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Solid oxide fuel cell modeling using numerical method and neural network

نمذجة خلايا الوقود ذات الأكسيد الصلب باستخدام طريقة عددية والشبكة العصبية

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المخلص

الهدف الرئيسي لهذه الورقة البحثية هو دراسة نمذجة خلية أكسيد الوقود الصلبة SOFC بطريقة عددية وباستخدام تقنية تستند على الذكاء الصناعي. ويهتم البحث باختبار موثوقية نموذج ثنائي الأبعاد لخلايا الوقود باستخدام برنامج (COMSOL 3.1 FEMLAB) ومقارنة النتائج بنموذج الشبكة العصبية. في الدراسة المقترحة تم اختبار شبكة عصبية بطبقتين ذو تغذية أمامية لغرض نمذجة خلية أكسيد الوقود الصلبة. تم تدريب نموذج الشبكة العصبية المستخدم مع طبقة واحدة خفية مكونة من عشرة عقد باستخدام خوارزم Levenberg-Marquardt ذو عودة الانتشار. نموذج الشبكة العصبية ذات التغذية الأمامية تطابق بشكل جيد للغاية مع البيانات التجريبية وأثبت تفوقه على النموذج العددي. وأثبتت كذلك النتائج المختلفة لهذا التطبيق أن المحاكاة العددية لخلية أكسيد الوقود الصلبة باستخدام 3.1 FEMLAB احتاجت فقط لتعديلات طفيفة.

Abstract

Modeling Solid Oxide Fuel cell SOFC numerically and by AI-based technique is the main objective of this paper. Testing the reliability of a two dimensional numerical model of SOFC using COMSOL (FEMLAB 3.1) software against neural network model is another important issue that will be considered in this paper. In the proposed study, two layers feed forward neural network was examined for the purpose of modeling the Solid Oxide Fuel Cell (SOFC) system. The examined neural network model with one hidden layer of ten nodes was trained with the Levenberg-Marquardt back propagation algorithm. The presented feed forward neural network model is fitted very well with the experimental data and proved to outperform a numerical model. The various outcomes of this application indicate that numerical simulation of SOFC by using FEMLAB 3.1 needs minor modifications. A more general investigation into the potential role of neural network in modeling SOFC is conducted in this research.

Keywords

Neural Network, Two-dimensional Numerical Model, SOFC.

1. Introduction

The Solid oxide fuel cell has the potential for application in transportation, for example, in vehicular auxiliary power units (APU). Current SOFC technology demonstrates viable manufacture, feasible power ranges and applications. This has been accompanied by developments of new concepts, cell and stack designs, advanced processing methods as well as, improved and novel materials [1]. The structure of fuel cell is relatively simple. However, the difficulty of modeling such cell

arises from the way it operates [2]. This is due to the large quantity of coefficients to be determined. Several variants of SOFCs are currently being built (e.g. electrolyte, anode or cathode supported, planar, tubular etc.). Additionally, fuel cell layers can be made from many various materials (YSZ, SDC, etc.) and are still under development. In addition, the layers forming the anode and cathode can have different porosities, and even consist of several different layers. SOFC technology is widely studied by researchers due to its merits. SOFC directly converts chemical energy of fuel into electric

current and heat. In spite of its high efficiency, low pollution emissions and sound, it suffers from high cost, thermo-mechanical issues, sealing requirements under high temperature, performance reduction due to rapid degradation of elements, the need of extra equipment as well as long startup time [3,4].

The SOFC models developed thus far are mainly based on the Nernst equation, activation, ohmic, and concentration losses. The performance of an anode-supported solid oxide fuel cell (SOFC) is considered in this work [5].

Generally, mathematical modeling of SOFCs, require knowledge about many parameters of the microstructure and electrochemical properties of component materials, the exact multi-physicochemical processes, the operating conditions increasing difficulty of problem solving [6].

