UDC 620.93:681.3.06
Original scientific paper
Received: 03.09.2001.

Nonlinear modelling of MCFC stack based on RBF neural networks identification

Cheng Shen, Guang-yi Cao and **Xin-jian Zhu**
Institute of Fuel Cell, Department of Automation, Shanghai Jiaotong University, Shanghai 200030, P.R. CHINA
e-mail: smacao@263.net

SUMMARY

Modelling Molten Carbonate Fuel Cells (MCFC) is very difficult and the existing models are too complicated to be used for controlling design, especially for on-line control design. This paper presents the application of neural networks identification method to develop the nonlinear temperature model of MCFC stack. The hidden layer units of the neural networks consist of a set of nonlinear radial basis functions (RBF). The temperature characters of MCFC stack are briefly analyzed. A summary of RBF neural networks for the multi-input and multi-output (MIMO) nonlinear system modelling is introduced. The simulation tests reveal that it is feasible to establish the model of MCFC stack using RBF neural networks identification. The most important thing is that the modelling process avoids complex analytical modelling that uses complicated differential equations to describe the stack. After being tested, the model can be used to predict the temperature responses on-line which makes it possible to design online controller of MCFC stack.

Key words: *Molten Carbonate Fuel Cells (MCFC), Radial Basis Function (RBF), modelling, neural networks, identification.*

1. INTRODUCTION

Nowadays, the increasing energy demands as well as preserving the global environment make it more and more urgent to develop energy systems with readily available fuels, high efficiency and minimal environmental pollution. A fuel cell system is expected to meet such demands for it is a chemical power generation device that converts the chemical energy of fuel directly into electrical energy without combustion as an intermediate step. The fuel cell system has many advantages over conventional power generation equipment, such as high energy conversion efficiency, modular design and very low environmental pollution. A fuel cell system can get an overall efficiency up to *80%* and a net electrical efficiency ranging from *40%* to *60%*, which is higher than that of almost all other energy conversion systems [1].

MCFC is now the most hopeful model to reach commercialization after phosphoric acid fuel cell (PAFC) [2]. The MCFC has undeniable advantages over PAFC. MCFC can use various fuels such as coal gasification and nature gas. No expensive metals such as Platinum etc. are needed as a catalyst and the costs of the main materials are relatively low. These characteristics allow a wide spectrum of applications for an MCFC varying from central power generation to industrial or commercial integrated power-generation.

The performance and lifespan of MCFC stack are greatly dependent on the operating temperature. The temperature range allowed for a stable cell performance of MCFC is *600* to *700 °C*, and the normal operating temperature is *650°C* [3]. Operating at a temperature lower than *600°C* the activities of molten salts decrease and the cell performance drops significantly. A higher operating temperature is favorable for improving the working voltage and output performance of MCFC. However, when the operating temperature is higher than *700°C*, material corrosion accelerates and electrolyte loss enlarges which increases the risk of short-circuit and shortens the stack lifespan. Hence, tight control of the operating temperature within a specified range and reducing its temperature fluctuation are indispensable.

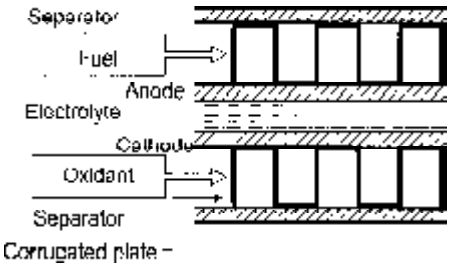
Unfortunately, an accurate mathematical model is indispensable either in classical control theories or modern control theories. MCFC systems are worked under high-temperature, closed, complicated environments. An MCFC system integrates various components, including entirely new components (e.g. fuel cell) and new applications of conventional components (e.g. reformer and heat exchanger) as well as multiple recycling gas flow loops and multiple phase flows and complex chemical and electro-chemical reactions [4]. According to the analysis of MCFC systems, it is known that MCFC systems is a nonlinear system with MIMO and it is very difficult to model MCFC systems [5]. Extensive studies on MCFC stack modelling have been carried out for decades [6]. However, all the models developed are based on matters, energy and momentum conservation laws, with expressions that are too complicated to be used to design a control system, especially for online control.

