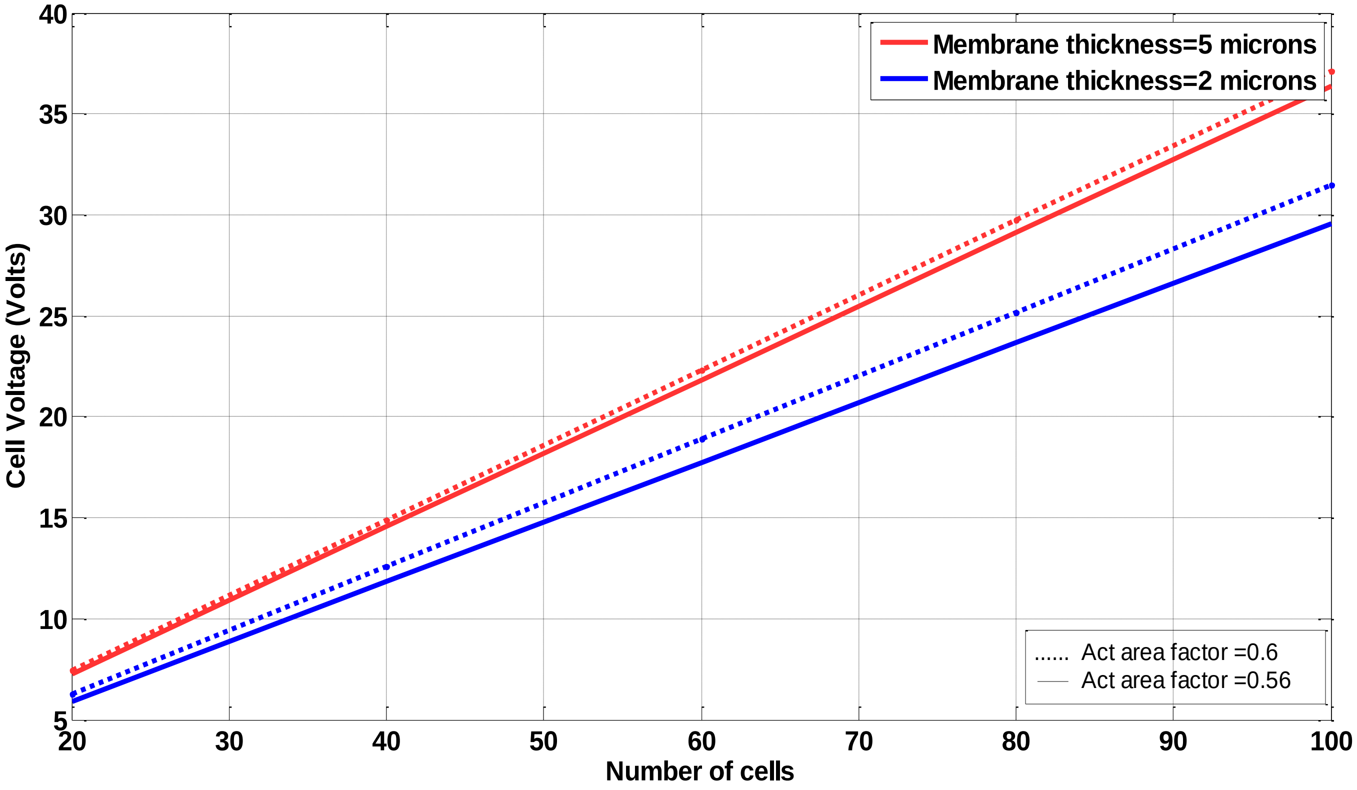


Fig 6.7: Cell voltage at variable membrane thickness and number of cells

Fig 6.7 illustrates the effect of fuel cell voltage at different membrane thickness, active area factor and number of cells is shown in the above figure. The voltage decreases as the membrane thickness is increased leading to an increase in ohmic losses. The protonic resistance which depends on current density, membrane material and thickness increases with a thicker membrane. While the active area factor allows for a larger active area increasing the reaction sites. The voltage increases from 5 volts to 38 volts as the number of cells is increased. This explains for the reason why Polymer electrolyte fuel cells are arranged in a stack for most of the stationary power or automobile applications.

6.3 VOLTAGE OPTIMIZATION BY GENETIC ALGORITHM

The electro chemical model has been optimized using toolbox of Genetic algorithm MATLAB. The algorithm is first applied to maximize the fuel cell voltage on the basis of temperature, pressure and cell area. These optimum values are used to find new optimized design variables active area factor, number of cells and membrane thickness limit. The optimization procedure initiates with a random population size of 550 as the design variables are three the algorithm creates a matrix of chromosomes size 550 by 3 which are then evaluated according to their fitness value at each iteration, the selection technique chosen for the study is Roulette which selects the individuals with the best fitness values according to the elitism technique. The elite count for the study is default which is 2 that removes the individual with worst values. The crossover and mutation operator subsequently produce offspring by altering the genes of the parents (chromosomes). The number of crossover children depends on the crossover probability which is 0.8560. Fig 6.8 shows the best fitness value of 1.233 and a mean value of 0.1978.Process of selection, crossover and mutation continues until the maximum voltage is reached after 200 generations.

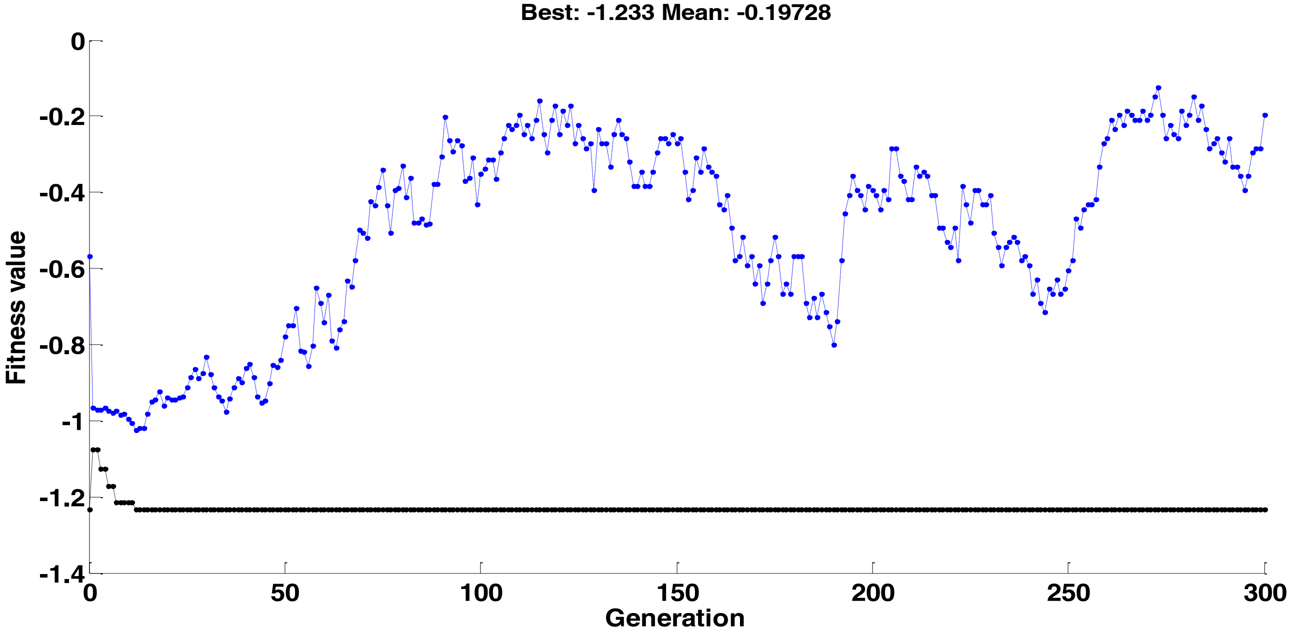


Fig 6.8: Convergence graph of best and mean fitness values

The following plots display the best individuals that provided the optimum value of fuel cell voltage.