Classical mathematical models are based on physical process description of the fuel cells and required details information of that description administrate both chemical and electrical reaction. Advanced Methods of Solid Oxide Fuel Cell Modeling provides a comprehensive description of modern fuel cell theory and a guide to the mathematical modeling of SOFCs, with particular emphasis on the use of ANNs. Up to now, most of the equations involved in SOFC models have required the addition of numerous factors that are difficult to determine. The artificial neural network (ANN) can be applied to simulate an object's behavior without an algorithmic solution, merely by utilizing available experimental data. Up to now, most of the equations involved in SOFC models have required the addition of numerous factors that are difficult to determine. The artificial neural network (ANN) can be applied to simulate an object's behavior without an algorithmic solution, merely by utilizing available experimental data.

Artificial neural network (ANN) has been widely used for modeling due to its ability to simulate a system as a black-box, while avoiding the solution of physical equations.

Moreover, the performance of ANN depends upon its generalization capability. This means that a trained network could classify data from the same class as the learning data that it has never seen before [7].

Usually, data are obtained from experimental measurements or physical models. However, good selection of training data is essential for the reason of covering all aspects of the problem. Moreover, randomness of input information should guarantee better training power of the neural network.

ANN is one of the most common approaches in modeling chemical and physical systems [8]. The precision of obtained ANN model could be attained to the desired accuracy. Applications of ANN in chemistry include electrochemistry, spectral analysis thermal analysis, gas sensors, phase diagram, estimation of kinetic analytical parameters, etc [9-12]. Levenberg-Marquardt back propagation algorithm is applied in this work to train a feed forward neural network FFNN for modeling SOFC at two different temperatures.

Numerical modeling of solid oxide fuel cells has been demonstrated by [13]. A detailed numerical model has been formulated for, and applied to solid oxide fuel cells (SOFCs). In this model, the transport of oxygen ions was modeled as a Fickian diffusion process mimicking the effect of the potential in the cell. The output cell voltage was based on the electric potential difference between the cathode and anode current collectors, which were fixed as constants. The "effective concentration" of ions was computed and then converted into ionic phase potential, making it possible to determine the potential losses due to activation and ohmic resistance. In this paper, the 2-D numerical simulation of a node-supported SOFC has been developed by using FEMLAB 3.1 commercial software. The parametric study has been carried out by using the developed model to achieve the optimum operating conditions at different circumferences of SOFC operations. Moreover, the performance of SOFC is compared to the

ANN model trained by Levenberg-Marquardt back propagation algorithm.

The rest of this paper is organized as follows. Section 2 covers neural network learning algorithm, namely Levenberg-Marquardt. Mathematical model for SOFC is investigated in section 3. Section 4 covers computer simulation and results. Finally the conclusion is presented

2. Levenberg-Marquardt model

The mentioned back propagation algorithm uses the gradient of the performance function to determine how to adjust the network weights to optimize the performance. An iteration of this algorithm is as follows:

$$X_{i+1} = X_i - \eta_i \nabla f(x) \quad (1)$$

Where

X_i is a vector of current weights and biases, $\nabla f(x)$ is the current gradient, and $\eta_i =$ learning rate

Levenberg-Marquardt learning algorithm (LMA) was used in this paper [14]. LMA operates in batch mode (all inputs are applied to the network before weights are updated). It is faster and more accurate than standard back propagation algorithms in which it outperforms simple gradient descent and other conjugate methods in a wide variety of problem [15]. LMA can locate the minimum of a multivariable function that is expressed as the sum of squares of non-linear real-valued functions [16,17]. It has become a standard technique for non-linear least-squares problems [18].

LMA interpolates gradient descent and the Gauss-Newton method. When the current solution is close to the correct one, it becomes a Gauss-Newton method. When the current solution is far from the correct one, the algorithm becomes slow but guaranteed to converge behaving like a steepest descent method.