An alternative approach is to establish the mathematical relationship of the dynamic system based on input-output data. Neural networks have been an attractive structure in such an approach. A large number of identification and control structures and algorithms based on neural networks have been proposed [7]. However, practical applications of neural networks for modelling and prediction of MCFC stack can not be found in prior papers.

In the present work, the internal complexes of MCFC stack are avoided, and RBF neural networks identification technology is applied to set up the nonlinear temperature model of MCFC stack. Firstly, the main characters of MCFC stack are briefly analyzed in Section 2. Then, a summary of RBF neural networks for the MIMO nonlinear system modelling is introduced in Section 3. Training and simulation tests are given in Section 4. Finally, conclusions are given in Section 5.

2. DESCRIPTION AND ANALYSIS OF MCFC STACK

A single cell's structure is shown in Figure l. A single cell consists of an anode, cathode, electrolyte plate, separator plates, corrugated plates, and current collectors. The fuel and oxidant gases flow in the anode and cathode side channel along the corrugated plates. O_2 and CO_2 in oxidant gas react with the electron at the cathode, and produce CO_3^{2-}. CO_3^{2-} moves within the electrolyte plate perpendicularly from cathode to anode by the driving force of concentration difference. At the anode, H_2 in the fuel gas reacts with CO_3^{2-} and produces CO_2, H_2O and electrons by electro-chemical reaction. Electrons released from the reaction site are collected by the current collector and pass the corrugated plate and separator perpendicularly. The top and the bottom separators are connected to external load equipments [8].



Cathode reaction: $CO_2+O_2+2e^- \rightarrow CO_3^{-2}$
Anode reaction: $H_2+CO_3^{-2} \rightarrow H_2O+CO_2+2e^-$
Shift reaction: $H_2+CO_2 \rightarrow H_2O+CO$

Fig. 1 Conceptual structure of a single cell

A single fuel cell has a potential of about *0.8 V* with a current of about *200~500 mA/cm²*. To supply a higher power, MCFC are used superimposed into the stack where cells are electrically connected in series and separated from each other by bipolar plates [4].

According to MCFC stack dynamic characteristic [9], the temperature model of MCFC stack can be described as:

$$\frac{d\boldsymbol{T}(t)}{dt} = \dot{\boldsymbol{T}}(t) = F\left[\boldsymbol{T}(t), \boldsymbol{v}(t)\right] \tag{1}$$

Here, $\boldsymbol{v} = \left[v_a(t), v_c(t)\right]^T$ is the input vector, i.e., the anode and cathode gas flowrates.

$\boldsymbol{T}(t) = \left[T_a(t), T_c(t), T_e(t), T_s(t)\right]^T$ is the output vector, i.e., the temperatures of anode, cathode, electrolyte plate and separator.

The temperature responses of anode, cathode, electrolyte plate and separator are mainly dependent on three factors: the heat emitted by electro-chemical reactions that cause the temperatures increase, the convection heat loss with the exited gases that lowers the temperatures, and the conduction loss by the stack hardware. When the gases flow slowly, on the one hand the reaction is adequate and less heat is lost, and on the other hand, less heat is produced. On the contrary, when the gases flow fast, on the one hand, the reaction is inadequate and part of heat flows away with the remnant gases, and on the other hand, more reaction heat is produced so the ultimately stabilized temperature is variable at different anode and cathode gas flow rates. In general, in order to cool the stack and ensure the fuel to be utilized completely, it is assumed that the oxidant (i.e. compressed air to cathode) is excessive and the fuel supply rate is not beyond the maxim reaction rate capacity of the stack.

