ELSEVIER

Journal of Power Sources 112 (2002) 54–60

JOURNAL OF POWER SOURCES

www.elsevier.com/locate/jpowsour

Artificial neural network simulator for SOFC performance prediction☆

Jaime Arriagada*, Pernilla Olausson, Azra Selimovic

Department of Heat and Power Engineering, Division of Thermal Power Engineering, Lund University, Box 118, S-221 00 Lund, Sweden

Accepted 31 May 2002

Abstract

This paper describes the development of a novel modelling tool for evaluation of solid oxide fuel cell (SOFC) performance. An artificial neural network (ANN) is trained with a reduced amount of data generated by a validated cell model, and it is then capable of learning the generic functional relationship between inputs and outputs of the system. Once the network is trained, the ANN-driven simulator can predict different operational parameters of the SOFC (i.e. gas flows, operational voltages, current density, etc.) avoiding the detailed description of the fuel cell processes. The highly parallel connectivity within the ANN further reduces the computational time. In a real case, the necessary data for training the ANN simulator would be extracted from experiments. This simulator could be suitable for different applications in the fuel cell field, such as, the construction of performance maps and operating point optimisation and analysis. All this is performed with minimum time demand and good accuracy. This intelligent model together with the operational conditions may provide useful insight into SOFC operating characteristics and improved means of selecting operating conditions, reducing costs and the need for extensive experiments.

Keywords: Fuel cell; Solid oxide fuel cells (SOFC); Artificial neural network (ANN); Neural network; Feed-forward network; Backpropagation

1. Introduction

Solid oxide fuel cell (SOFC) technology is under development for distributed generation (DG) of power at load centres. The SOFC offers high electric efficiencies in excess of 45% (natural gas, full load) for normal cycle operation and over 55% for a combined cycle pressurised SOFC-gas turbine system [1]. An important tool in the fuel cell development is mathematical modelling, which has the capability of predicting the fuel cell performance. To avoid extensive and costly experiments, the fuel cell developers use detailed cell and stack models for economic assessments and development purposes. From the results of the model simulations, conducted for a broad range of operating conditions, performance charts can be constructed. Since these models are rather detailed descriptions of the physical processes and conditions occurring in the fuel cell, they are unnecessarily complex and cumbersome, especially when the goal is operating point analysis and optimisation.

In this work, a statistical data-driven approach, i.e. artificial neural networks (ANNs), is introduced as an alternative to these mathematical models. ANNs are used in a wide range of engineering and non-engineering applications, such as, pattern recognition (spectroscopy, protein analysis, fingerprint identification), as well as behaviour prediction and function approximation (stock market forecasting, energy demand forecasting, process control systems). These methods are inspired by the central nervous system, exploiting features such as high connectivity and parallel information processing, exactly like in the human brain. The characteristic feature of ANNs is that they are not programmed; they are trained to learn *by experience* [6].

In this work, a two-layer feed-forward network has been trained (with the backpropagation (BP) algorithm) to learn the performance parameters in a planar SOFC. The data used during the training has been generated with a validated physical model, which is presented in detail in [2]. In future applications, it is hoped that the data will be available from various fuel cell experiments. However, encouraging results from this study demonstrate that there is a potential to introduce this tool in the development of fuel cells, in order to reduce the calculation time compared with the physical models, and to save time and money in both the

☆ This paper was presented at the Seventh Grove Fuel Cell Symposium held in London between 11 and 13 September 2001.

* Corresponding author. Fax: +46-46-222-4717.
E-mail address: jaime.arriagada@vok.lth.se (J. Arriagada).

PII: S0378-7753(02)00314-2

Nomenclature

e	actual error
E	error function
F	activation or transfer function
H	number of hidden neurons
M	number of input signals
N	number of output signals
w	weight
x	input signal
y	output signal
$\sum$	summation function
Subscripts	
0	bias
h	hidden layer
i	arbitrary node in the input layer
j	arbitrary neuron in the hidden layer
k	arbitrary neuron in output layer
o	output layer

experimental phase and the manufacturing process of these units.

The first part of this paper deals with a general overview of the chosen method, while the second part reports the results of the ANN model applied to the SOFC.

