

Neural Network-Based Modeling of PEM fuel cell and Controller Synthesis of a stand-alone system for residential application

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Abstract

The paper is focused especially on presenting possibilities of applying artificial neural networks at creating the optimal model PEM fuel cell. Various ANN approaches have been tested; the back-propagation feed-forward networks show satisfactory performance with regard to cell voltage prediction. The model is then used in a power system for residential application. This models include an ANN fuel cell stack model, reformer model and DC/AC inverter model. Furthermore a neural network (NNTC) and fuzzy logic (FLC) controllers are used to control active power of PEM fuel cell system. The controllers modifies the hydrogen flow feedback from the terminal load. The validity of the controller is verified when the fuel cell system model is used in conjunction with the NNT controller to predict the response of the active power to: (a) computer-simulated step changes in the load active and reactive power demand, and (b) actual active and reactive load demand of a single family residence. Simulation results confirmed the high performance capability of the neural network (NNTC) to control power generation.

Keywords: *Fuel Cell; Polymer-electrolyte fuel cell PEMFC; Electrochemical model; Modelling and Simulation; Fuzzy Logic Controller (FLC); Neural Network controller (NNTC)*

1. Introduction

Proton exchange membrane (PEM) fuel cell is one of the promising technologies for alternative power source of residential power generation in future. However, a fuel cell system is large, complex and expensive. Designing and building prototypes is difficult and expensive. The alternative is modelling the fuel cell system for the simulation. The modelling of fuel cell is very important for power system, because it facilitates the understanding of the involved phenomena. Many models have been proposed to simulate fuel cells in the literature [1]-[8], which have generally each the own specificities and

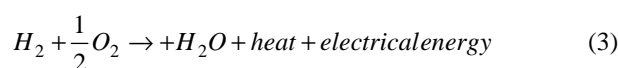
utilities, following the studied phenomena. A PEMFC converts the chemical energy of a fuel O_2 , in electrical energy. The outline of a typical PEMFC is illustrated in Figure 1. On one side of the cell, referred to as the anode, the fuel is supplied under certain pressure. The fuel for this model is the pure gas H_2 , although other compositions of gases can be used. In these cases, the hydrogen concentration should be determined in the mixture. The fuel spreads through the electrode until it reaches the catalytic layer of the anode where it reacts to form protons and electrons, as shown below in the reaction given in Eq. (1.1) [1]-[9]:



The protons are transferred through the electrolyte (solid membrane) to the catalytic layer of the cathode. On the other side of the cell, the oxidizer flows through the channels of the plate and it spreads through the electrode until it reaches the catalytic layer of the cathode. The oxidizer used in this model is air or O_2 . The oxygen is consumed with the protons and electrons and the product, liquid water, is produced with residual heat on the surface of the catalytic particles. The electrochemical reaction that happens in the cathode is



Then, the full physical-chemical FC reaction is:



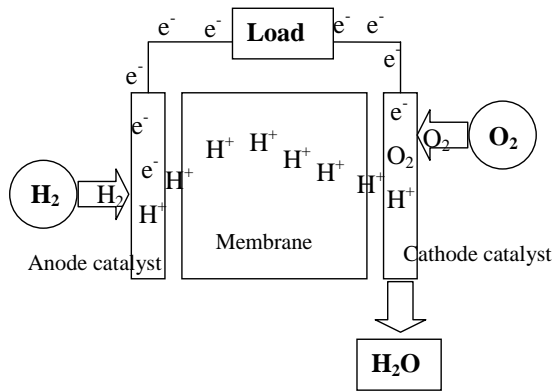


Figure 1. Basic Fuel Cell Operation

2. Fuel Cell Model Formulation

In [1], [2] and [3] a performance model for a proton exchange membrane (PEM) fuel cell stack was previously developed. The model incorporated both the mechanistic and empirical properties to describe the electrochemical phenomena of combining oxygen and hydrogen over a platinum catalyst to produce an electrical current and water. The previous model predicted the cell voltage in terms of inlet partial pressures of hydrogen and oxygen, stack temperature, and operating current. The cell voltage was defined as:

$$V_{Fc} = E_{Nerst} - V_{act} - V_{ohm} - V_{act} \quad (4)$$

In (2.1), E_{Nerst} is the thermodynamic potential of the cell and its represents reversible voltage; V_{act} is the voltage drop due to the activation of the anode and of the cathode; V_{ohm} is the ohmic voltage drop, a measure of the ohmic voltage drop associated with the conduction of the protons through the solid electrolyte and electrons through the internal electronic resistances; V_{conc} represents the voltage drop resulting from the concentration or mass transportation of the reacting gases [5]. The first term of (2) represents the FC open circuit voltage, while the three last terms represent reductions in this voltage to supply the useful voltage of the cell, for a certain operating condition. Each one of the terms in (2) can be calculated by the following equations [6]:

$$E_{nerst} = 1,229 - 0.85 \cdot 10^{-3} (T - 298,15) + 4,31 \cdot 10^{-5} \cdot T \cdot \left[\ln(P_{H_2}) + \frac{1}{2} \ln(P_{O_2}) \right] \quad (5)$$

