

Modelling Architecture Parameters Of A Solid Oxide Fuel Cell Using A Hybrid-Artificial Neural Network

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Abstract— An Artificial Neural Network (ANN) can predict and be applied to simulate an object's behavior with no algorithmic solution merely by utilizing available experimental data. The error back-propagation algorithm was used for an ANN training procedure. There are SOFC features that cannot be expressed in numerical form or where numerical expression is difficult to obtain, i.e. electrolyte type, anode type, cathode type etc. In those situations, a hybrid model can be applied. The hybrid model (H-ANN) consists of the ANN model and mathematical expressions. The H-ANN can predict cell voltage with knowledge of minimum physical factors.

Keywords— Solid Oxide Fuel Cell; Hybrid Model; Artificial Neural Network; Architecture Parameters.

I. INTRODUCTION

Fuel cells are very promising technology for power generation in the future due to the direct conversion of fuel into electricity. High temperature fuel cells [4] can be coupled with other devices, such as gas turbines [37, 10, 11, 34, 3] (making a hybrid system), and can be used in poly-generation [23] or even as CO₂ separators [30, 13] in coal fired power plants [27]. Their high working temperatures enable the use of fuels other than pure hydrogen—even biofuels [6, 31]. Solid Oxide Fuel Cells (in contrast to Molten Carbonate Fuel Cells—MCFC [19]) are characterized by electrolyte in solid form [1], allowing a certain flexibility of design.

There are many mathematical models of the solid oxide fuel cell (SOFC) [9, 7, 17, 33,

28, 24, 29]. SOFC performance modeling is related to the multi-physic processes taking place on the fuel cell surfaces. Heat transfer together with electrochemical reactions, mass and charge transport are conducted inside the cell. The SOFC models found in the literature are based mainly on mathematical descriptions of these physical, chemical and electrochemical properties. The SOFC models developed thus far are mainly based on the Nernst equation, activation, ohmic, and concentration losses. Often, most of the equations used require the addition of numerous factors which are difficult or impossible to determine. There are many parameters which impact cell working conditions, e.g. electrolyte material, electrolyte thickness, cell temperature, inlet and outlet gas compositions at anode and cathode, anode and cathode porosity etc.

The Artificial Neural Network (ANN) can be applied to simulate an object's behavior without an algorithmic solution merely by utilizing available experimental data. Moreover, the ANN can make the model more general, which means that the model gives accurate results for other data not used in the training processes.

A description of the development of the ANN for evaluating SOFC performance can be found in [2]. The ANN was trained with a reduced amount of data generated by a physical cell model. No experimental data were taken in the training or validating procedures. A two-layer feed-forward network was trained, and the back-propagation algorithm was utilized. The input parameters were: fuel utilization factor, gas inlet temperature, voltage, and fuel flow; whereas the output parameters were air flow, current density, air outlet temperature, fuel outlet temperature, mean solid temperature and reversible voltage. Those sets of parameters can be used to seek the operating point and system optimization. The potential of ANN utilization to improve the quality of power supply was shown in [21]. The ANN was used to control the SOFC plant in case of systems failure. The influence of the fuel utilization factor on cell voltage was successfully

modeled in [18] by using a least squares support vector machine (LS-SVM). The radial basis function (RBF) neural network based on a genetic algorithm (GA) for establishing a black-box model for the SOFC was shown in [36, 35]. The RBF neural network was a feed-forward neural network with a singular hidden layer. As in [2], the ANN was trained using data generated by the other model previously made by the authors. The network architecture consisted of an input layer with two nodes, a singular hidden layer with three nodes, and an output layer with one node. Validation data were taken from the other model as well. The ANN was used to predict SOFC performances in residential micro-generation installations [14]. The ANN was trained using real data from a 5-kW system with three modes of operation: start-up, steady-state, and shutdown. The input parameters were stack fuel flow, stack temperature, stack air flow, stack air inlet temperature, burner fuel flow, burner combustion temperature, burner air flow, and burner air inlet temperature; whereas there were two output parameters: stack current and stack voltage. Several network architectures were tested to determine the most efficient network structure. Utilization of an ANN trained with real experimental data to simulate single solid oxide fuel cell behaviour is presented in [25, 26]. Fuzzy modeling of the fuel cell based on mutual information between variables is presented in [22]. Modeling and optimization of anode-supported solid oxide fuel cells on cell parameters via artificial neural network and genetic algorithm is presented in [5], whereas a neural network hybrid model of a direct internal reforming solid oxide fuel cell was analyzed in [8].