2. Brief description of feed-forward neural networks

An ANN can be regarded as a black box which is able to produce certain output data as a response to a specific combination of input data. By receiving the data for *an existing* system, the ANN can be trained to learn the internal relationships that govern that system, and predict its behaviour without any physical equations. The major advantage of ANNs, compared to traditional polynomial mapping, is that they are able to perform non-linear mapping of multi-dimensional functions [3], i.e. relationships from many inputs to many outputs. The drawback of this technique is that the solution space becomes non-linear as well, containing many solutions and increasing the risk of getting stuck in a non-optimal solution, or local minimum. In any event, once the ANN is trained, there are several techniques for validating it and ensuring its generalisation ability.

Fig. 1 illustrates the structure of a feed-forward multi-layer neural network, which in this case consists of an input layer, a hidden layer and an output layer. The ANN is denominated feed-forward, because the data flow is strictly forward through the entire network.

Each input parameter is indicated by a node in the input layer, and no data processing occurs here, i.e. the input nodes only act as collectors of the input signals ($x_1, \ldots, x_M$). After that, the information is distributed from every input node to every unit in the hidden layer, and it is amplified or debilitated by the synaptic connections between them, i.e. the *weights* (w_{ji}). The pieces of information that arrive at the hidden units are summed up by the summation function, $\sum$, and transformed by the transfer function, F. From the hidden layer, the data is re-distributed and weighted by a new set of weights (w_{kj}), and then passed on to the processing units in the output layer, where the information is summed up and transformed once again, generating the output signals ($y_1, \ldots, y_N$). An extra input equal to unity is fed both to the hidden and the output layers, and its corresponding weight introduces an off-set or bias to the transfer function. The ANN shown in Fig. 1 is a two-layer network, since only two layers have processing units or *artificial neurons*. Eventually, every output can be represented by a generic expression of the inputs, e.g. for a network with M input signals, H neurons in the hidden layer and N outputs:

$$y_k = F_o\left(\sum_{j=0}^{H} w_{kj} F_h\left(\sum_{i=0}^{M} w_{ji} x_i\right)\right) \quad \text{where} \quad k = 1, \ldots, N. \tag{1}$$

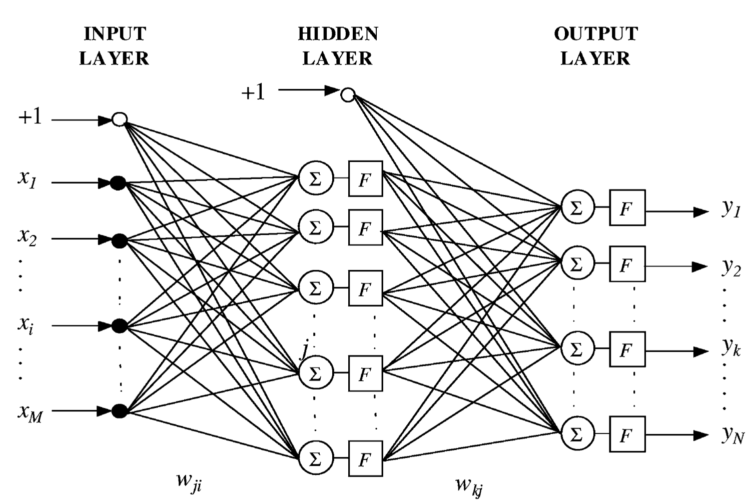

Fig. 1. The feed-forward multi-layer neural network.

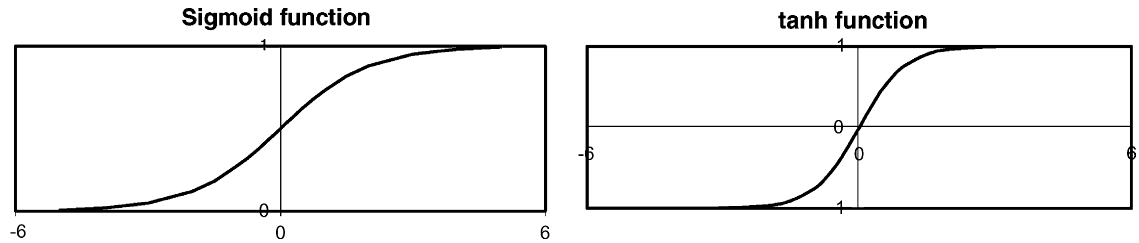

Fig. 2. The sigmoidal transfer functions.