Where P_{H_2} and P_{O_2} while and are the partial pressures of hydrogen and oxygen (atm), respectively, T the cell operation temperature (K)

$$V_{act} = -[\xi_1 + \xi_2 \cdot T + \xi_3 \cdot T \cdot (CO_2) + \xi_4 \ln(I_{stack})] \quad (6)$$

Where I_{stack} is the cell operating current (A), and the ξ_i 's represent parametric coefficients for each cell model, whose values are defined based on theoretical equations with kinetic, thermodynamic, and electrochemical foundations [6]. CO_2 is the concentration of oxygen in the catalytic interface of the cathode mol/cm, determined by

$$CO_2 = \frac{PO_2}{5,08 \cdot 10^6 \cdot e^{(-498/T)}} \quad (7)$$

$$V_{ohmic} = I_{stack} \cdot (R_m + R_c) \quad (8)$$

Where R_c represents the resistance to the transfer of protons through the membrane, usually considered constant and:

$$R_m = \frac{\rho_M \cdot l}{A} \quad \text{with:}$$

$$\rho_M = \frac{181,6 \left[1 + 0,03 \left(\frac{I_{stack}}{A} \right) + 0,062 \left(\frac{T}{303} \right)^2 \cdot \left(\frac{I_{stack}}{A} \right) \cdot \left(\frac{I_{stack}}{A} \right)^{2,5} \right]}{\left[\psi - 0,634 - 3 \left(\frac{I_{stack}}{A} \right) \right] \exp \left[4,18 \left(\frac{T - 303}{T} \right) \right]} : \text{ is}$$

the specific resistivity of the membrane for the electron flow Ω/cm , A is the cell active area cm and l is the thickness of the membrane (cm), which serves as the electrolyte of the cell. Where $181,6/(\psi - 0,634)$ the term is the specific resistivity Ω/cm at no current and at $30^\circ C$ [6];

$$V_{con} = -B \cdot \ln \left(1 - \frac{J}{J_{max}} \right) \quad (9)$$

Where B (V) is a parametric coefficient, which depends on the cell and its operation state, and J represents the actual current density of the cell (A/cm).

2.1 Artificial Neural Network (ANN) Model

Artificial neural network is a type of artificial intelligence technique that mimics the behaviour of human brain. It can approximate any linear or nonlinear function well. A feed-forward neural network with supervised

training [14] was utilized in this study. The structure of the feedforward is three-layer. The network consists of an input layer, a hidden layer and an output layer. The transfer function for the hidden layer is a sigmoid function, whose form is defined by [17]:

$$f(u) = \frac{1}{1 + e^{-(d.u)}} \quad (10)$$

where d is the slope parameter. The input of the hidden layer can be described by the following equation:

$$u = \sum_{j=1}^n (w_{ij}x_j + b_i) \quad (11)$$

where w_{ij} is the weight from the j th input x_j to the i th neuron in the hidden layer, and b_i is the bias. If the function in the output layer is linear, the model equation for the entire network can be expressed as follows[17]:

$$y_k u = \sum_{j=1}^N (w_{ij}^o u_j + b_i) = u = \sum_{j=1}^N w_{ij}^o f \left(\sum_{j=1}^N (w_{ij} x_j + b_i) \right) \quad (12)$$

where y_k is the output signal from the k_{th} output neuron, and w_{ki}^o is the weight from the i th output u_i to the k_{th} neuron in the output layer. In this study, the weights and bias values of ANN are updated according to the gradient descent momentum algorithm, which is considered to be one of the best training algorithms for the ANN [16].

Fig 2 shows the architecture of the developed neural network model. The ANN network has an input layer with 3 inputs (partial pressures of hydrogen P_{H_2} , partial of oxygen P_{O_2} and cell operating current I_{stack}), 1 hidden layer with 10 neurons and an output layer with 1 outputs (PEMFC cell voltage). MATLAB \S (The MathWorks Inc.) Neural Networks Toolbox was used to build ANN models. The hyperbolic tangent sigmoid transfer function (``tansig'`) was used in the hidden layer and linear transfer function (``purelin'`) was applied in the output layer. The two-layer sigmoid/linear network usually can represent any functional relationship between inputs and outputs if the sigmoid layer has enough neurons [16].

The nonlinear transfer function in the hidden layer allows the network to learn nonlinear and linear relationships between input and output vectors and the linear output layer lets the network produce values outside the range -1 to + 1. The weights and biases were initialized using ``init'` function which calculates the weight and bias values using the Nguyen--Widrow initialization method. The data from the semi-empirical model was used for training the

network. Lavenberg--Marquart backpropagation training algorithms (``trainlm'`) was used as a training function to update weight and bias values, as it is the fastest training algorithm for networks of moderate size although it can require additional memory. Memory problems did not occur during the simulations for all developed ANN models. Neural network simulation blocks for use in Simulink can be automatically generated with the (`gensim`) command [18].