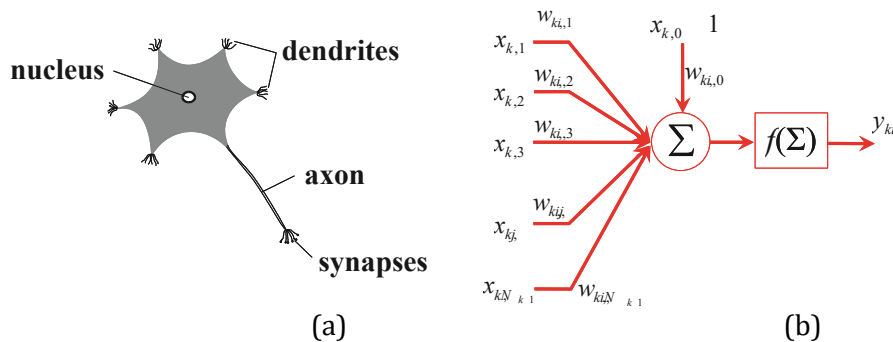


Figure 1: Neuron scheme (a) and its mathematical model (b)

SOFCs are able to operate in reverse mode (i.e. electrolysis), where the neural network was utilized for cathodic process description in [16].

There are SOFC features that cannot be expressed in numerical form or where numerical expression is difficult to obtain, i.e. electrolyte type, anode type, cathode type etc. In those situations, a hybrid model can be applied. The hybrid model consists of the ANN model and mathematical expressions (H-ANN). The H-ANN is able to predict cell voltage with knowledge of minimum physical factors.

This paper focuses on the quality of the modeling of architecture parameters of Solid Oxide Fuel Cell.

II. THEORY

An ANN is a black-box model which produces certain output data as a response to a specific combination of input data. The ANN can be trained to learn the internal relationships and predict system behavior without any physical equations. The ANN consists of neurons gathered into layers. Information is delivered to the neurons by dendrites, and the activation function is realized (by the nucleus). Then modified information is transferred forward by the axon and synapses (see Fig. 1) to other neurons.

Each neuron in the first layer takes the input values, multiplies them by the corresponding weights ($w_{k,i,1}$) and summarizes all these multiplications. Bias ($x_{k,0}$) is added to the sum ($s_{k,i}$). The sum ($s_{k,i}$) is recalculated by the neuron activation function, which gives the neuron answer: $y_{k,i}$.

A hyperbolic tangent sigmoid transfer function was used as the neuron activation function in the first layer, whereas a linear transfer function was used in the output layer (see Fig. 2).

During the model calculations, information proceeds step by step from the first layer to the last one. The answers of the neurons in the last layer are the output parameters of the ANN model (see Fig. 3).

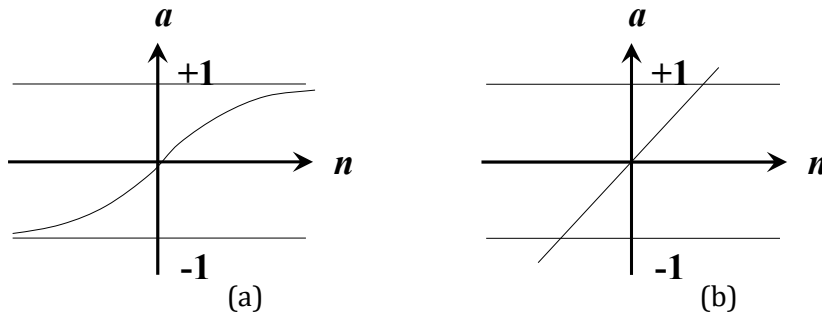


Figure 2: Hyperbolic tangent sigmoid (a) and linear transfer functions (b) [12]