The object of the identification model is to simulate dynamically the variant trails of temperature under various gas flowrates. Thus, the identification model can be described by a nonlinear discrete equation:

$$\boldsymbol{T}(k+1) = F\left[\boldsymbol{T}(k), \boldsymbol{v}(k)\right] \tag{2}$$

Here, k is discrete-time variable.

3. THE IDENTIFICATION STRUCTURE AND ALGORITHM

3.1 Radial basis function neural networks

Feedforward neural networks trained with back propagation algorithm (BPNN) have been widely applied to system identification and control. However, they have several drawbacks such as their proneness to get stuck in local minima, their relatively slow convergence rate and their difficulties to determine a minimal but adequate architecture, etc. [10].

Similar to BPNN, the radial basis function neural network (RBFNN) has the universal approximation ability. Unlike the BPNN, RBFNN has the best approximation property. Its approximation accuracy properties are better than the other methods, including multilayer perceptron networks [11]. Even more important, the connection weights from the hidden layer to the output layer are linear, which means that the linear optimal algorithms can be used in RBFNNs and that guarantees the convergence of the parameters to the global minimum. In addition, while training RBFNNs, only a part of the nodes will be affected by any given input, and only a portion of the model parameters may need to be adjusted, thus reducing the training time and computational burden [8].

Similar to most feedforward networks, RBF neural networks have an input layer, a nonlinear hidden layer and a linear output layer. The nodes within each layer are fully connected to the previous layer nodes. The input variables are each assigned a node in the input layer and connected directly to the hidden layer without weights. The hidden layer nodes are RBF units. The nodes calculate the Euclidean distances between the centers and the network input vector and pass the results through a nonlinear function [7]. The output layer nodes are weighted linear combinations the RBFs in a hidden layer. The structure diagram of RBF neural networks with m inputs, p outputs and N hidden nodes is given in Figure 2.

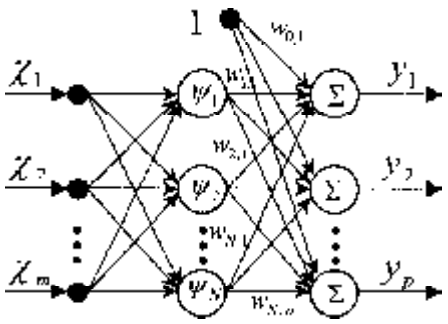


Fig. 2 RBF neural networks structure

For a data set consisting of m inputs, p outputs and N hidden elements, the hidden unit can be expressed as a matrix:

$$\boldsymbol{\Phi} = \begin{bmatrix} Y_{1,1} & Y_{1,2} & \cdots & Y_{1,N} \\ Y_{2,1} & Y_{2,2} & \cdots & Y_{2,N} \\ \vdots & \vdots & \vdots & \vdots \\ Y_{m,1} & Y_{m,2} & \cdots & Y_{m,N} \end{bmatrix}$$

and the network weight:

$$\boldsymbol{W} = \begin{bmatrix} w_{1,1} & w_{1,2} & \cdots & w_{1,N} \\ w_{2,1} & w_{2,2} & \cdots & w_{2,N} \\ \vdots & \vdots & \vdots & \vdots \\ w_{p,1} & w_{p,2} & \cdots & w_{p,N} \end{bmatrix}$$

where $Y_j(X(k))$ is a nonlinear function. Here it is chosen to be a Gaussian activation function:

$$Y_j(X(k)) = exp\left(\left\|X(k) - Cj\right\|^2 \Big/ l_j^2\right) \qquad (3)$$

where: C_j $(j=1,2,...,N) \in R^N$ is the center of the j-th hidden node, which is a vector having the same dimension as the input vector $X(k)$; and l_j is the width of the j-th RBF hidden unit.