Fig 3 show A typical PEMFC (NNT model) cell voltage response surface. With simultaneous changes in the inlet partial pressure of hydrogen and current at a constant stack temperature of 70°

Fig 4 show the relative difference between semi-empirical model and neural network model. The simulation results show good agreement with the empirical and experimental ones. The absolute error was less than 0.4%. This result prove the ability of NNT model to replace the analytical model for simulink

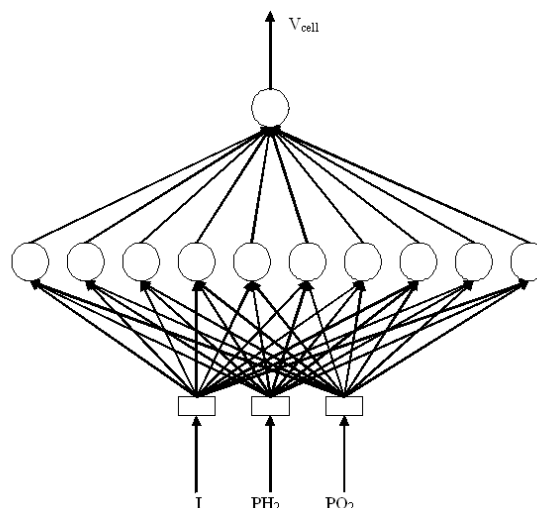


Fig 2: PEMFC NNT model

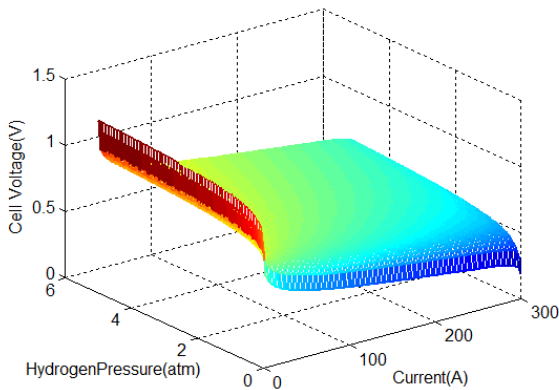


Fig 3: Polarization curve

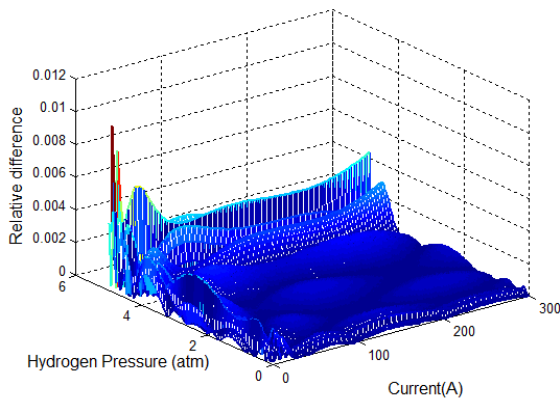


Fig 4: Relative difference between semi-empirical model and neural network model

3. Fuel Cell System Model

3.1 Fuel Cell Dynamic Model

Choose the partial pressure of hydrogen and oxygen on the cathode side as three states; hydrogen inlet flow rate, oxygen inlet flow rate and output current density as three inputs as well. Using the ideal gas law, the state equations become[9]:

$$\frac{d}{dt}(P_{H_2}) = \frac{RT}{V_{an}}(q_{H_2}^{in} - q_{H_2}^{out} - q_{H_2}^r) \quad (13)$$

$$\frac{d}{dt}(P_{O_2}) = \frac{RT}{V_{an}}(q_{O_2}^{in} - q_{O_2}^{out} - q_{O_2}^r) \quad (14)$$

$$\frac{d}{dt}(P_{H_2O}) = \frac{RT}{V_{an}}(-q_{H_2O}^{out} - q_{H_2O}^r) \quad (15)$$

Where: P_{H_2} , P_{O_2} and P_{H_2O} : the partial pressures of each gas inside cell; $q_{H_2}^{in}$, $q_{O_2}^{in}$: the inlet flow rates of hydrogen and oxygen of the cathode and anode; $q_{H_2}^{out}$, $q_{O_2}^{out}$ and $q_{H_2O}^{out}$: the outlet flow rates of each gas and water vapor; $q_{H_2}^r$, $q_{O_2}^r$ and $q_{H_2O}^r$: usage and production of the gases and water.

Based on the electrochemical relationships, we have[6]:

$$q_{H_2}^r = 2q_{O_2}^r = q_{H_2O}^r = \frac{N_0 \cdot I_{stack}}{2 \cdot F} = 2 \cdot K_r \cdot I_{stack} \quad (16)$$

$$q_{H_2}^{out} = K_{H_2} P_{H_2}; q_{O_2}^{out} = K_{O_2} P_{O_2}; q_{H_2O}^{out} = K_{H_2O} P_{H_2O} \quad (17)$$

Where:

K_{H_2} : hydrogen valve molar constant [kmol/(atm s)];

K_{O_2} : oxygen valve molar constant (kmol/(atm s));

N_0 : number of series fuel cells in the stack; I_{stack} : stack

current (A); K_r : constant = $\frac{N_0}{4F}$ Kmole/ (s.A) and F :

Farady constant 9684600 C/Kmole.