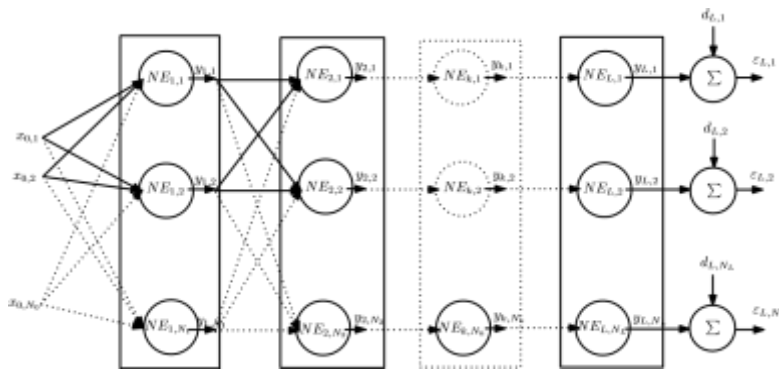


Figure 3: Artificial Neural Network model

Backpropagation was chosen as the learning process of the ANN. Backpropagation is the generalization of the Widrow-Hoff learning rule to multiple-layer networks and nonlinear differentiable transfer functions. A detailed description of backpropagation can be found in [12]. The governing equations of the process are presented below.

$$w_{k,i,j} = x_{k,j} \cdot s_{k,i}$$

$$j=0$$

$$y_{k,i} = f(s_{k,i})$$

$$\varepsilon_{L,i} = d_{L,i} - y_{L,i}$$

$$\delta_{k,i} = \varepsilon_{k,i} \cdot \frac{\partial f(s_{k,i})}{\partial (s_{k,i})}$$

$$w_{k,i,j}^{n+1} = w_{k,i,j}^n + 2 \cdot \eta \cdot \delta_{k,i} \cdot x_{k,j} + \alpha \cdot (w_{k,i,j}^n - w_{k,i,j}^{n-1})$$

where: η —learning rate; α —momentum parameter; for a description of the other

parameters see Fig. 1b and 3.

Commercially available software [12] was used for the ANN calculations. The LevenbergMarquardt algorithm was used to accelerate the training procedure. An overly complex network can be trained with extraordinary accuracy, which means that the network becomes noise dependent (overfitting).

Overfitting means the network has memorized the training examples but has not learned to generalize to new situations. To improve network generalization a network can be used that is just large enough to provide an adequate fit.

The simplest architecture of the network was found in each case to avoid overfitting. If a small enough network is used, it has insufficient power to overfit the data.

Further, optimal regularization parameters were applied in automated fashion (Bayesian). This approach does not require dividing the database into two parts: training and testing. Bayesian regularization makes a model generalized, which is the main advantage of applying this algorithm in the network teaching process. This means that the model can be validated using the same batches of data.

The initial value of the weights of the network was assumed to be 1. The regularization parameters are related to the unknown variances associated with these distributions. Estimation of these parameters can be made using statistical techniques. A detailed discussion of the use of Bayesian regularization, in combination with Levenberg-Marquardt training, can be found in [15]. When using Levenberg-Marquardt training with Bayesian regularization, it is important to let the algorithm run until the effective number of parameters has converged. The training was stopped with the message “Maximum MU reached”. This is typical and is a good indication that the algorithm was truly converged.