The Levenberg-Marquardt algorithm was designed to approach second-order training speed without having to compute the Hessian

matrix just like the Newton method[16]. When the performance function has the form of a sum of squares as it is typical in training feed forward networks equation (2), then the Hessian matrix can be approximated as depicted in equation (3)

$$f(x) = \frac{1}{2} \sum_{j=1}^m e_j^2(x) \quad (2)$$

$$\nabla^2 f(x) = J^T(x)J(x) \quad (3)$$

and the gradient can be computed as

$$\nabla f(x) = \sum_{j=1}^m e_j(x) \nabla e_j(x) = J^T(x)e(x) \quad (4)$$

where

J is the Jacobian matrix that contains first derivatives of the network errors with respect to the weights and biases, and e is a vector of network errors. The Jacobian matrix can be computed through a standard back propagation technique that is much less complex than computing the Hessian matrix. The Levenberg-Marquardt algorithm uses this approximation to the Hessian matrix in the following Newton-like update:

$$X_{i+1} = X_i - [J^T J + \mu I]^{-1} J^T(x)e(x) \quad (5)$$

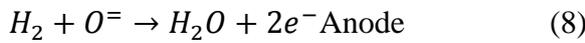
$$X_{i+1} = X_i - [J^T J + \mu \text{diag}[J^T J]]^{-1} J^T(x)e \quad (6)$$

When the scalar μ is zero, it is just Newton's method, using the approximate Hessian matrix. When μ is large, this becomes gradient descent with a low step size. Newton's method is faster and more accurate near an error minimum, so the aim is to shift towards Newton's method as quickly as possible. Thus, μ is decreased after each successful step (reduction in performance function) and is increased only when a

tentative step would increase the performance function. In this way, the performance function will always be reduced at each iteration of the algorithm.

3. Proposed SOFC Mathematical Model

This section is dedicated to introduce how to derive the different parameters of the proposed mathematical model. A solid oxide fuel cell (SOFC) consists of anode, cathode and an ionic conductor (electrolyte). The oxygen diffuses through the porous cathode and fuel, (hydrogen) diffuses through the porous anode. The oxygen at cathode accepts the electrons from the external circuit to form oxide ions. The oxide ions conducted through the electrolyte interface surface and combine with the hydrogen to form water. Then the electrons are released in this process flow through the external circuit back to cathode. The reactions in a hydrogen consuming SOFC are:



The open cell voltage can be calculated by using Nernst equation as follows [19]:

$$E = E_o + \left(\frac{R_g \cdot T}{n \cdot F}\right) \ln \left[\frac{P_{H_2} \cdot P_{O_2}^{1/2}}{P_{H_2O}} \right] \quad (9)$$

The governing equations which will be used to study mass transport and electrochemical reaction in SOFC are as follows:

Electronic current balance in cathode and anode by using conductive media DC equation; (1) Ionic current balance in electrolyte and the two electrodes by using conductive media DC equation; (2) Mass balance, Maxwell-Stefan equation will be used at the two electrodes, electrodes, and (3) Momentum equation, Darcy's law applied to study the flow in porous media, electrodes

The mass balance at steady state in the macroscopic structure is according the following equation [19]:

$$\nabla N_i = R_i \quad (10)$$

For species $i = N_2, O_2$ in the cathode and, $i = H_2, H_2O$ in the anode.

Where N_i denotes the flux vector and R_i denotes the consumption term. For nitrogen (N_2), the consumption term R_i is equal to zero. The flux vector is given by Fickian formulation, obtained from Maxwell-Stefan equations, so that mass balance can be calculated as the following equation depicts:

$$\nabla \left[-\rho \omega_i \sum_{j=1}^n D_{ij} \frac{M}{M_j} \left(\nabla \omega_j + \omega_j \frac{\nabla M}{M} \right) \right] = R_i \quad (11)$$

in the two electrodes

The density of the oxidizer (air) in the cathode can be calculated as follows:

$$\rho_{cat} = \frac{P_{atm}}{R_g T (\omega_{O_2} M_{O_2} + \omega_{N_2} M_{N_2})} \quad (12)$$