By substituting equations (16) and (17) into equation (15), applying the Laplace transform, and isolating the partial pressure term, the following equation can be written as:

$$P_{H_2} = \frac{1/K_{H_2}}{1 + \tau_{H_2}s} (q_{H_2} - 2K_r I_{stack}) \quad (18)$$

where τ_{H_2} : the system pole associated with the hydrogen flow. and for partial pressure of oxygen:

$$P_{O_2} = \frac{1/K_{O_2}}{1 + \tau_{O_2}s} (q_{O_2} - K_r I_{stack}) \quad (19)$$

This model is based on simulating the relationship between output voltage and partial pressure of hydrogen and oxygen.

3.2 Reformer Model

In [9]and[10] the authors introduced a simple model of a reformer that generates hydrogen through reforming methane. The model is a second-order transfer function. The mathematical form of the model can be written as follows:

$$\frac{q_{H_2}}{q_{methane}} = \frac{CV}{\tau_1 \tau_2 \cdot s^2 + (\tau_1 + \tau_2) \cdot s + 1} \quad (20)$$

Were:

CV: conversion factor[kmol of hydrogen per kmol of methane]; $q_{methane}$ methane flow rate (kmol/s); τ_1 , τ_2 : reformer time constants [s]

3.3 DC/AC inverter Model

In this paper, only a simple model of a DC/AC inverter is considered for the following reasons: the dynamic time constant of inverters is of the order of microseconds or at the most milliseconds. The time constants for the reformer and stack are of the order of seconds model of the inverter is given in [11], where output voltage and output power are controlled using the inverter modulation index and the phase angle of the AC voltage.

Considering the fuel cell as a source, the output voltage and the output power as a function of the modulation index and the phase angle can be written as:

$$V_{ac} = m.V_{cell}\angle\delta \quad (21)$$

$$P_{ac} = \frac{m.V_{cell}}{X} \sin(\delta) \quad (22)$$

$$P_{ac} = \frac{m.V_{cell}}{X} \sin(\delta) \quad (23)$$

$$Q_{ac} = \frac{m.V_{cell}^2 - m.V_{cell}.V_s \cos(\delta)}{X} \quad (24)$$

$$I_L = \frac{P_L}{V_s \cos(\theta)} \quad (25)$$

$$I_{stack} = m.I_L \cos(\theta + \delta) \quad (26)$$

Where the model parameter are as follows:

V_{ac} : AC output voltage of the inverter ; m : inverter modulation index; δ :phase angle of the AC voltage [rad] ; P_{ac} : AC output power from the inverter; Q_{ac} :reactive output power from the inverter; V_s :load terminal voltage; X : reactance of the line connecting the fuel cell to the load I_L :load current ; θ :load phase angle [rad]; P_L :load power; I_{stack} :stack current.

PI controllers are used to control the modulation index. The transfer function of the modulation index can be expressed as:

$$m = \frac{k_5 + k_6 s}{s} (V_r - V_{ac}) \quad (27)$$

Were :

k_5 , and k_6 : are the PI gain, and V_r is the reference voltage signal.

In traditional synchronous generators, the amount of steam input to the turbine controls the power angle, which controls the active output power from the generator. In synchronous machines, the power angle is not measured but the adjustment of the power angle occurs following changes in steam input and rotor speed. In the fuel cell system, there is no speed control but a similar relationship between the output voltage phase angle and the flow of

hydrogen can be adopted as follows. Given that the load voltage is constant and the AC source voltage out of the inverter is as given in [11] , the angle controls the power flow from the fuel cell to the load, as in [10]. The phase angle can be controlled using the input flow of hydrogen. The expression for, therefore, provides the relationship between the power output as a regulated quantity, and the amount of flow of fuel input. This relationship is described by the following equations:

$$P_{ac} = P_{dc} = V_{cell}.I_{stack} \quad (28)$$

Assuming a lossless inverter, we get According to electrochemical relationships, a relationship between the stack current and the molar flow of hydrogen can be written as

$$q_{H2} = \frac{N_0.I_{stack}}{2F.U} \quad (29)$$

Were U is a utilization factor

From equation (21), (22) and (29)

$$\sin(\delta) = \frac{2F.U.X}{m.V_s N_0} q_{H2} \quad (30)$$

Assuming a small phase angle

$$\delta = \frac{2.F.U.X}{m.V_s N_0} q_{H2} \quad (31)$$

The equation (31) describes the relationship between output voltage phase angle and hydrogen flow. Equations (21) and (31) indicate that the active power as a function of the voltage phase angle can be controlled by controlling the amount of hydrogen flow.