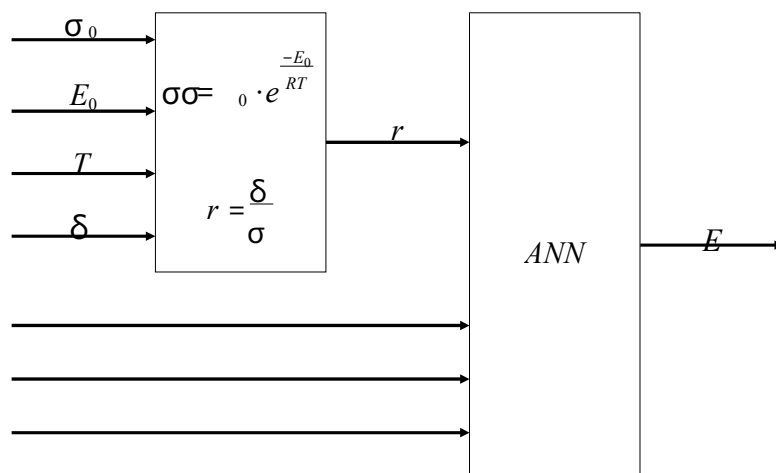


Figure 4: Hybrid-Artificial Neural Network (H-ANN) model

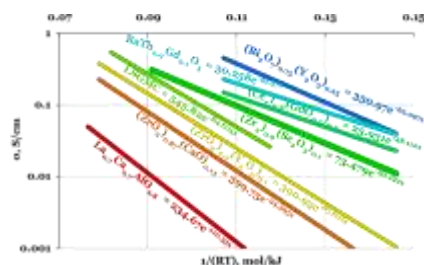


Figure 5: Ionic conductivities of solid oxides

The network architecture is indicated in the following way: “number of inputs–number of neurons in the first layer–number of neurons in the second layer”; e.g. 9–7–1 means that the two-layer network consists of nine inputs, seven neurons in the first layer and one neuron in the second layer (the number of neurons in the last layer equals the number of outputs).

In situations where there is no numerical representation of the inlet values, a hybrid model can be applied. The hybrid model consists of the ANN model and mathematical expressions (see Fig. 4).

A hybrid model combines known relationships and ANN model. The ionic conductivities of solid oxides as adequate equations (see Fig. 4) were applied. Adequate factors for those equations are shown in Fig. 5.

TABLE 1: MAIN PARAMETERS OF EXPERIMENTAL DATA USED FOR TRAINING PROCEDURES

Electrolyte	Temperature, C	800	550-800
	Thickness, m	10	4-20
	Type	YSZ	YSZ/SDC
Anode	Thickness, mm	1.1	0.5-2.45
	Porosity	0.54	0.48-0.76
	Type	n/a	Ni/YSZ
Cathode	Type	LSM	LSC/SDC
	Thickness, m	50	n/a
Area	cm2	1.1	2
Experimental data source		Jiang Y., Virkar A.V. (2003) [20]	Zhao F., Virkar A.V. (2005) [38]

III. EXPERIMENTAL DATA

For training procedures, the experimental data were taken from three papers: [38] (cell architecture variations), [20] (fuel composition variations) and [32] (oxidant composition variations). It was assumed that the experimental results taken from both [20] and [32] were obtained from the same laboratory set. This assumption was made based on analysis of a cell voltage-current density ($E - i$) curve (H_2 /Air, $800^\circ C$), which is presented identically in both papers. The main parameters of the experimental data used for training procedures are listed in Table 1.