Equation (12) is also applicable for the anode by replacing O_2 and N_2 by H_2 and H_2O

The Maxwell-Stefan diffusivities can be described for cathode and anode with an empirical equation as showed by [19], based on kinetic gas theory for the gas mixture in the cathode as follows:

$$D_{O_2-N_2} = K_D \frac{T^{1.75}}{P_{atm} (V_{O_2}^{1/3} + V_{N_2}^{1/3})} \left[\frac{1}{M_{O_2}} + \frac{1}{M_{N_2}} \right]^{1/2} \quad (13)$$

Moreover, the gas mixture in the anode can be represented by equation (13) by replacing (O_2 and N_2) by (H_2 and H_2O). Where K_D is constant, V_i denotes the molar diffusion volume of species i ($m^3 \text{ mole}^{-1}$)

In the porous cathode and anode, the effective binary diffusivities depend on the porosity (ε), of the two electrodes according to:

$$D_{i-j}^{eff} = D_{i-j} \varepsilon^{1.5} \quad (14)$$

The balance of the current induced by the migration of oxide ions and hydrogen ions in the two electrodes can be written as:

$$\nabla(-K_i \nabla \varphi_i) = Q \quad (15)$$

Where K_i denotes the ionic electrode conductivity (Sm^{-1}), φ_i is the ionic potential (V) and Q is the current source term, as shown by [20] can be defined according the Tafel equation as follows:

$$Q_{cat} = i_{o,cat} S_a \left\{ \exp \left[\frac{0.5 F (\varphi_e - \varphi_i - \Delta \varphi_{e-cat})}{RT} \right] - \right. \\ \left. X_{O_2} X_{O_2-o} \exp - 0.5 F \varphi_i - \varphi_e RT \right\} \quad (16)$$

The equation (16) is also applicable for the anode by replacing O_2 by H_2 and cat by an .

Where $i_{o,an}$ is the exchange current density for reaction (Am^{-2}), X_{O_2} , X_{H_2} , is the actual concentration of oxygen and hydrogen respectively and X_{O_2-o} , X_{H_2-o} are reference concentration of oxygen in air and hydrogen in fuel, and φ_e is the electronic potential (V), S_a is specific surface area ($\text{m}^2 \text{m}^{-3}$).

The consumption term can be calculated as follows:

$$R_{i,cat} = \frac{Q_{cat} M_{O_2}}{4F} \text{(Oxygen reduction)} \quad (17)$$

$$R_{i,an} = \frac{Q_{an} M_{H_2}}{2F} \text{(Hydrogenoxidation)} \quad (18)$$

$$R_{i,an} = -\frac{Q_{an} M_{H_2O}}{2F} \text{(Water formation)} \quad (19)$$

The exchange current density for the reaction can be computed as follows:

$$i_{o,cat} = \gamma_{cat} \left(\frac{P_{O_2}}{P_{atm}} \right)^{0.25} \exp \left(\frac{-E_{act,cat}}{R_g T} \right) \quad (20)$$

$$i_{o,an} = \gamma_{an} \left(\frac{P_{H_2}}{P_{atm}} \right) \left(\frac{P_{H_2O}}{P_{atm}} \right)^m \exp \left(\frac{-E_{act,an}}{R_g T} \right) \quad (21)$$

Equation (20), (21) were used in several papers [21, 22, 23].