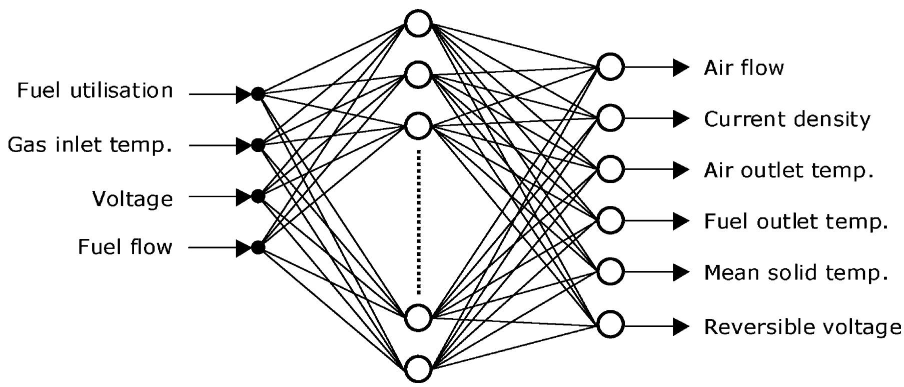

Fig. 3. Neural network for the performance maps of a fuel cell.

In order to be able to store the internal representations of the actual problem in the weights, the ANN must be trained. This is done by feeding the network with a suitable set of training data for which the correct outputs or targets are available. This way of training is called *supervised training*, since the targets are known. The most used method for training multi-layer ANNs is the *backpropagation* algorithm. The BP algorithm was popularised by Rumelhart et al. [5] in 1986, but it was previously proposed by Bryson and Ho in 1969 and Werbos in 1974 [3,4,7].

The idea with the backpropagation algorithm is to send back through the network the errors (e_k) generated, when the actual

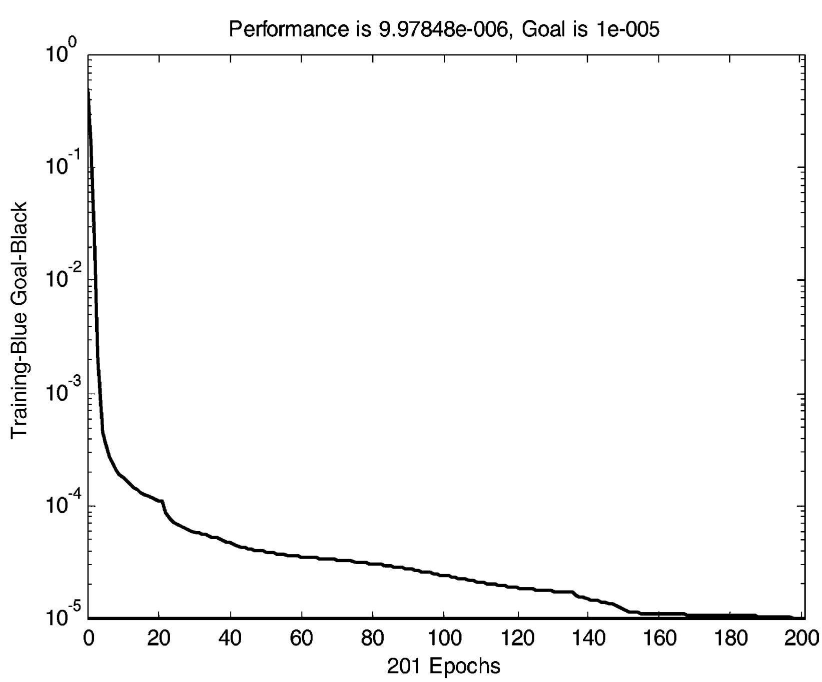

Fig. 4. LMS training error during the learning process.