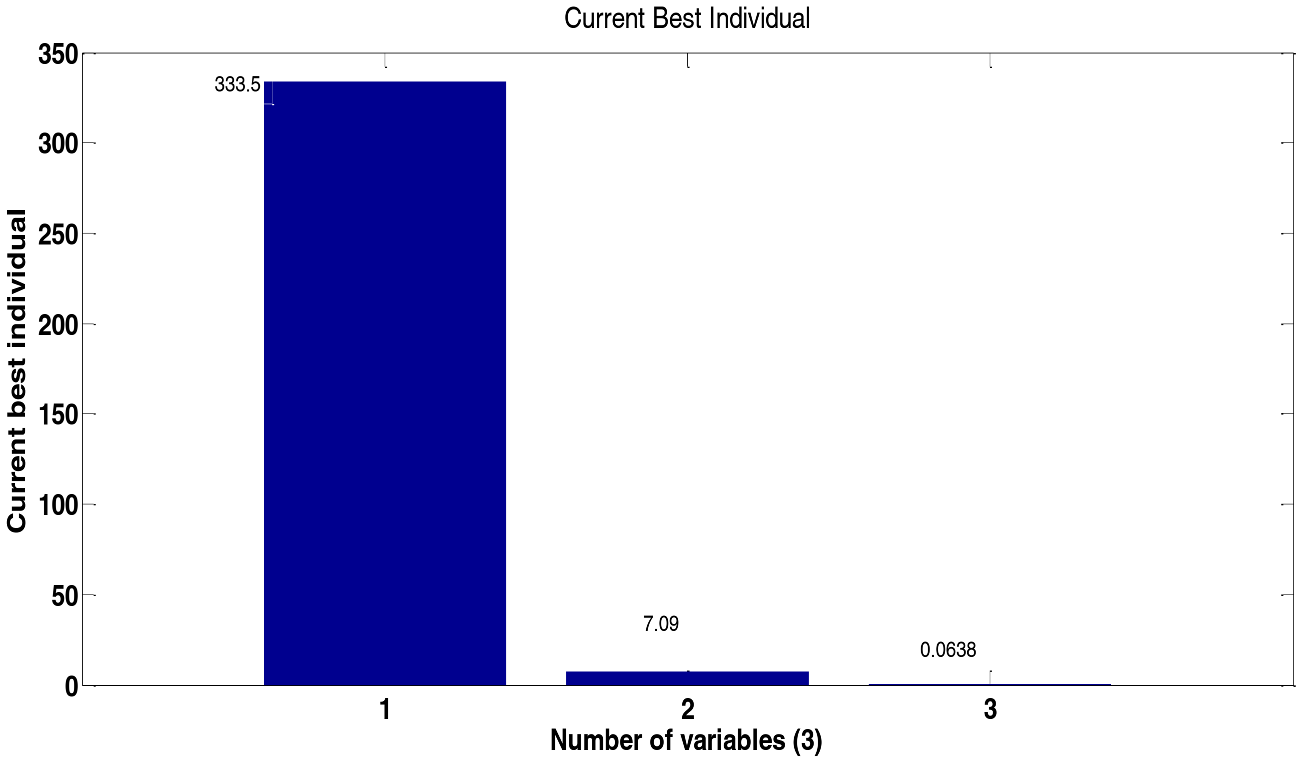


Fig 6.9: Best individual values for the objective function

The optimum design area is 0.0623 m ^{2} with a fuel cell operating temperature of 333.5 Kelvin and a cell pressure of 7 bars. A larger cell area and a pressure with a moderate temperature value provide the optimum voltage of 1.233 volts.

Table 6.1: Optimized PEM fuel cell parameters

Parameter	**Minimum limit**	**Maximum limit**	**Optimum value**
Temperature (Kelvin)	313	360	333.5188
Pressure (bars)	1.013	10.013	7.09
Area (m^2)	0.016	0.064	0.0638
Optimized voltage 1.2330 volts			

As mentioned earlier the negative sign indicates the maximized quantity since the Genetic algorithm by default searches the global minima. These values are validated against the optimized values of Narendar *et al* [3] which depict a good agreement with their results.

Table 6.2: Results validation

Parameter	**Reference [3]**	**Obtained Values**
Voltage (Volts)	1.223	1.233
Temperature(Kelvin)	334.890	333.5188
Pressure (bars)	4.554	7.09
Area (m^2)	0.053	0.0638

The genetic algorithm in Fig also displays the range of best, mean and worst scores at each generation giving an overview of the fitness function during the search space. The worst and best values range from 0 to 1.233 with the mean varying rapidly at each generation as shown below.

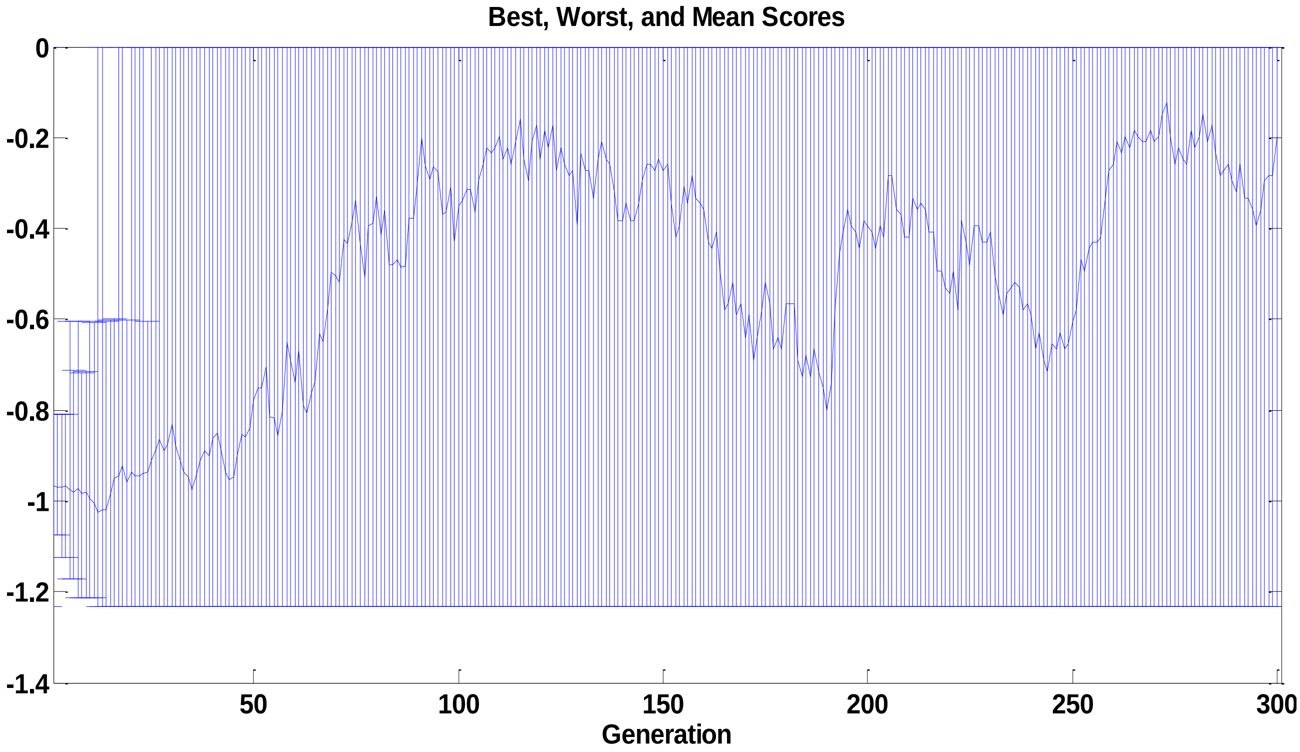


Fig 6.10: Best, worst and mean scores at each generation

Fig 6.11 illustrates the algorithm searches the individuals from the population whose fitness values are closer to the fitness limit, as it directs its search the average distance between the individuals converges to a minimum with successive generations. Here the distance varies till 180 generations after which the population of chromosomes has no diversity. Once the algorithm observes no major improvement in the optimum value the solution converges.

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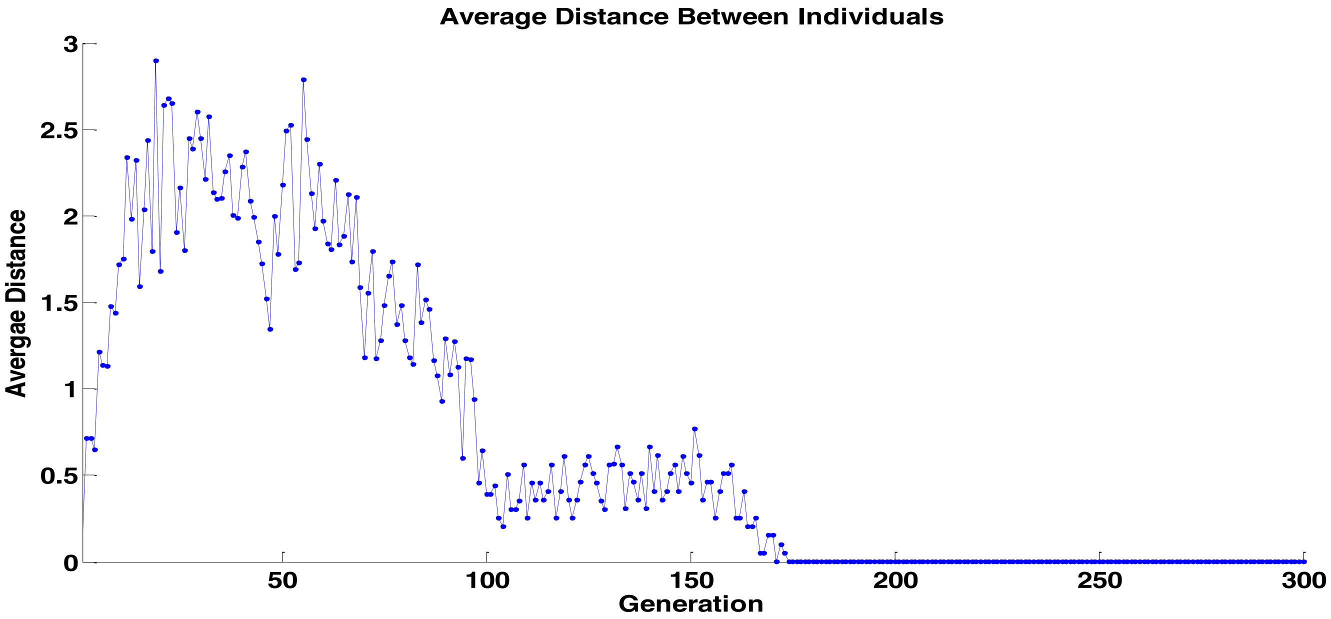