In the electrolyte, the reaction term Q is eliminated and equation (15) can be used for electrolyte:

The electronic conduction at the two electrodes is defined as follows:

$$\nabla(-K_{e,cat} \nabla \varphi_e) = -Q_{cat} \quad (22)$$

And for anode, cat is replaced by an ; the momentum equation for flow in porous media, Darcy's law will be used, which states that the velocity vector is determined by the pressure gradient, the fluid viscosity and the structure of the porous media as follows:

$$\bar{u} = -\frac{K_p}{\mu} \nabla P \quad (23)$$

The Darcy's law application mode combines with continuity equation and equation of state for ideal gas to obtain the following equation

$$\nabla \cdot \left(-\frac{K_p M_i}{\mu R_g T} P \nabla P \right) = 0 \quad (24)$$

The permeability (K_p) of the porous media can be calculated as shown by [24] as follows:

$$K_p = \frac{\varepsilon^3}{5(1-\varepsilon)^2 (3 \times 10^5)^2} \quad (25)$$

3.1 Boundary Conditions

Both of Dirchlit and Neumann boundary conditions at different physics mode will be used in this study as following; Darcy's law boundary conditions

$$P = P_0 \text{ Pressure condition} \quad (26)$$

$$-\frac{K_p}{\mu} \nabla P \cdot n = 0 \quad (27)$$

An impervious or symmetric boundary condition

And equation (27) can be used for specific flow perpendicular to the boundary by substituting the RHS of the equation by u_0

3.2 Maxwell-Stefan equation boundary conditions

$$\omega = \omega_0 \text{ for given mass fraction} \quad (28)$$

$$-n \cdot \left[\rho \omega_k \bar{u} - \rho \omega_k \sum_{l=1}^n \tilde{D}_{kl} \left(\nabla x_l + x_l - \omega_l \right) \right] + D^T \left(\frac{\nabla T}{T} \right) = R_i \quad (29)$$

For given flux; and equation (23) can be used for insulation/symmetry by eliminating R_i

$$-n \cdot \left[-\rho \omega_k \sum_{l=1}^n \tilde{D}_{kl} \left(\nabla x_l + (x_l - \omega_l) \frac{\nabla P}{P} \right) + D^T \left(\frac{\nabla T}{T} \right) \right] \quad (30)$$

For convective flow
Conductive media DC application boundary conditions

$$-n \cdot J = J_n \text{ For inward current flow (31)}$$

$$-n \cdot J = 0 \text{ For electric insulation/no current across the boundary (32)}$$

$$V = V_0 \text{ For electric-potential (33)}$$

4. Results and Discussion

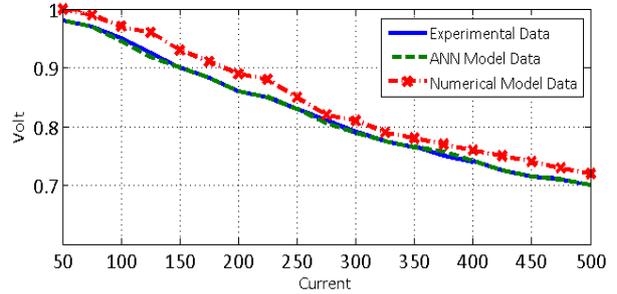
In the proposed work, two layers feed forward neural network with five nodes in hidden layer were employed. Levenberg-Marquardt learning algorithm was used to adjust the network weights provided 19 sampled data with 60% of samples used for training, 20% for testing and 20% for validation. The designed feed forward neural network has one input node representing current density (mA / cm²) and one output node representing voltage.

The proposed NN model was applied to SOFC considering one input (current) and one output which is the voltage. Training process provides a high learning capability with an acceptable ability to model the SOFC system as shown below through Table 1, and figures 1- 4 for cell operating temperatures 750 °C, and 800 °C respectively.

Table 1: MSE of SOFC at different temperatures for both numerical and neural models.

MSE	Numerical	Neural
Voltage at 750 °C	0.00053	0.000064
Voltage at 800 °C	0.000916	0.000096

The best-fit line that can correlate the experimental data to the ANN model data has



correlation factor $R = 0.9996$ at 750°C and $R = 0.9924$ at 800°C respectively. These lines are plotted below in figures 5-6.