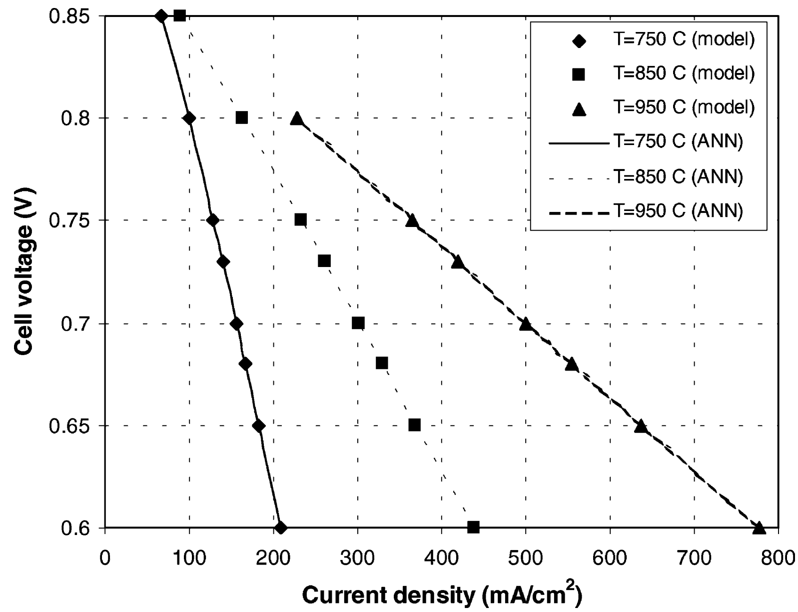

Fig. 5. *I–V* chart for H_2, utilisation = 85% at 5 bar.

output differs from the target. For this reason, a least mean square (LMS) error function, E, is introduced, according to:

$$E = \frac{1}{2}\sum_{k=1}^{N}(e_k)^2. \tag{2}$$

During this procedure, local gradients of E with respect to the weights, i.e. *delta terms*, are calculated, which later can be used for adjusting the old weights. The weights, which at the beginning are random numbers close to zero, are successively updated in the direction of the decreasing error gradient. The major assumption is that the weight correction is proportional to this gradient, with a constant, η, also known as the *learning rate*:

$$\Delta w_{ji} = -\eta \frac{\partial E}{\partial w_{ji}}, \tag{3}$$

$$\Delta w_{kj} = -\eta \frac{\partial E}{\partial w_{kj}}. \tag{4}$$

The BP algorithm requires the use of differentiable transfer functions, because of the calculation of the local gradients, and the most widely used are the *sigmoidal functions* (logistic-sigmoid and tanh-sigmoid) shown in Fig. 2.

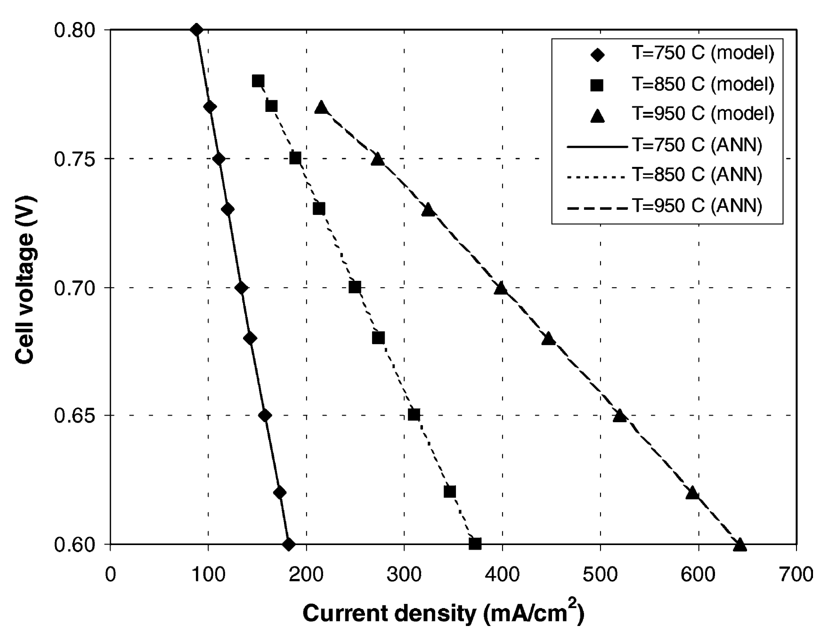

Fig. 6. *I–V* chart for CH_4, utilisation = 85% at 5 bar.