3.4 Fuzzy Logic Controller

The active power flow from the PEMFC to the load is controlled thought controlling the flow hydrogen. The proposed fuzzy logic controller controls the active power by controlling the hydrogen flow.

The fuzzy controller consists of five different steps [12] , [11]

Step 1) definition of input-output variables of controller

Step 2) design of fuzzy control rule

Step 3) fuzzification

Step4) inference

Step 5) defuzzification

The fuzzy controller inputs are the error $e(k)$, and change of error $ce(k)$. The output of the controller is the duty ratio of hydrogen flow $u_{H2}(k)$. The error, change of error, and the output of the controller are given as follows:

$$e(k) = q_{H2} + q_{meth_{ref}} - q_{H2b} \quad (32)$$

Where q_{H2} is the flow hydrogen from the current feedback signal were is proportional to the terminal load, $q_{methane}$ is the methane reference signal and q_{H2b} is the hydrogen flow feedback signal.

$$ce(k) = e(k) - e(k-1) \quad (33)$$

$$u_{H2}(k) = u_{H2}(k-1) + \rho \Delta u_{H2}(k) \quad (34)$$

Where $\Delta u_{H2}(k)$ is the inferred change of duty ratio by fuzzy controller and ρ is the gain factor of the controller[13],[11]. Fig 6, 7 and 8 shows the basic fuzzy partition of membership function for error, change of error, and change of control action. And fuzzy variables are expressed by linguistic variables such as "positive big(PB)", "positive medium(PM)", "zero(ZO)", "negative medium(NM)", "negative big(NB)". Table 1 shows the fuzzy model based on fuzzy rules[9].

Exemple fuzzy rules are:

Ruel 1 `` If $e(k)$ is PM and $ce(k)$ ZO then $u(k)$ is PM

Ruel 2 `` If $e(k)$ is NB and $ce(k)$ NM then $u(k)$ is NB

The inference methode used is basic and simple, it is developed from the minimum operation function rule as a fuzzy implementing function. The membership function of e , ce and u_{H2} are given by μ_{E_i} , μ_{CE_i} , $\mu_{U_{H2}^i}$ μ_{C_i} . The commonly use Min-Max method is given as:

$$\mu_{R_i}(e, ce) = \min[\mu_{E_i}(e), \mu_{CE_i}(ce)] \quad i=1..n \quad (34)$$

$$\mu_{C_i}(u_{H2}) = \max[\mu_{R_i}(e, ce), \mu_{u_{H2}^i}(u_{H2})] \quad (35)$$

Table 1. Linguistic Rule.

		CHANGE OF ERROR(ce)					
		U	NB	NM	ZO	PM	PB
E R R O R	NB	NB	NB	NM	NM	ZO	
	NM	NB	NM	NM	ZO	PM	
	ZO	NM	NM	ZO	PM	PM	
	PM	NM	ZO	PM	PM	PB	
	PB	ZO	PM	PM	PB	PB	
	U						

The centroid defuzzification method determines the output value from center of gravity of the output membership function and is given by the expression[12].

$$\Delta u_{H2} = \frac{\sum_{i=0}^n \mu_{C_i}(u_{H2i})u_{H2i}}{\sum_{i=0}^n \mu_{C_i}(u_{H2i})} \quad (36)$$

Based on table 1 and fig9, the 3-dimensional representation of control input (u_{H2}) for fuzzy variables (e, ce) is shown in figure 7

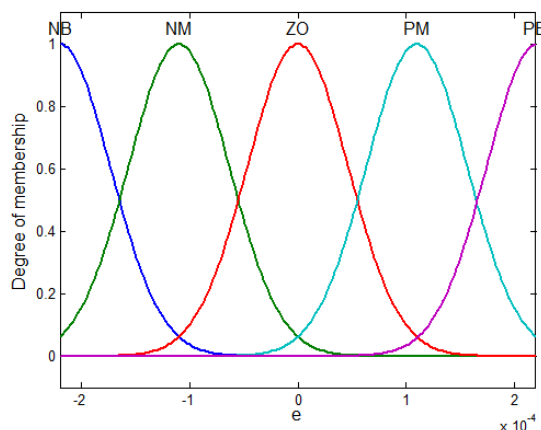


Fig 6: Membership fonction for error(e)

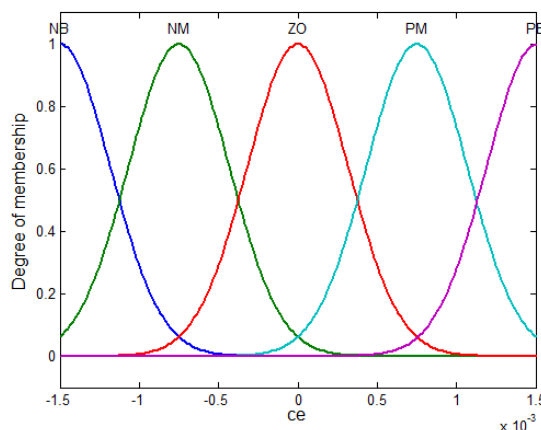


Fig 7: Membership fonction for change of error(ce)