Fig 6.11: Average distance between the individuals at each generation

The optimum values of cell pressure, temperature and area are applied to the electrochemical equations again to predict the effect of three more dimensional design parameters number of cells, membrane thickness and active area factor on the fuel cell voltage. The lower and upper bound for thickness, area factor and number of cells is kept as Xmin = [0.0015, 0.56, 1] to Xmax= [0.05, 0.60, 100] respectively.

Table 6.3: Upper and lower limits of three more design variables

S.No	Parameter	Upper limit	Lower limit	Unit
1	tm	0.0015	0.05	nm
2	Af	0.56	0.60	
3	ncell	1	100	Number of cells

The optimization is again applied with the limits mentioned in Table 6.3 combined with the optimum values of temperature, pressure and cell area obtained previously. Fig shows a voltage output of 101.78 volts with these new parameters as shown

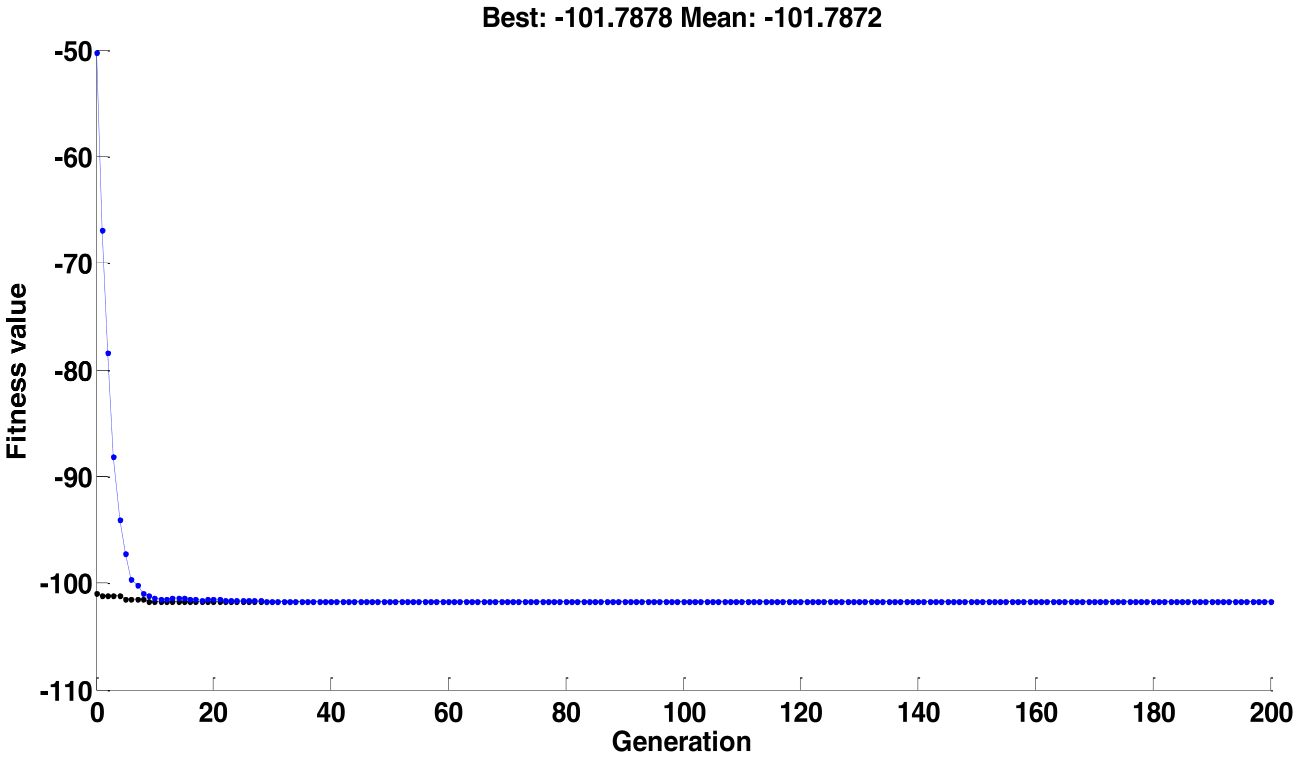

Fig 6.12: Best fitness value after optimization of geometrical fuel cell design parameters

Fig 6.12 shows the best fitness value has now changed to 102 volts after optimizing three more design variables. Here the mean value after 15 generations converges with the best fitness value. The algorithm stops when there is no change in the fitness value till 200 generations. The voltage from the optimized design can be calculated as

Voltage = 101.79 volts and Power = Vcell x I x ncell = 20 KWatt

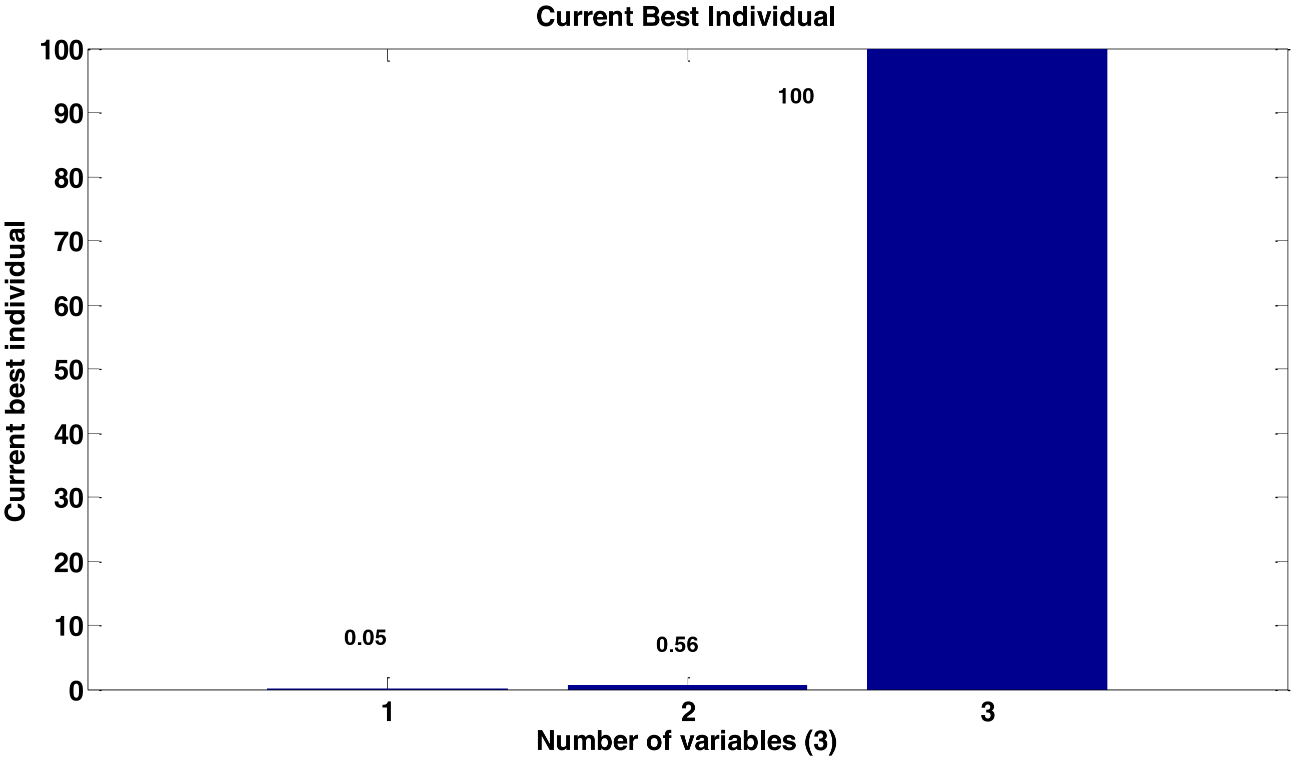

Fig 6.13: Best individual values for thickness, area factor and number of cells

The optimum values of temperature, pressure and cell area are again employed in the electrochemical equations and effect of three new variables membrane thickness, active area factor and number of cells on fuel cell voltage is established.