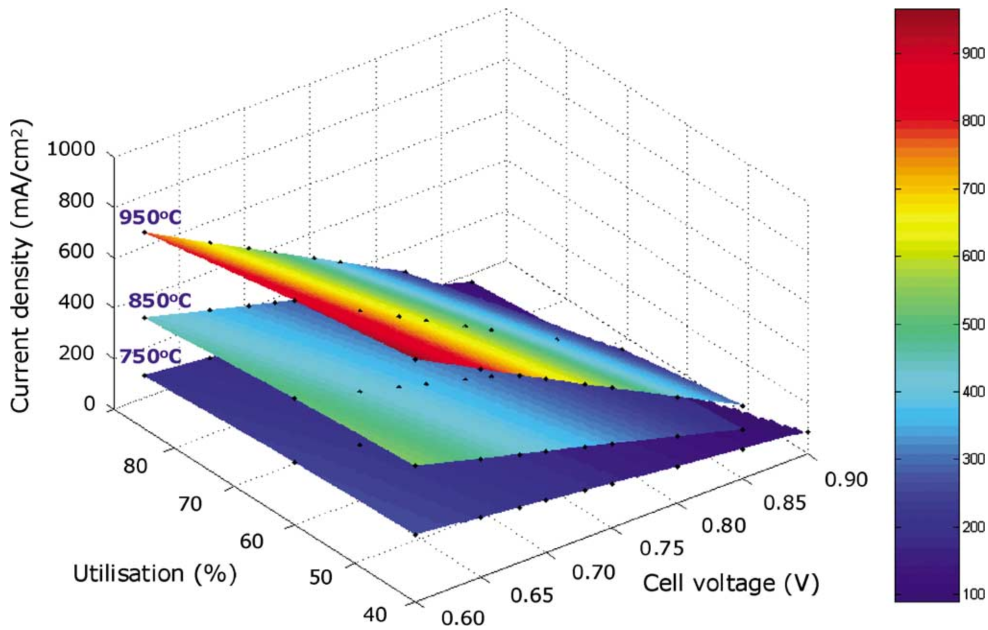

Fig. 7. I–V chart for H_2 fuel, by the ANN model at 5 bar.

3. Creation of the ANN model

3.1. The architecture of the ANN

The artificial neural network used in this study is a two-layer feed-forward network, as shown in Fig. 3. The input parameters are fuel utilisation, gas inlet temperature, voltage and fuel flow. These inputs are passed forward to produce the output parameters, air flow, current density, air outlet temperature, fuel outlet temperature, mean solid temperature and finally the reversible voltage.

To optimise the network, the number of hidden neurons, the number of training epochs and the learning rate are altered during the training phase by a trial-and-error method. A network is produced, which is used for both hydrogen and methane as fuel.

3.2. Data set for training and validation

Since the data on operating fuel cells is not available at the present, a physical SOFC model is used to generate the data required for the training of the ANN-based simulator.