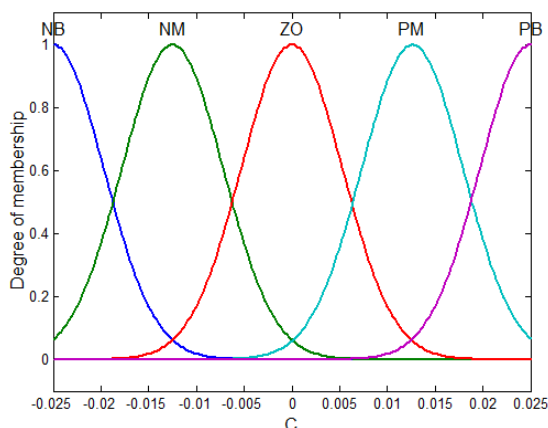


Fig 8: Membership function for control(u)

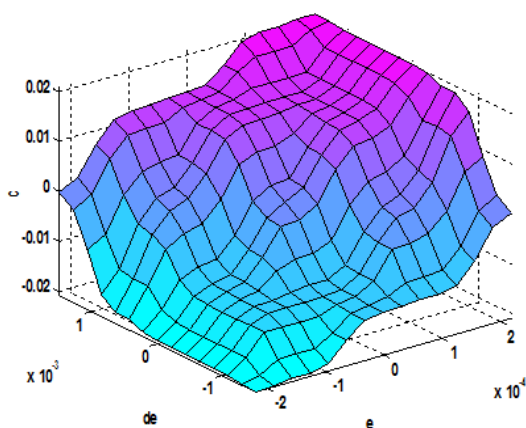


Fig 9: FLC control input

3.4 Neural Network Controller

The structure of the Neural Network Controller (NNTC) is similar to one of the Neural Network Identifier. The objective of NNTC is to develop a back-propagation algorithm such that the output of the plant can track the output of fuzzy logic controller FLC (fig 10) .

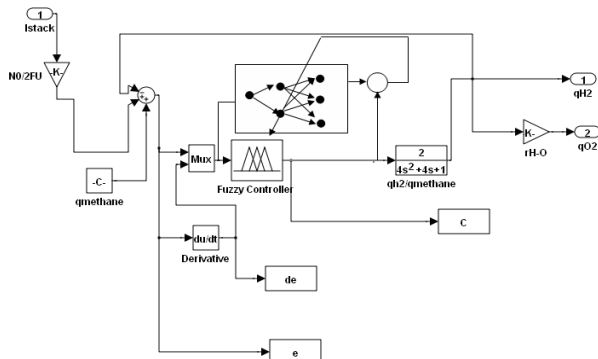


Fig 10: Block diagram of the proposed controller.

The 3-dimensional representation of control input for NNTC u_{H_2} (e, ce) is shown in Fig11

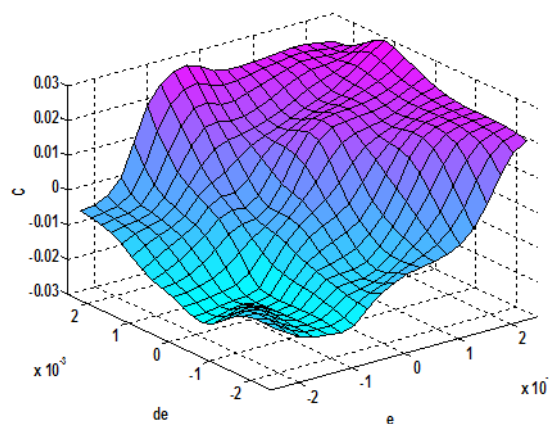


Fig11: NNT control input

4. Simulation Results

The model parameter are given in Table 2. The model of Fuel cell system for residential power generations shown in Fig 12 is tested with step change in the load as shown in Fig13. These abrupt changes in the active and reactive power are for testing the dynamic response of the system and do not necessarily represent change in residential load.

In a practical system, the response time of the reformer can be longer than tens second [8], [9]. Therefore the reformer controller parameters have significant effect on the active power control. In this simulation the Neural Network controller (NNTC) was able to modify hydrogen flow for controlling active power to the load change fig13. The Neural Network controller (NNTC) is characterized by faster time response compared to the fuzzy logic controller and PID controllers used in fig14

Fig15 and Fig 16 shows the change of hydrogen flow and phase angle. we note that this change is similar to the change of active power because the active power flow from the PEMFC to the load is controlled thought controlling the flow hydrogen.

The reactive power Q_{ac} follows immediately the change of the reactive power load (fig17). Because the reactive power is controlled directly by modulation index (fig 18) from DC/AC inverter and the response of DC/AC inverter is not considerable. We notice that, the reactive power value is superior to the reactive power. This is due to inductive effect losses of the line (x).