IV. MODELING ARCHITECTURE PARAMETERS OF SOLID OXIDE FUEL CELL BY ANN-BASED MODEL

The cell architecture parameters investigated were:

1. temperature,
2. electrolyte thickness,
3. anode thickness,
4. anode porosity,
5. electrolyte type

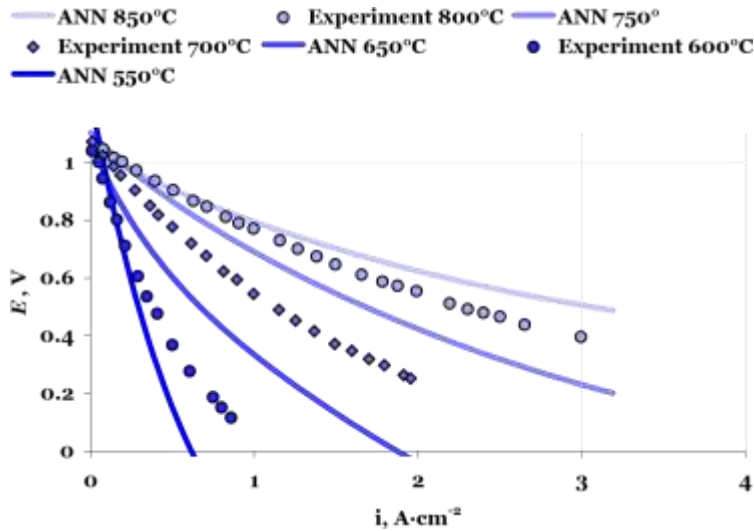


Figure 6: Temperature dependence modelled by the 2-3-1 ANN for experimental data taken from [38]

Temperature dependence on the SOFC performance is modeled by a network which has two input parameters: current density, $A \cdot cm^{-2}$ and cell temperature, $^{\circ}C$. The minimum network architecture for this purpose is 2-3-1, which was taught with relative error of 0.7%. The quality of the model was tested at four temperatures (550 $^{\circ}C$, 650 $^{\circ}C$, 750 $^{\circ}C$, and 850 $^{\circ}C$). The network extrapolates the temperature dependence in a relatively regular way (see Fig. 6).

The electrolyte thickness dependence on solid oxide fuel cell performance is modeled by a network which has two inlet parameters: current density, $A \cdot cm^{-2}$, and electrolyte thickness, m. A 2-3-1 network is the minimum network architecture allowing a reasonable level of relative error (0.7%). Three electrolyte thicknesses were tested to check network modeling quality. In fact, the change in electrolyte thickness has little impact on voltage. Consequently, there is limited impact when testing values of electrolyte thickness. The ANN gives few inaccurate results as regards extrapolation where the model estimates higher voltage for electrolyte thickness of 25 m than for the electrolyte thickness of 20 m (see Fig. 8).

The data given in Fig. 8 are very difficult to judge, thus an additional graph is made to show modeling quality—see Fig. 8. The ANN follows the behavior of SOFC as regards electrolyte thickness.

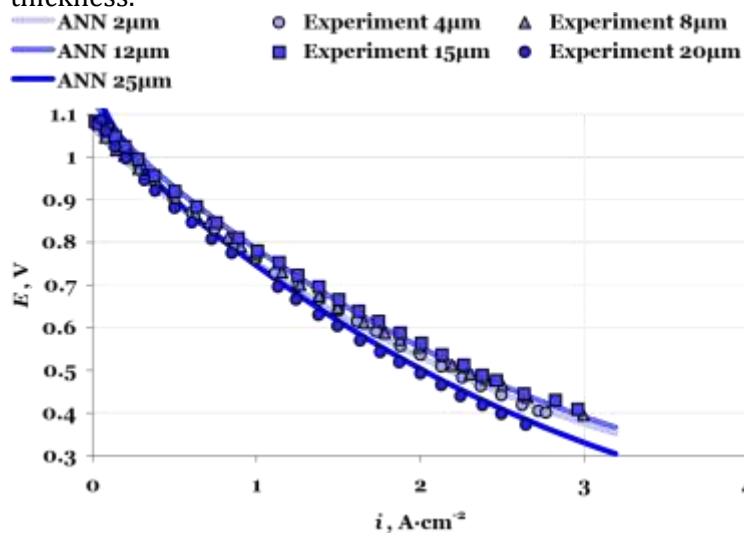


Figure 7: Electrolyte thickness dependence modelled by the 2-3-1 ANN. Experimental data were taken from [38]