Fig 6.13 shows the best individual values obtained for membrane thickness as 0.05 nm or 50 microns, active area factor 0f 0.56 and number of cells 100. Hence the genetic algorithm provides four dimensional and two optimum design operating conditions of operating pressure and cell temperature where a Polymer electrolyte fuel cell can deliver its highest output. The system can now be assumed as a stack of 100 fuel cells providing a power output of 20 KWatt.

Table 6.4: Optimized PEM fuel cell parameters

Parameter	**Minimum limit**	**Maximum limit**	**Optimum value**
Membrane thickness(µm)	1.5	50	50
Active area factor	0.56	0.6	0.56
Number of cells	1	100	100
Optimized voltage 101.79 volts			

Table 6.4 presents the new optimized variables obtained after repeating the optimization process Previous values of membrane thickness 1.5µm active area factor 0.56 and number of cell as 1 cell provided the value of 1.233 volts with a combination of optimum cell operating temperature, operating pressure and cell area as 333.5 Kelvin, 7.09 bars and 0.0638 m^2 respectively. The optimization procedure when repeated by applying these optimum values and setting a new maximum and minimum limit of membrane thickness, active area factor and number of cells gave a new set of six optimized parameters that presented an increase in the optimized cell voltage from 1.233 volts to 101.78 volts.

Table 6.5: Optimization of three variables

Parameter	Minimum limit	Maximum limit	Optimum value
Temperature (Kelvin)	313	360	333.5188
Pressure (bars)	1.013	10.013	7.09
Area (m^2)	0.016	0.064	0.0638
Membrane thickness	1.5µm		
Active area factor	0.56		
Number of cells	1		
Optimized voltage 1.2330 volts			

Table 6.6 Set of all six optimized parameters

Parameter	Minimum limit	Maximum limit	Optimum value
Membrane thickness (µm)	2	50	50
Active area factor	0.56	0.60	0.56
Number of cells	1	100	100
Temperature (Kelvin)	333.5188		
Pressure (bars)	7.09		
Area (m^2)	0.0638		
Optimized voltage 101.78 volts			

Table 6.5 and Table 6.6 present a comparison between the optimized results. The three design variables chosen for the first study were temperature, pressure and cell area. New design variables of membrane thickness, active area factor and number of cells were optimized in the second study.

Fig 6.14 shows the plot of best worst and mean individuals in each generation which depicts the search direction converging from 0 to 100 in the initial 50 generations after which all of the values are converged to the mean value of 100.

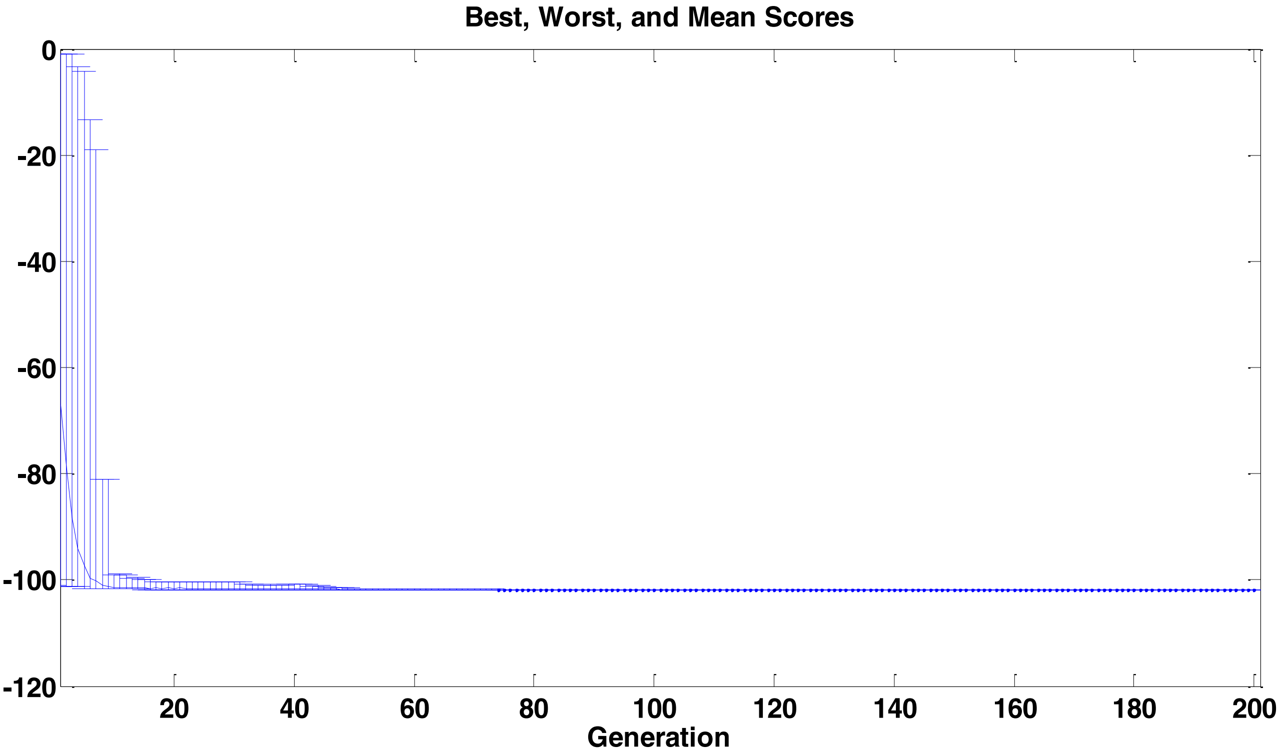

Fig 6.14: Best, worst and mean values of fuel cell voltage after optimization of geometrical parameters

6.4 PARAMETRIC STUDY OF RELATIVE HUMIDITY

The calculations of limit operating temperature and desired relative humidity are done with the equations of thermo dynamical model. The limit operating temperature is the highest temperature in which a PEM Fuel cell can operate preserving a recommended output relative humidity and a minimum recommended stoichiometry. Effects of inlet temperature, air pressure and stoichiometry have been studied to obtain the operating conditions which allow the fuel cell to operate without drying and with sufficient supply of air.

6.3.1 Model validation

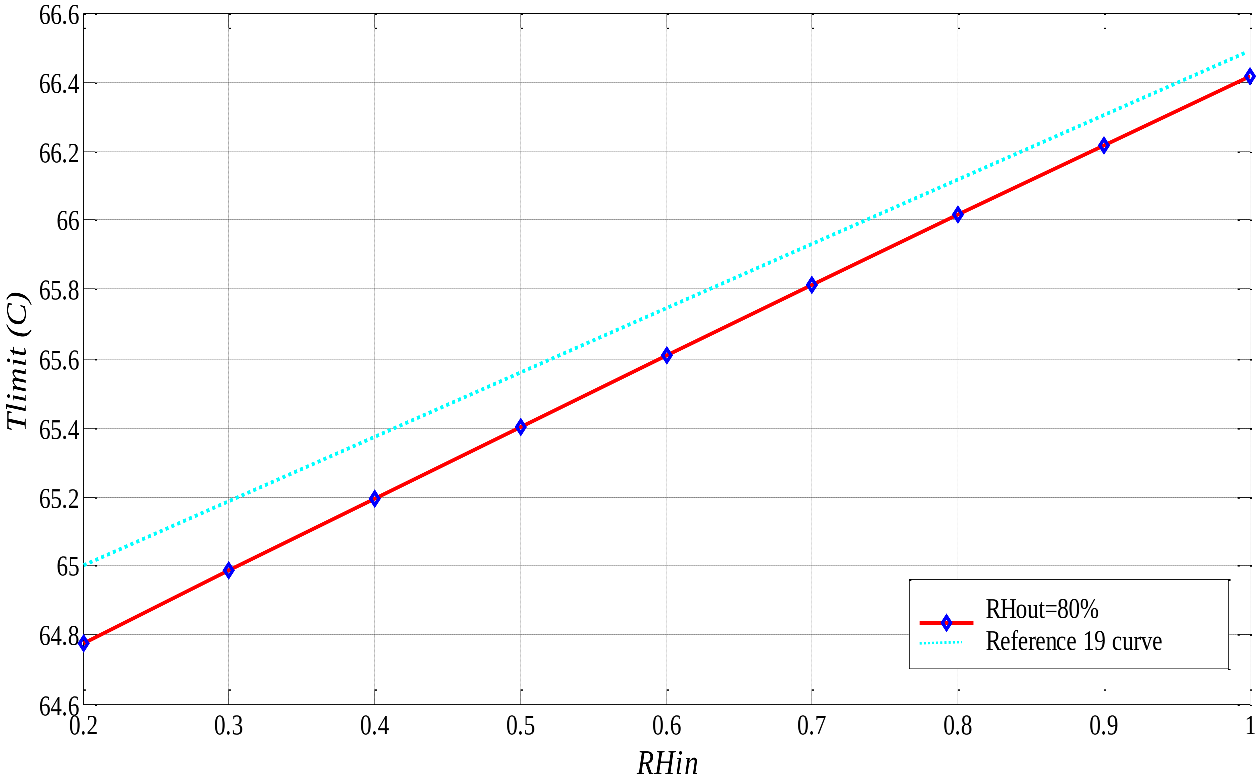

Fig 6.15: Model validation using reference

The above figure shows the Tlimit at output relative humidity 80% with comparison to the values of Luis A.M Riascos [19]. The equations are validated as it shows good agreement with their model as they have also tested it experimentally.