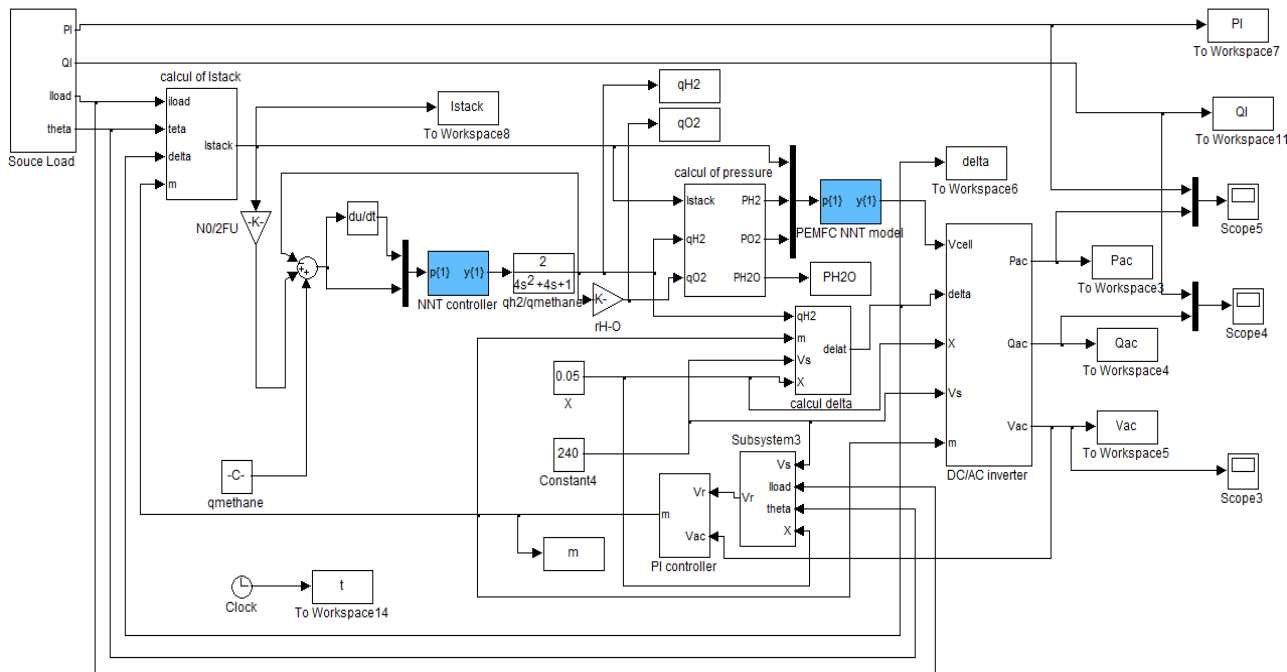


Fig 12: Simulink implementation of Fuel Cell control system architecture

Table2. Model Parameter

Parameters	Values
Facteur de conversion CV	2
farady,s Constant, F	9684600 C/Kmol
Universal gas Constant R	8314.47 j/Kmol.K
Number of cells N_0	333
Hydrogen valve constant K_{H2}	$4.22 \cdot 10^{-5}$ Kmole/(s.A)
Oxygen valve constant K_{O2}	$2.11 \cdot 10^{-5}$ Kmole/ (s.atm)
Hydrogen time constant, τ_{H2}	3.37 (s)
Oxygen time constant, τ_{O2}	6.74 (s)
Utilization factor, U	0.8
PI gain constants K_5, K_6	10
Hydrogen –Oxygen flow ratio r_{H-O}	1.168
Methane reference signal, q_{ref}	0.000015 Kmole/ s
Reformer time constants τ_1, τ_2	2, 2
Line reactance, X	0.05Ω
Voltage reference signal V_r	240 V
K_r constant = $\frac{N_0}{4F}$	$0.996 \cdot 10^{-6}$ Kmole/ (s.A)

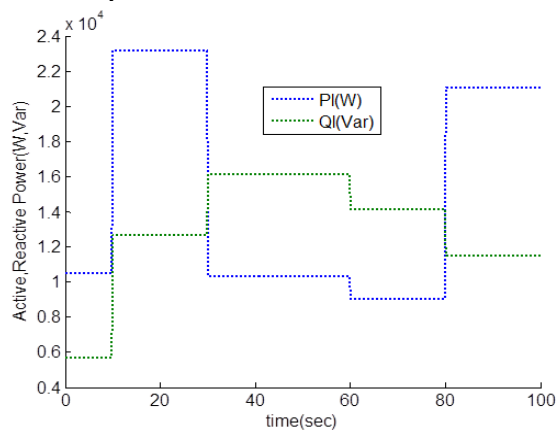


Fig 13: Load step

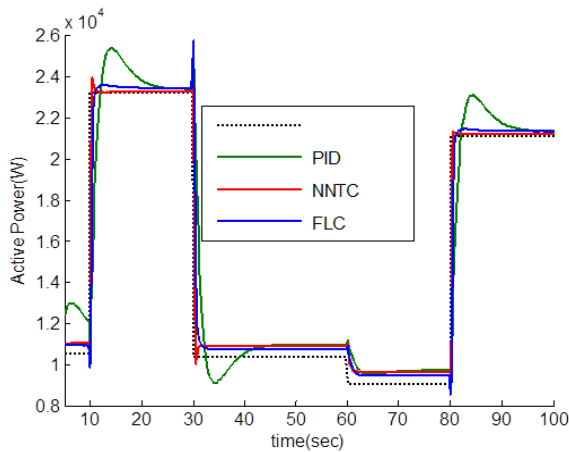


Fig 14: Active output power change (with,PID, FLC,and NNTC)