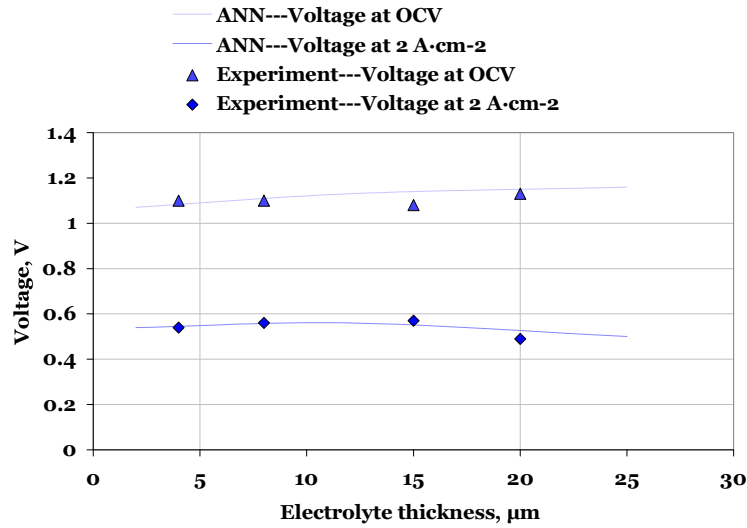


Figure 8: Electrolyte thickness dependence modeled by the 2-3-1 ANN for two current density values: 0 and 2 A·cm⁻²

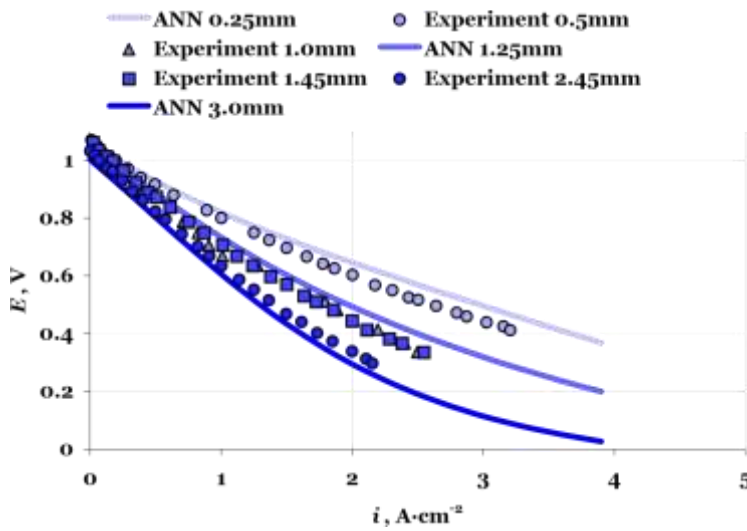


Figure 9: Anode thickness dependence modeled by the 2-2-1 ANN. Experimental data were taken from [38]

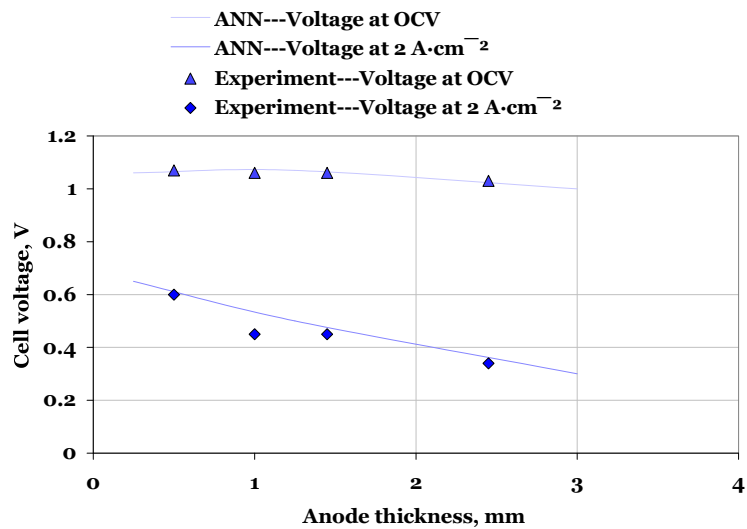


Figure 10: Anode thickness influence for two current density values 0 and 2 A·cm⁻²