6.3.1 Effect of inlet relative humidity, pressure and stoichiometry on output humidity

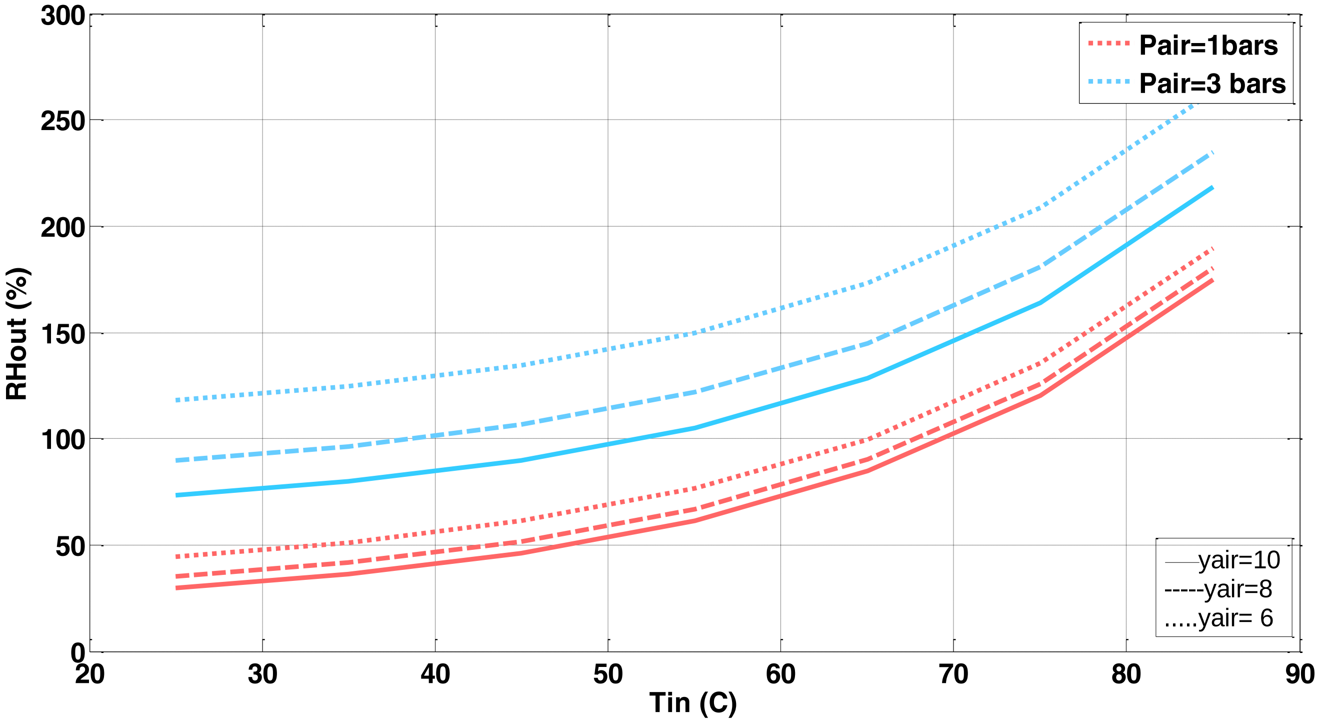

Fig 6.16: RHout at variable pressure, stoichiometry and temperature

The water content of a Polymer electrolyte fuel cell is monitored through the output relative humidity of the air. It is desired to maintain at greater than 85% to prevent the membrane from drying out and greater than 100% to restrict the flooding. The relative humidity shows a sharp increase with the increase in temperature due to increased saturation pressure of the inlet air.

Fig 6.16 shows that air pressure and stoichiometry have a coupled effect on the output relative humidity. Higher stoichiometry at greater air pressure predicts a sudden decrease in the humidity therefore at higher flow rates drying can occur in the membrane. The key to balanced humidity is a moderately pressurized system at ambient temperature. Lowering the stoichiometry too much is also not desirable as it increases the concentration losses.

6.3.2 Effect of inlet relative humidity, pressure and stoichiometry on humidity

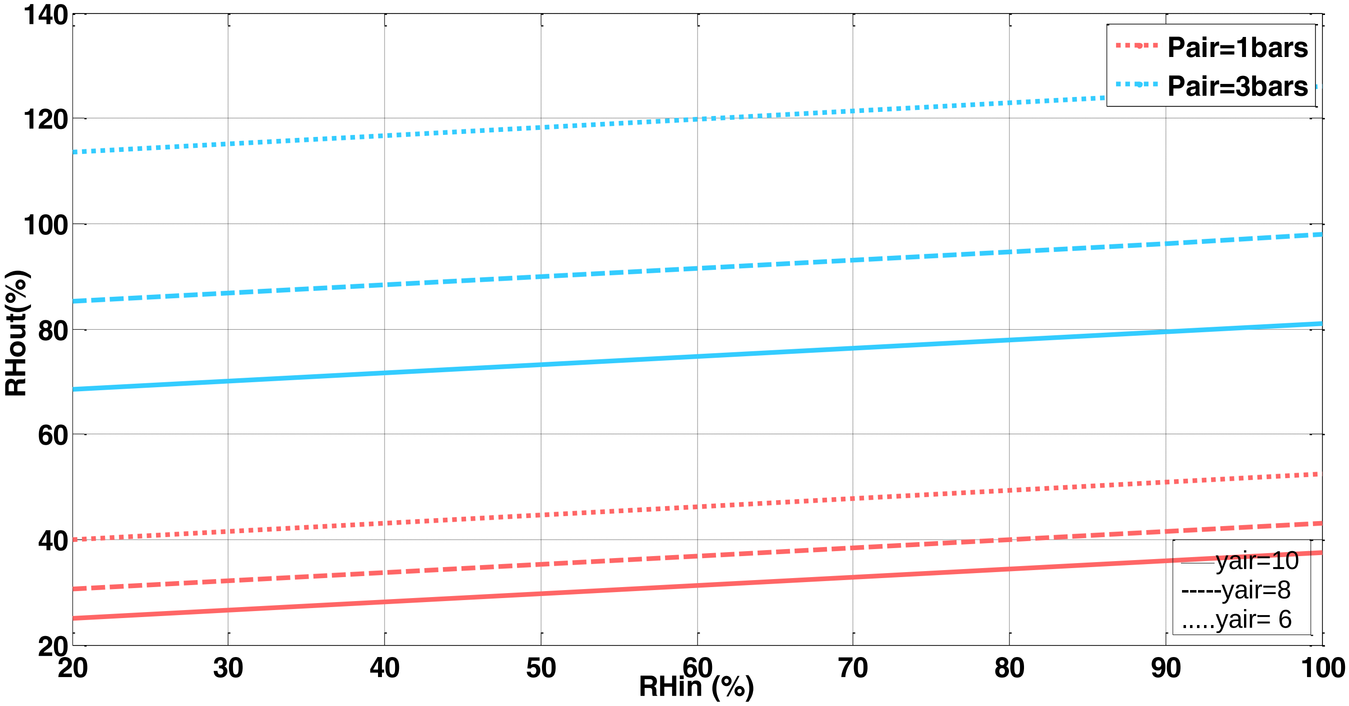

Fig 6.17: RHout at variable inlet relative humidity, stoichiometry and pressure

Fig 6.17 depicts that fuel cell relative humidity shows an increase with the increase in relative humidity but the rise is not as sharp with that compared with inlet temperature. The water partial pressure in the inlet air has more pronounced effect with the increase in inlet temperature as compared to the change in relative humidity. Although at lower stoichiometry and high pressure output humidity can be increased to an optimum level. Hence it is a common practice to humidify and pressurize the stream of inlet air prior to its entry in the fuel cell. The inlet temperature is mostly kept constant at ambient temperature of 25- 30 ^{0}C.