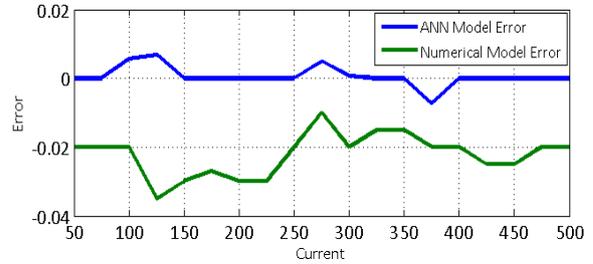


Fig. 1: Numerical profile compared to NN model and experimental model of SOFC voltage at 750 °C.

Fig. 2: Numerical profile error compared to NN model of SOFC voltage at 750 °C.

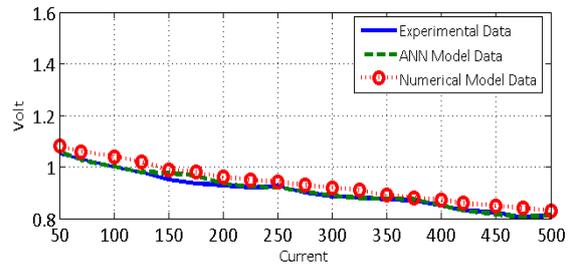


Fig. 3: Numerical profile compared to NN model and experimental model of SOFC voltage at 800 °C.

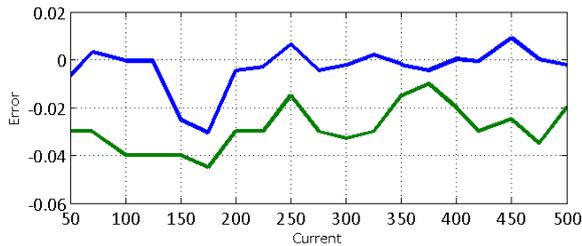


Fig. 4: Numerical profile error compared to NN model of SOFC voltage at 800 °C.

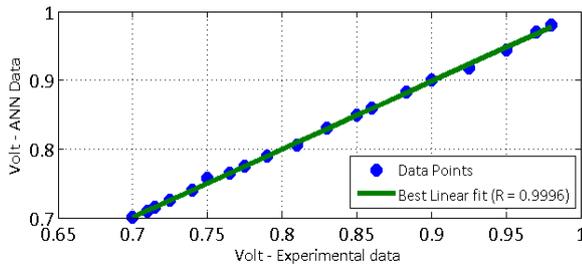


Fig. 5: Best-fit line between Numerical data and ANN model at 750 °C.

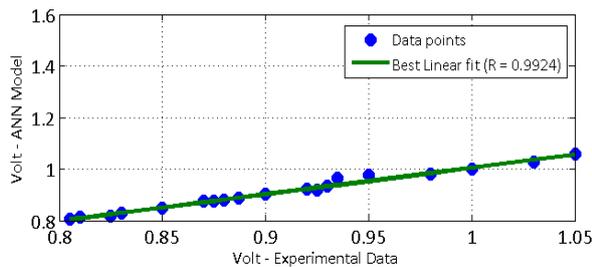


Fig. 6: Best-fit line between Numerical data and ANN model at 800 °C.

It is observed that the proposed NN with Levenberg-Marquardt learning algorithm behaves very well in modeling SOFC at the two temperatures compared to the measured experimental data. Modeling SOFC using suggested Numerical model using FEMLAB 3.1 commercial software showed acceptable performance compared to the experimental data.

The deviation between numerical data and experimental data was due to considering the temperature is constant inside the SOFC.

5. Conclusions

Two layers feed forward neural network was examined for the purpose of modeling the Solid Oxide Fuel Cell (SOFC) to test the reliability of a two dimensional numerical model of SOFC.

The proposed NN model using Levenberg-Marquardt learning algorithm showed high performance in modeling SOFC. However, the suggested numerical model using FEMLAB 3.1 commercial software demonstrated acceptable performance in modeling SOFC and to increase the performance of this model, it is important to consider the energy equation for the SOFC.

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