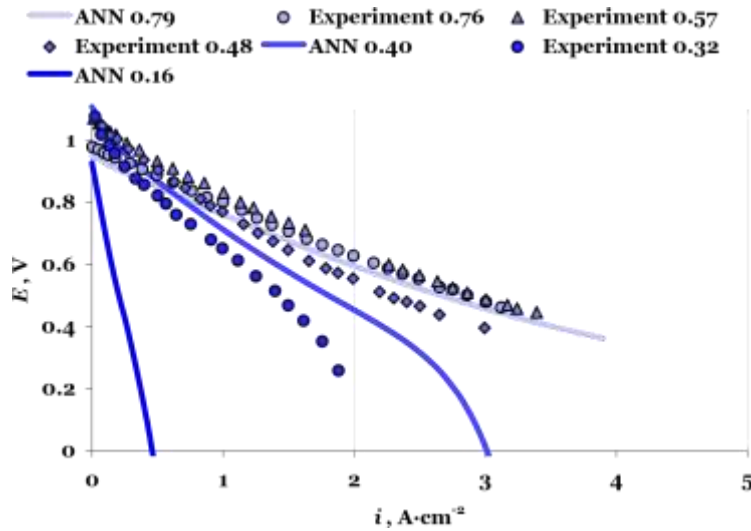


Figure 11: Anode porosity dependence modelled by the 2-5-1 ANN for experimental data taken from [38]

Anode thickness dependence is modeled by a network which has two inlet parameters: current density, $A \cdot cm^{-2}$, and anode thickness, mm. A 2-2-1 network is the minimum network architecture allowing a reasonable level of relative error (0.4%). Three anode thicknesses (0.25, 1.25 and 3.0 mm) were tested to check network modeling quality— see Fig. 9, the network was observed to model the voltages appropriately. This conclusion is also validated by data shown in Fig. 10.

Anode porosity dependence is modeled by a network which has two inlet parameters: current density, $A \cdot cm^{-2}$, and anode porosity. A 2-5-1 network is the minimum network architecture allowing a reasonable level of relative error (0.3%). The network was tested for three anode porosities to check network modeling quality, the network was observed to model the voltage appropriately apart from extrapolated porosity of 0.16—which seems to be too far from the rest of the curves. A better view of porosity influence is presented in Fig. 12.

Electrolyte type is difficult to express in numerical form; thus a hybrid model is applied here. The electrolyte type is modeled by area specific internal resistance:

$$r = \frac{\delta}{\sigma} \quad (1)$$

where: δ —electrolyte thickness, cm; σ —conductivity, S/cm.

Ionic conductivity of solid oxides is shown in Fig. 5 and can be approximated by the following relationship:

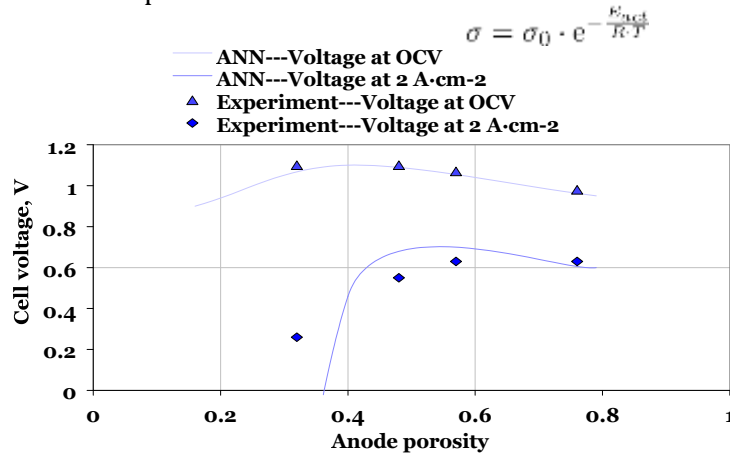


Figure 12: Anode porosity influence at OCV and 2 A·cm-2

where: R —ideal gas constant; T —absolute temperature; σ_0 , E_{act} —factors depend on electrolyte type.