6.5 GA BASED OPTIMIZATION OF RELATIVE HUMIDITY

The Genetic algorithm is also employed to obtain the operating conditions at the inlet for a balanced water content in the fuel cell. As stated earlier a humidity level from 85 to 100% if maintained is beneficial for the fuel cell performance as well as a stable water management.

The cell operating temperature and pressure where the PEM fuel cell exhibited a maximum voltage output was Tcell= 60 C and Pcell= 7.09 bars. These variables were used to find out the optimum inlet conditions for the optimized relative humidity of the outlet air. The design variables chosen are inlet relative humidity, air stoichiometry and exit air pressure which is always less than the cell pressure. [27]

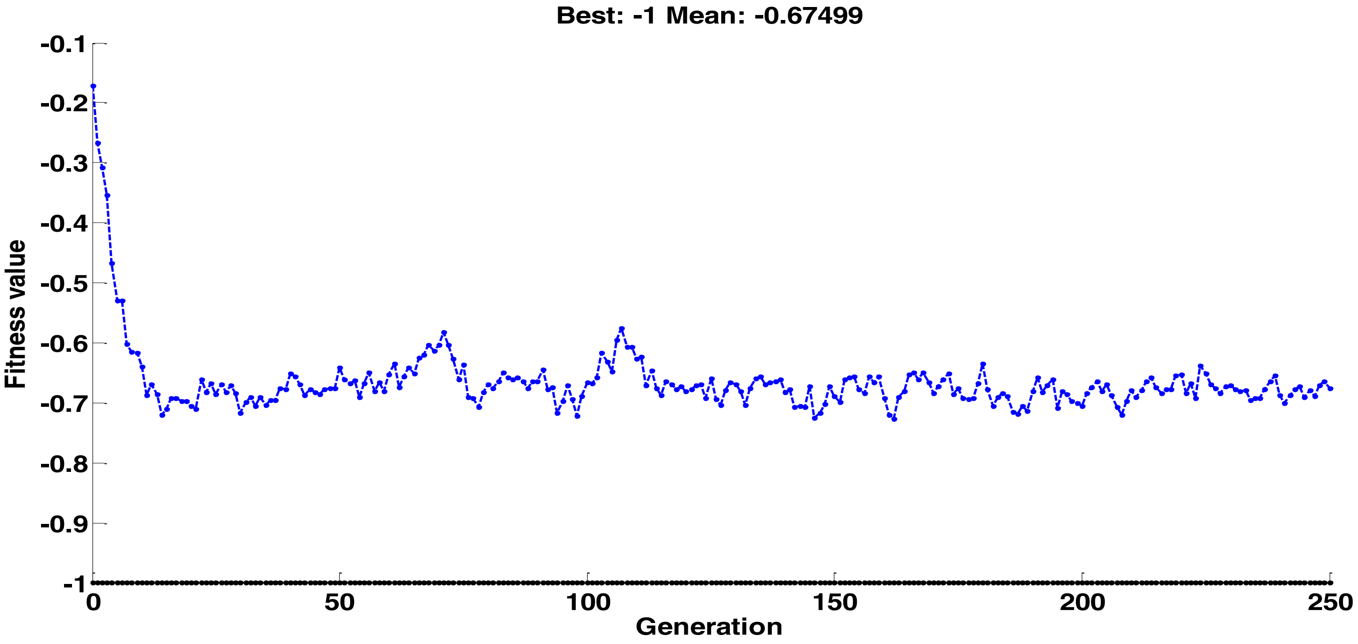

Fig 6.18: Best fitness value for the output relative humidity

Fig 6.18 shows the algorithm returned an optimized value of 100% relative humidity after 250 generations when no significant improvement in the fitness value was detected.

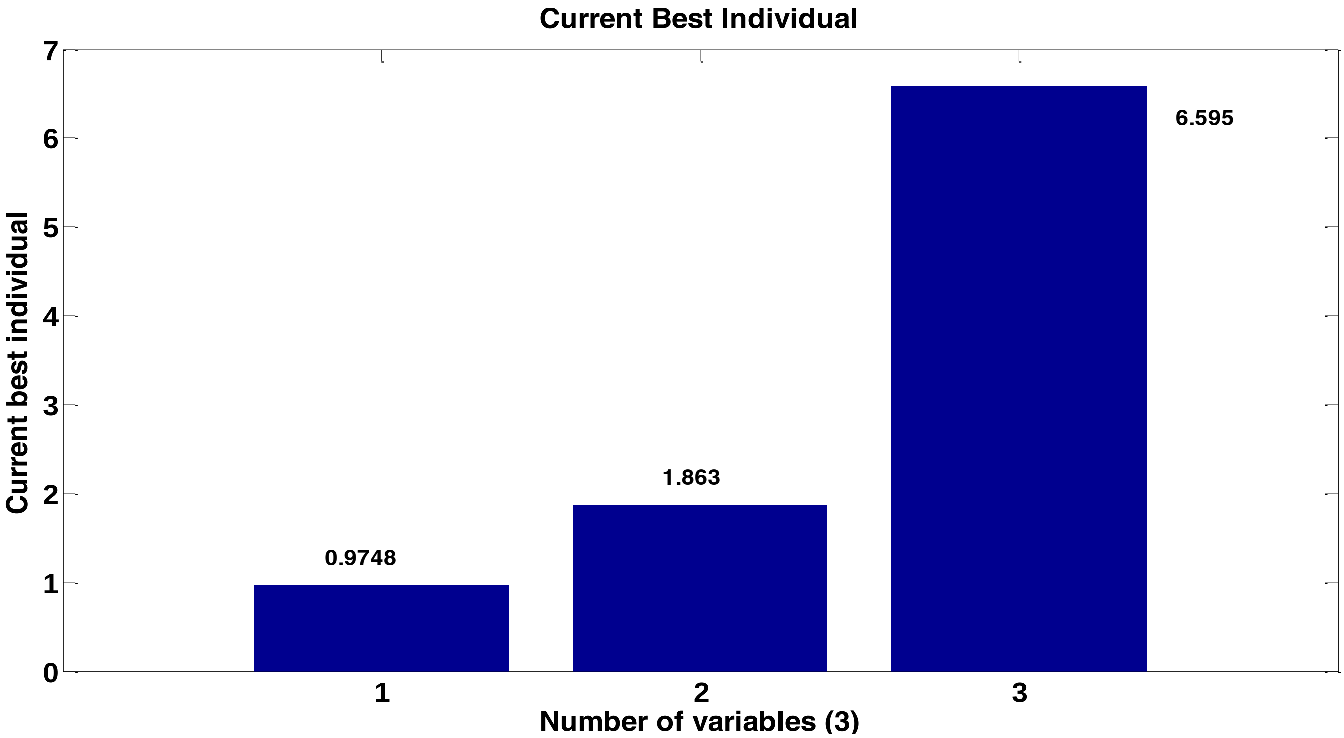

Fig 6.19: Best individual values for the fitness function of RHout

Fig 6.19 presents the design variables for optimizing the output relative humidity of the air are found as follows which are in good agreement with the results of electrochemical model

Table 6.7: Best operating conditions for output humidity

Parameter	**Minimum limit**	**Maximum limit**	**Optimum value**
Relative humidity	0.2	1	0.9748
Air stoichiometry	2	10	2
Air pressure (bars)	1	8	6.5
Optimized output humidity (RHout) 100%			

The design variables where the model is minmized can also be found using the built in minimize function of the genetic algorithm toolbox. The negative sign when removed form the objective function provides the local minima, which is used to establish the conditions where output relative humidity falls to the least value of 54.6% which can severely affect and can cause the cell to dry out.