Then the i-th RBF network output can be represented as a linearly weighted sum of N basis functions:

$$Y_i^{net}(k) = w_{0,i} + \sum_{j=1}^{N} w_{j,i} \cdot Y_j(X(k)) \quad i = 1,2,...,p \qquad (4)$$

where: $w_{j,i}$ and $w_{0,i}$ are the weights. $w_{0,i}$ is used to compensate for the difference between the average value over the data set of the RBFs activation and the corresponding average value of the target outputs [7].

With the structure described above, the transformation from the input layer to the hidden layer is nonlinear, due to the use of Gaussian functions $Y(\cdot)$ for RBFs. The hidden layer connected to the output layer is linear.

3.2 Identification system of MCFC stack with RBF networks

It has been proved that a wide class of nonlinear systems can be represented by the following difference equation model, i.e., nonlinear autoregressive model with exogenous inputs (NARX) or named one-step ahead predictor or series-parallel model [3, 12]:

$$\begin{aligned} Y(k) = F(&Y(k-1),...,Y(k-n_y), \\ &U(k-1),...,U(k-n_u)) \end{aligned} \qquad (5)$$

Here, $Y(k)$ is the output vector, $U(k)$ is the input vector. n_y and n_u are the lags of the output and input respectively. $F(\cdot)$ is a nonlinear function.

For the MCFC stack, $U(k)=[v_a(k),v_c(k)]^T$ is the input manipulated vector, i.e., the anode and cathode gas flowrates. $Y(k)=[T_a(k),T_c(k),T_e(k),T_s(k)]^T$ is the output vector, i.e., the temperatures of anode, cathode, electrolyte plate and separator of the MCFC stack.

The objective of this paper is to use RBF neural networks to model the MCFC stack as described by Eq. (1). Define the input vector of the network at sample k as:

$$X(k)=[Y(k),Y(k-1),...,Y(k-n_y), U(k),U(k-1),...,U(k-n_u)]^T \quad (6)$$

Here the dimension of the input vector, and also the dimension of the centers of the hidden layer nodes, is given by:

$$N = pn_y + mn_u \quad (7)$$

where p and m are the number of outputs and inputs of the system respectively, and N is the input vector dimension.

The structure of the RBFNN identification system is shown in Figure 3 [13]. TDL is the tapped delay line that the output vector has for its elements, the delayed values of the input signal.

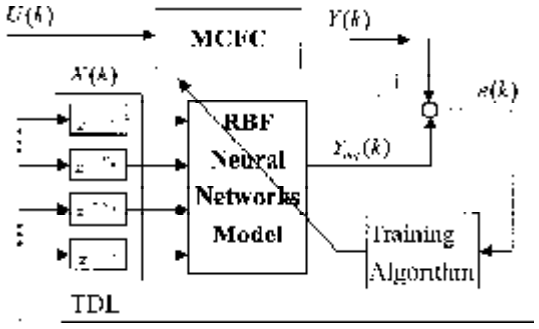


Fig. 3 The identification structure of MCFC stack with RBF networks

3.3 Training algorithm of the RBF networks

In Figure 3, the predictive error or residual is $e(k)=Y(k)-Y^{net}(k)$, where $Y^{net}(k)$ is the predictive output of the networks. In this paper, the criterion of training an RBF network is to minimize the sum of squared errors (SSE) below [7]:

$$E_{SSE} = \sum_j \sum_k \left[Y_j^d(k) - Y_j^{net}(k) \right]^2 \quad (8)$$

where $Y_j^d(k)$ are the destination values of the network output; here it is the sampled data from the experiments.

Training of RBF neural networks can be divided into a two-stage procedure [14]. The first stage involves selecting the basis function centre vectors C_j ($j=1,2,...,N$). The selection principle is that they should be chosen to form a representation of the probability density of the input data [7]. Most published papers simply assume that the centers are arbitrarily selected from input data points, which will often result in that either the RBF neural networks perform poorly or the computational burden of network training increases largely. Moreover, numerical ill-conditioning frequently occurs owing to a nearly linear dependency caused by some centers being too close. Hence, an adequate technique to determine RBF network centers, i.e., the orthogonal least-squares (OLS) method has been adopted here [14, 15].