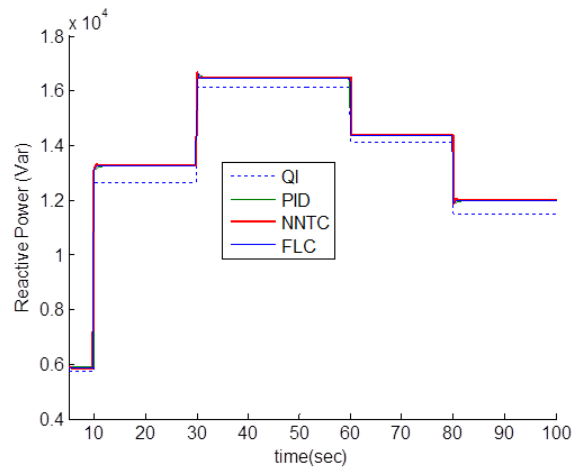


Fig17: Reactive output power change

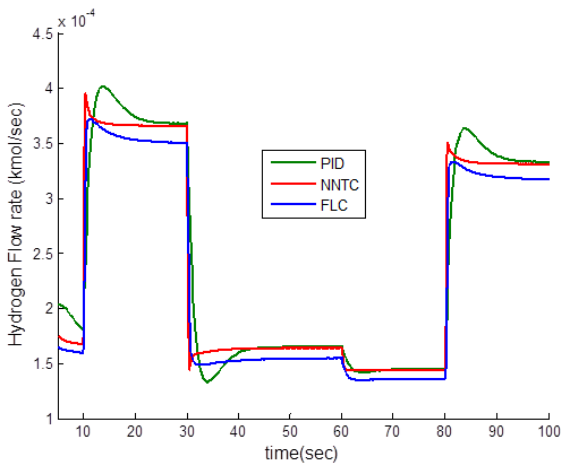


Fig 15: Hydrogen flow rate change(with,PID, FLC,and NNTC)

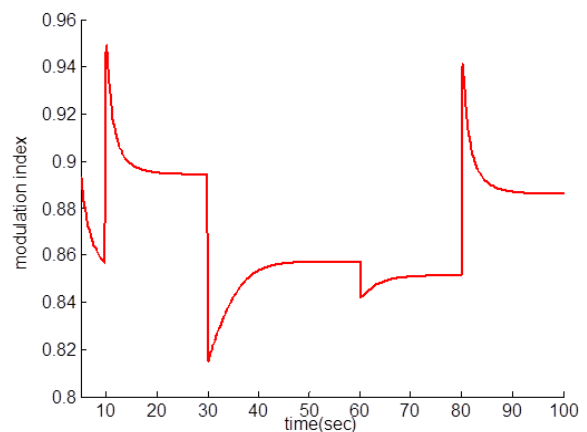


Fig 18: Modulation index change

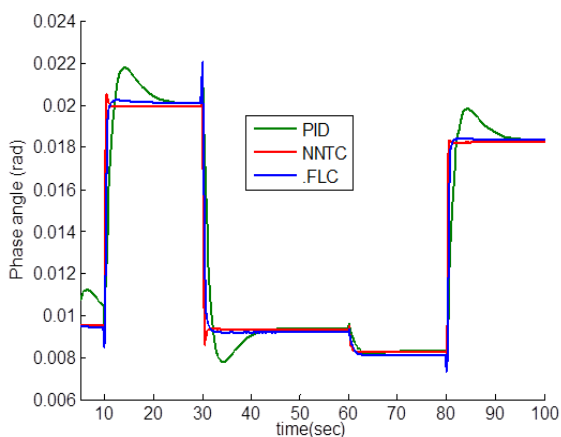


Fig 16: Output voltage phase angle change change(with,PID, FLC,and NNTC)

Conclusions

This paper introduces a technique based on neural network to control the active power output from fuel cell system power generation. The proposed model includes a neural network PEMFC model, a dynamic fuel cell model, a gas reformer model, DC/AC inverter model, and NNT controller unit block. Artificial neural networks can be trained to simulate the performance of a fuel cell with great accuracy; consequently, the same concept could be extended to other components and thus bigger and more complex cycles can be simulated at reduced time. The developed models are tested using computer-simulated step change in the load active and reactive power demands. The simulation results indicate that converter and fuel quantities have to be controlled simultaneously to control the active and reactive power. It also indicates that the

neural network controller (NNTC) and fuzzy logic controller (FLC) are very effective to control hydrogen flow for active power load variation.

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