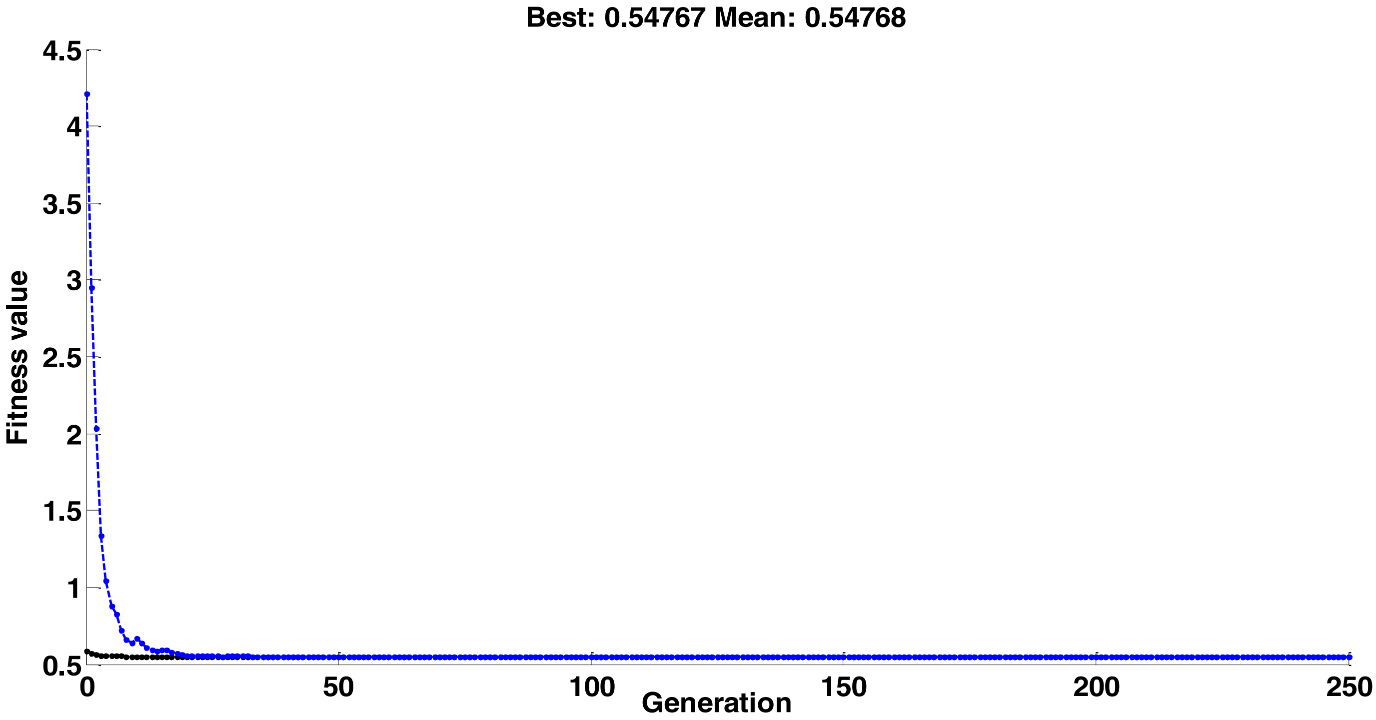

Fig 6.20: The fitness value for the least RHout

Fig 6.20 displays after the initial 20 generations the best fitness and mean values concide and the solution converges at 250 generations. The output air when depleted of water vapours causes drying of air as well of the fuel cell due to which high voltage losses are encountered in addition if the humidity falls below 70%, the fuel cell ceases to work. Here 54% is too less than the minimum desired value of 85%. The optimum values where the global minima is found reflects a combination of very low inlet relative humidity, high pressure and a stoichiometry of 2.

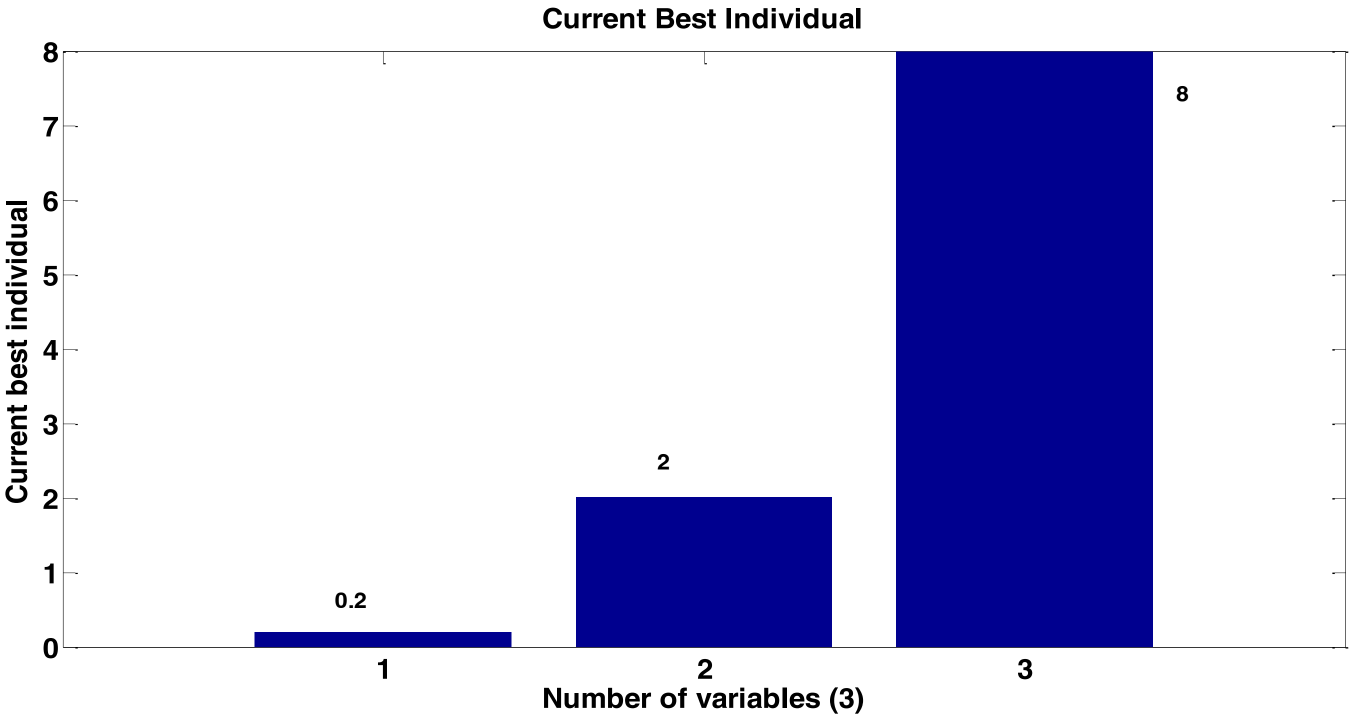

Fig 6.21: The individual values for the least RHout of 54%

The worst conditions for minimum relative humidity of output air found from the genetic algorithm are as follows

Table 6.8: Worst operating conditions for output humidity

Parameter	**Minimum limit**	**Maximum limit**	**Optimum value**
Relative humidity	0.2	1	0.2
Air stoichiometry	2	10	2
Air pressure (bars)	1	8	8
Optimized output humidity (RHout) 54.8%			

Fig 6.21 illustrates that an increase in air pressure with a decrease in water content of the inlet air causes the output air to dry out faster. Hence it is essential to enter discreetly pressurize air with a suitable water content so that during the fuel cell operation it does not creates a drying effect. The water produced at the cathode can be used to humidify the air entering the fuel cell.

Using relations for water production and water required [28] the water produced at the modeled fuel cell can be obtained. For the design fuel cell with power of 20 KW and fuel cell voltage of 1.01 volts the rate of water production will be 0.00185 kg/sec.

$$mwp = 9.34 * 10^{-8} \quad \left(\frac{Power}{Cellvoltage}\right)$$

$$mwp = 9.34 * 10^{-8} \quad \left(\frac{20{,}000}{1.01}\right)$$

$$mwp = 9.34 * 10^{-8} \quad \left(\frac{20{,}000}{1.01}\right)$$

0.00185 kilograms of water per second will be generated in the designed fuel cell which can be used to humidify the input air. The mass of water required in the inlet air to retain a humidity of 97.48% at an ambient temperature of 30 ^{0} C can be given using 5.28 and 5.19

$$mwr = 0.622 \left(\frac{Pw}{P - Pw}\right) ma$$

Where mass of air for a fuel cell of power 20 KW and fuel cell voltage 1.01 volts at a stoichiometry of 2, can be given using 5.27 as

$$ma = 0.0141 kg/sec$$

which gives mass of water required for a 97 % humid air stream entering at a flow rate of 0.0141 kg/sec, pressure of 6.5 bars and temperature of 30^0 C as

$$mwr = 0.622 \left(\frac{Pw}{P - Pw}\right) ma$$

$$mwr = 0.0000562\ kg/sec$$

Hence the water being produced at the cathode side can be utilized for humidifying the air stream thus eliminating the need for any external humidification. At higher temperatures and high current densities the mass of water required increases as the saturation pressure of the water vapor increases at higher temperatures.