After the network centers have been chosen, the values of weights are also determined at the same time from the solution of the following group of equations:

$$\begin{cases} Y_1(k) = w_{0,1} + y_{1,1}w_{1,1} + \cdots + y_{1,N}w_{1,N} \\ \quad \vdots \quad \vdots \quad \vdots \\ Y_p(k) = w_{0,p} + y_{p,1}w_{p,1} + \cdots + y_{p,N}w_{p,N} \end{cases} \quad (9)$$

The width parameters l_j of the RBFs may be calculated by many techniques. Here we chose all widths to be equal to about twice the average space between the basis function centers [7].

4. TRAINING AND SIMULATION TEST

Use the MATLAB neural network toolbox to perform the training and simulation. Firstly, all the experimental sampled data points are divided into a training set and a testing set [15]. The former is used in networks training procedure and the latter is used in testing the validities of the networks model trained.

The training samples (training set) are *960* temperature response values under various gas velocities. They are stored in a training data file and will be supplied for the neural networks during the training process. Based on satisfying the minimum SSE conditions in Eq. (8) and shorter training time, the neuron number is set to be *64*. The training time using a Pentium-II 266 MHZ computer was *61.38 seconds*. While the same set of data were used to train an MLP-BP network also with a hidden layer and *25* neurons, and on the same computer, the training time for obtaining the same error level of SSE is *198.64 s*. The desired SSE is *0.15*, and in the end of the training process the SSE obtained is *0.143664*. The adjustment curve of error in training is given in Figure 4. In fact, when the error decreases to about *0.14*, it no longer changes basically.

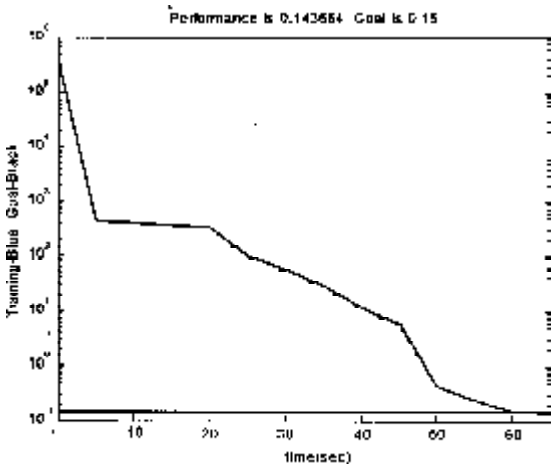
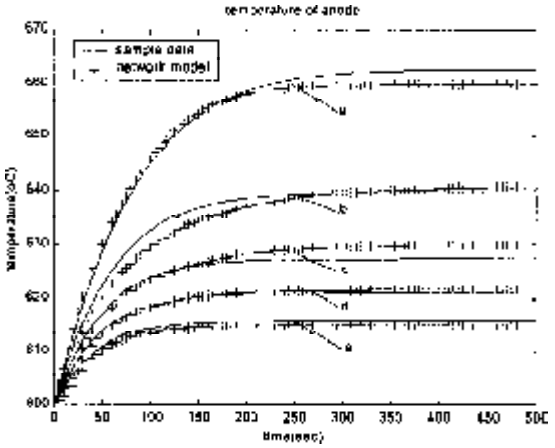