The H-ANN used for modeling electrolyte type is shown in Fig. 4. The trained network was used to generate the SOFC characteristics for two materials which were not used in the training procedures.

The influence of electrolyte material on SOFC performances obtained by the H-ANN is presented in Fig. 13. It should be noted that the experimental data concerns YSZ exclusively. In contrast to YSZ, the other two presented materials were not used during experimental procedures. There is no significant difference between LSGMC and YSZ, which means the network performed incorrectly extrapolation for higher ionic conductivities. With lower ionic conductors, the network gives more realistic values.

In fact, in the H-ANN model, the influence of electrolyte thickness has a similar effect on cell voltage as electrolyte material. From Fig. 8 it can be seen that electrolyte thickness has a very small impact on cell voltage, and this behavior is automatically translated by H-ANN into electrolyte type influence—thereby generating inaccuracies.

V. CONCLUSIONS

The presented results show that an artificial neural network can model the influences of: temperature, electrolyte thickness, anode thickness, anode porosity and electrolyte type. The (H-)ANN generalizes SOFC behaviors across a relatively wide range of conditions.

The network gives results with errors in the range of 0.3% (anode porosity) to 0.7% (electrolyte thickness). That seems comparable to errors in measurements made during experimental procedures.

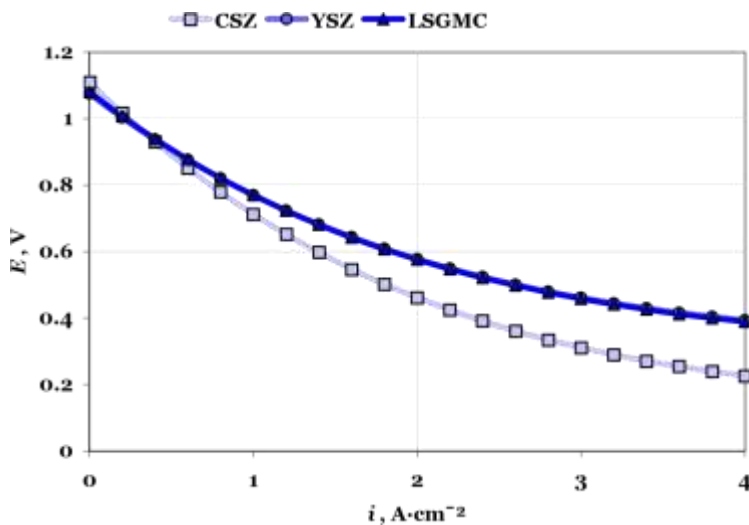


Figure 13: Electrolyte type dependence for three various materials modeled by H-ANN 4-2-1

The relatively low number of neurons used does not allow over-fitting of the network to occur, as is indicated by proper accordance in both: interpolation and extrapolation of the experimental data.

Utilization of (H-)ANNs for modeling the singular SOFC seems to be a promising way to obtain an advanced model of SOFC, as it makes rapid convergences (no iterations) and matches experimental data with little error. The model based on (H-)ANN is very useful for rapid calculation of SOFC, e.g. dynamic simulations, because it does not require iterations during the calculations. An ANN based SOFC model can be used for both cell and system simulations with timeless convergence.

An (H-)ANN based SOFC model gives results that are very close to the experimental data as well as for other working environments. This means that the model predicts SOFC

performances for various working environments. The model can be used in control and monitoring of a real system to predict performance prior to changing any of the control parameters.

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