The limit operating temperature is also an essential parameter of the fuel cell thermo dynamical model which is required to maintain a recommended relative humidity and a minimum stoichiometry.

$$Tlimit\ =\ 96.25\ +\ 23.55\ ln\ [\frac{1}{RHdesired}\left(\frac{0.421.Pair}{\lambda\ air\ +\ 0.188}\right)+Pwin+0.01751]$$

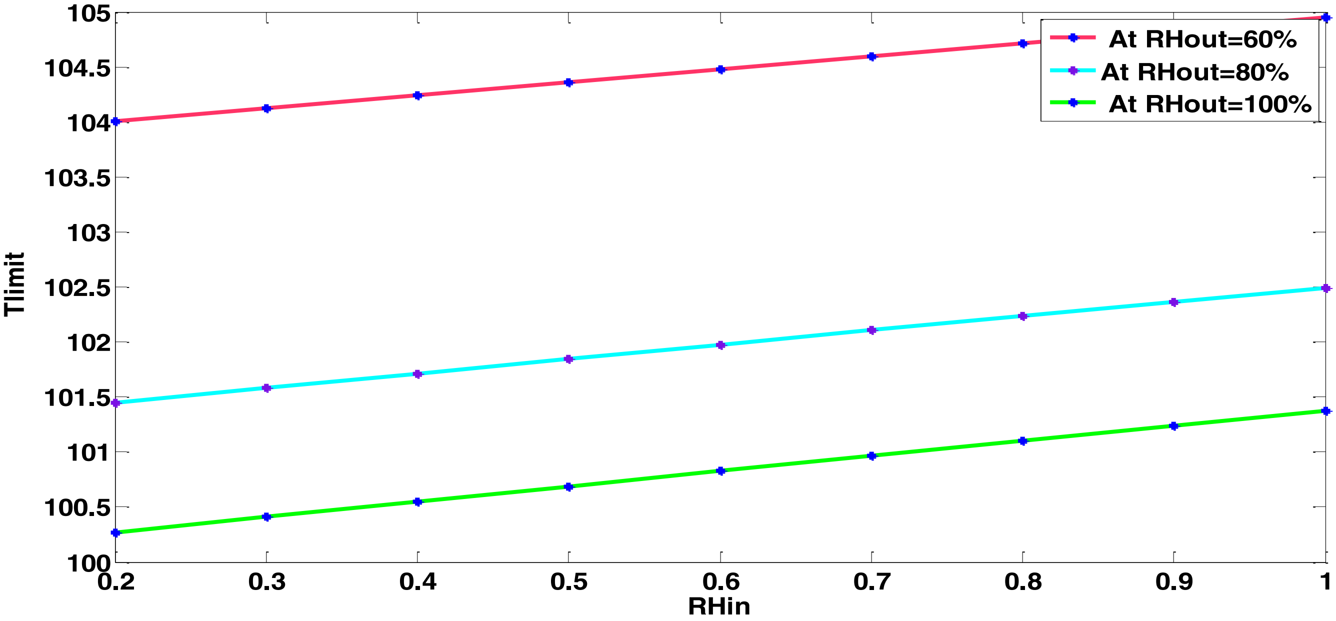

Fig 6.22: Tlimit at variable output relative humidity at an air pressure of 6.5 bars and Tin=30 C

Fig 6.22 shows the fuel cell is again restricted to operate at lower temperature if a high desired relative humidity is required. Temperatures from 60-65 C are suitable for desired air humidity of 90%. If operating temperatures greater than 70 C are required techniques for extra humidification are also needed.

6.6 Conclusion and suggestions for future work

Table 6.9 Comparison of electrochemical and thermo dynamical design

Optimized designs for PEM fuel cell voltage	**Optimum value**	**Optimized design for PEM fuel cell water content**	**Optimum value**
Temperature (Kelvin)	333.5188	Inlet relative humidity	0.9748
Cell operating Pressure (bars)	7.09	Air pressure(bars)	6.5
Area (m^2)	0.0638	Air stoichiometry	2
Membrane thickness µm	50	Inlet air temperature (C)	30
Active area factor	0.56	Operating temperature (C)	334
Number of cells	100	Optimized output humidity (RHout) 100%	
Current (Ampere)	200	Water produced 1.84 g/sec	
Optimized voltage 101.78 volts		Water required 0.0562 g/sec	
Optimized Power 20KW		Limit operating temperature - 100 C	

The work establishes a comparison between conditions at which maximum fuel cell performance can be achieved and the conditions where operating conditions are desirable permitting suitable water content and humidity for membrane hydration.

Although the fuel cell shows high voltage at some conditions but there are certain limitations to it

1- Higher temperatures produce high voltage but to sustain a relative humidity of more than 90% there is a limitation therefore the best temperature range lies below 65 C

2- Higher stoichiometry also show increase in performance but produces a drying effect at very high values of λair so it’s suitable to operate the cell with λair between 2 to 8 in combination with suitable values of temperature.

3- Increasing the pressure has significant effect on voltage of fuel cell but requires more energy and adds to the equipment cost. In addition higher air pressures coupled with higher values of stoichiometry produce a very severe drying effect on the cell membrane.

4- Cell areas can be increased to an optimum point which also increases the current density.

6.7 Suggestions

1- To maintain a desired humidity level from 80% to 100%, extra humidification techniques should be considered.

2- The analysis can be performed on a fuel cell of given area and should be tested experimentally to further observe the performance and water management.

3- The above electrochemical and thermo dynamical models can be utilized to predict the performance of a Polymer electrolyte fuel cell with the complete balance of plant to provide more realistic results with parasitic power losses.

Appendix 1- Modeling terms of PEM fuel cell electrochemical model

S.No	Term	Definition
1	Enernst	It is the reversible open circuit voltage of the fuel cell at a given temperature and pressure.
2	Activation over voltage(ηact)	These losses are due to the expanse of forcing the reaction to completion which is forcing the hydrogen to split into electrons and protons.
3	Ohmic overvoltage(ηohmic)	This is the voltage loss caused due to resistance to electron flow in the electrodes, graphite collector plates and resistance to ion flow in the electrolyte.
4	Concentration overvoltage (ηconc)	The losses that occur due to mass transport concentration problems. It occurs because the fuel cell is using fuel or oxygen faster than it can be supplied.
5	Membrane constant (λm)	It is an adjustable fitting parameter which depends on the method and manufacture of the membrane. It is the function of relative humidity, stoichiometric ratios at the anode and cathode and age and use of the membrane.
6	Stoichiometry of gases (λx)	The stoichiometry or stoichiometric ratio is the amount of gases (hydrogen or air) supplied to the amount of gas used.
7	Active cell area	The active cell area is only a portion of stack cross section area stack. Is usually 56 to 59% of the total cross section area. The other remaining 44% is used to accommodate the rods that hold the stack, the manifolds and seals.

8	Specific resistivity for membrane flow(r_M)	It is the membrane specific resistivity for the flow of hydrated protons.
9	Relectr	Electronic resistance which is assumes to be constant over the operation temperature of fuel cell and is inconsequential so is often ignored.
10	Rprotonic	Protonic resistance whose value depends on the distribution of water content in membrane.

Appendix 2- Modeling terms of PEM fuel cell thermo dynamical model

S.No	Term	Definition
1	Limit operating temperature (Tlimit)	It is the highest temperature in which a PEM Fuel cell can operate preserving a recommended output relative humidity and a minimum recommended stoichiometry
2	Generated Partial pressure (Pwgen)	The water partial pressure generated by the chemical reaction (internal generation).
3	Relative humidity (RHout)	The desired relative humidity of output air. It helps to predict the level of hydration of electrolyte.
4	Stoichiometric ratio (λair)	Stoichiometric ratio is the ratio between the actual amount/ flow rate of air supplied at the inlet to the amount/ flow rate of air used. In fuel cell literature it is an indicator of excess reactant supplied.

Appendix 3- Modeling terms of Genetic algorithm

S.No	**Term**	**Definition**
1	Fitness function	The fitness function is the function which is to be optimized, also known as the objective function. The toolbox tries to find the minimum of the toolbox.
2	Fitness limit	An individual is any point to which you apply the fitness function.
3	Individual	An individual is any point to which you apply the fitness function.
4	Score	The value of the fitness function for an individual is score
5	Population	A population is an array of individuals. For example if the size of the population is 100 and the number of variables in the function is 3, the population is represented by a 100x 3 matrix.
6	Generation	At each iteration, the genetic algorithm performs a series of computations on the current population to produce a new population. Each successive population is called a generation.
7	Selection Rule	It selects the individual called parents that contribute to the population at the next generation.
8	Fitness value	The fitness value of an individual is the value of the fitness function for that individual.
9	Best Fitness value	Since the MATLAB toolbox finds the minimum of the fitness function, the best fitness value for a population is the smallest fitness value for any individual in the population.

11	Parents and Children	To create the next generation the genetic algorithm selects certain individuals in the current population called parents and uses them to create individuals in the next generation called children.
12	Elite children	They are the individuals in the current generation with the best fitness values. These individuals automatically survive to the next generation.
13	Crossover children	These individuals are created by combining the vectors of a pair of parents.
14	Mutation children	These individuals are created by introducing random changes, or mutations, to a single parent.
15	Mutation	Mutation function makes small random changes in the individuals in the population, which provide genetic diversity and enable the genetic algorithm to search a broader space.
16	Crossover	Crossover combines two individuals, or parents, to form a new individual, or child, for the next generation.
17	Migration	Migration is the movement of individuals between subpopulations. The best individuals from one subpopulation replace the worst individuals in another subpopulation.
18	Reproduction	Reproduction options determine how the genetic algorithm creates children at each new generation.

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