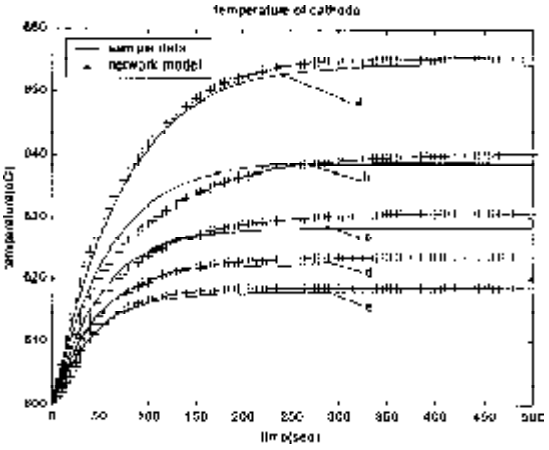
Fig. 4 Neural networks model error learning curve

To validate the RBF-network model, use the neural networks trained above to perform dynamic identification simulation of MCFC stack. Under various gases flowrates, comparing the discrete temperature values calculated by the neural networks and actual sampled temperature data (in testing set) obtained from the experiments of the MCFC stack, we obtain the results as Figure 5.

For simplicity and generality, in Figure 5, only the comparing results of the anode and cathode centers of co-flow MCFC stack at five different and typical gas flowrates are given. The identification results of electrolyte plate and separator have similarly variant trends and are omitted here.



(5a) Identification results of anode temperature



(5b) Identification results of cathode temperature

Fig. 5 Identification results under five different gas flowrates (m/s):
a) v_a=0.1, v_c=0.9; b) v_a=0.2, v_c=2.4;
c) v_a=0.3, v_c=3.5; d) v_a=0.4, v_c=4.2;
e) v_a=0.7, v_c=6.5

Figure 5 shows that the RBF neural networks model can imitate the dynamic temperature response of the actual stack, and the maximal error is not beyond *2°C*. The error is determined by the given error target in the training process, and the identification accuracy can be improved by trial-and-error to get the most suitable topologic structure.

5. CONCLUSION

Based on the RBF neural networks identification technology, a nonlinear temperature model of MCFC stack is developed. The simulation results have shown that the modelling accuracy is high and the RBF neural networks model can be trained faster than a BP neural networks model. The simulation results also reveal that it is feasible to set up the model of the complex nonlinear MCFC stack system based on RBF neural networks identification. The most important thing is that the modelling process avoids complex analytical modelling and also avoids using complicated differential equations groups to describe the stack so that the input-output performance can be effected quickly by neuro-calculation. The RBF-based model can be used to predict the temperature responses on-line which makes it possible to design online controller of MCFC stack.

6. ACKNOWLEDGEMENTS

This work was guided by the study of the Institute of Fuel Cells, Shanghai Jiaotong University. It was supported by Shanghai Science and Technology Development Funds, and by the National 985 Scientific Project Development Funds, P.R. China.

7. REFERENCES

[1] W. He, Dynamic model for molten carbonate fuel cell power-generation systems, *Energy Convers. Magmt.*, Vol. 39, No. 8, pp. 775-783, 1998.

[2] W. He, Operating characteristics of a molten carbonate fuel cell power-generation sytems, *Int. Journal of Energy Research*, Res., Vol. 23, pp. 1331-1344, 1999.

[3] J.-H. Koh, B.S. Kang and H.C. Lim, Effect of various stack parameters on temperature rise in molten carbonate fuel cell stack operation, *Journal of Power Sources*, Vol. 91, pp. 161-171, 2000.

[4] F. Yoshiba, N. Ono,Y. lzaki, Y. Watanabe and T. Abe, Numerical analyses of the internal conditions of a molten carbonate fuel cell stack: Comparison of stack performances for various gas flow types, *Journal of Power Sources*, Vol. 71, pp. 328-336, 1998.

[5] C. Guangyi and M. Masubuchi, Dynamic modelling and response in molten carbonate fuel cell, *Transactions of the Japan Society of Mechanical Engineers (JSME)*, Vol. 57, No. 535 (B), pp. 837-842, 1991.

[6] J.H. Lee and T.R. Lalk, Model fuel cell stack systems, *Journal of Power Sources*, Vol. 73, pp. 229-241, 1998.

[7] A. Ai-Amoudi and L. Zhang, Application of radial basis function network for solar-array modelling and maximum power-point prediction, *IEE Pro.-Gener, Transm. Distrib.*, Vol. 147, No. 5, pp. 310-316, September, 2000.
[8] S. Chen and S.A. Billings, Representation of nonlinear system: The NARMAX model, *Int. J. Control*, Vol. 49, No. 3, pp. 1013-1032, 1989.
[9] W. He and Q. Chen, Three-dimensional simulation of a molten carbonate fuel cell stack under transient conditions, *Journal of Power Sources*, Vol. 73, pp. 182-192, 1998.
[10] K. Warwick, An introduction to radial basis functions for system identification: A comparison with other neural network methods, Proc. of the 35th Conference on Decision and Control, Kobe, Japan, December, pp. 464-469, 1996.
[11] S. Chen and S.A. Billings, Neural network for nonlinear system modelling and identification, *Int. J. Control*, Vol. 56, No. 2, pp. 319-346, 1992.
[12] M.A. Abido and Y.L. Abdel-Magid, On-line identification of synchronous machines using radial basis function neural networks, *IEEE Trans. on Power Systems*, Vol. 12, No. 4, pp. 1500-1506, 1994.
[13] S.M. Ahmad, M.H. Shaheed, A.J. Chipperfield and M.O. Tokhi, Nonlinear modelling of a twin rotor MIMO system using radial basis function networks, National Aerospace and Electronics Conference, 2000 - NAECON 2000, Proc. of the IEEE 2000, pp. 313-320, 2000.
[14] J. Barry Gomm and Ding Li Yu, Selecting radial basis function network centers with recursive orthogonal least squares training, *IEEE Trans. on Neural Networks*, Vol. 11, No. 2, pp. 306-314, 2000.
[15] S. Chen, C.F.N. Cowan and P.M. Grant, Orthogonal least squares learning algorithm for radial basis function networks, *IEEE Trans. on Neural Networks*, Vol. 2, No. 2, pp. 302-309, 1991.
[16] B. Bosio, P. Costamagna and F. Parodi, Modelling and experiment of molten carbonate fuel cell reactors in a scale-up process, *Chemical Eng. Science*, Vol. 54, pp. 2907-2916, 1999.

NELINEARNO MODELIRANJE MCFC SKUPA ZASNOVANOG NA IDENTIFIKACIJI RBF NEURALNIH MREŽA

SAŽETAK

Modeliranje Molten Carbonate Fuel Cells (MCFC) je vrlo teško, a postojeæi modeli su previše složeni da bi se mogli koristiti za kontroliranje projektiranja, posebno za on-line kontrolu projektiranja. U ovom se radu opisuje primjena metode identificiranja neuralnih mreža kako bi se razvio nelinearni model temperature za MCFC skup. Jedinice skrivenih slojeva kod neuralnih mreža sastoje se od skupa nelinearnih radijalnih baznih funkcija (RBF). Ukratko se analiziraju temperaturne osobine MCFC skupa. Uvodi se kratki pregled RBF neuralnih mreža za višestruki input i višestruki output (MIMO) za nelinearni sistem modeliranja. Testovi simulacije pokazuju da je izvedivo uspostaviti model MCFC skupa koristeæi identifikaciju RBF neuralnih mreža. Najvažnija stvar je da ovaj proces modeliranja izbjegava složeno analitièko modeliranje koje koristi komplicirane diferencijalne jednadžbe za opisivanje skupa. Nakon testiranja model se može koristiti za on-line predviðanje temperaturnih reakcija što omoguæava projektiranje online kontrole za MCFC skup.

Ključne riječi: *Molten Carbonate Fuel Cells (MCFC), radijalne bazne funkcije (RBF), modeliranje, neuralne mreže, identifikacija.*