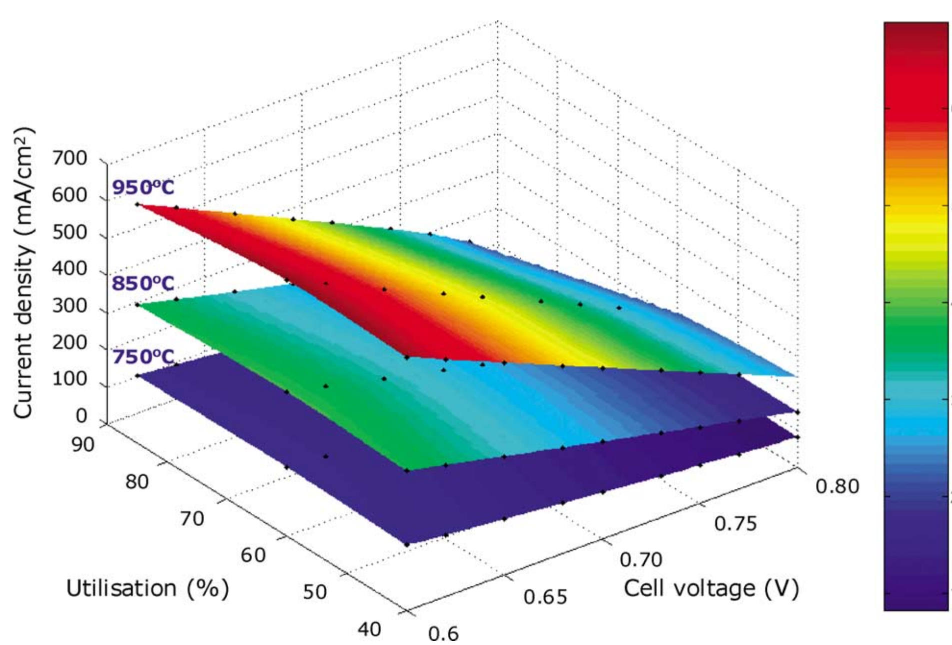

Fig. 8. I–V chart for CH_4 fuel, by the ANN model at 5 bar.

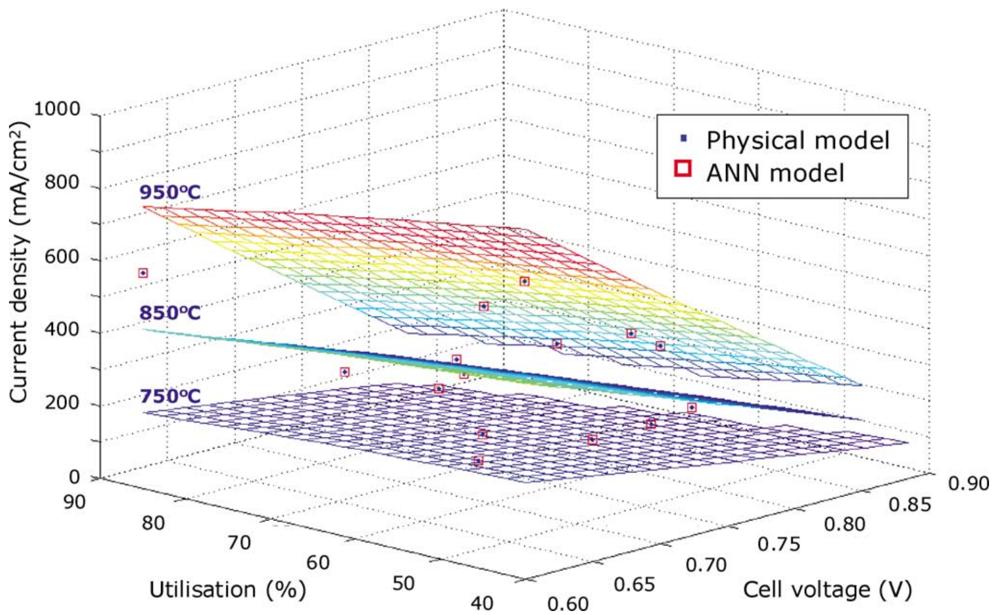

Fig. 9. Prediction of arbitrary operation points by ANN, using H_2 as fuel at 5 bar.

Also the data needed for validation of the simulator will be provided by the mentioned physical model. The physical model is a finite volume element model that has been developed for simulation of a planar SOFC with internal reforming [2]. The model calculates the temperature and current density distribution, the species concentration and the channel flows. This requires the solution of mass balances, chemical species, and energy balances of the gases in the gas channels and the solid structure for each volume element. This two-dimensional, steady-state model was validated against other models by comparing the simulated results obtained for a benchmark test. A standard benchmark test was defined for a flat plate cross-flow design, and the test input conditions have been set up according to IEA Annex II report [1]. The developed model showed good agreement with the other model results.

The physical model was used to calculate approximately eighty different operational cases. Main operational parameters of the cell were varied, such as, operating voltage (0.6–0.90 V), inlet gas temperature (750–950 °C) and gas flows, while the pressure was kept constant at 5 bar. The fuel flow, in each case, is varied in order to obtain the required fuel utilisation (40–85%), while the air flow is tuned to maintain the maximum solid temperature at a desired level. For each inlet gas temperature, the maximum cell temperature

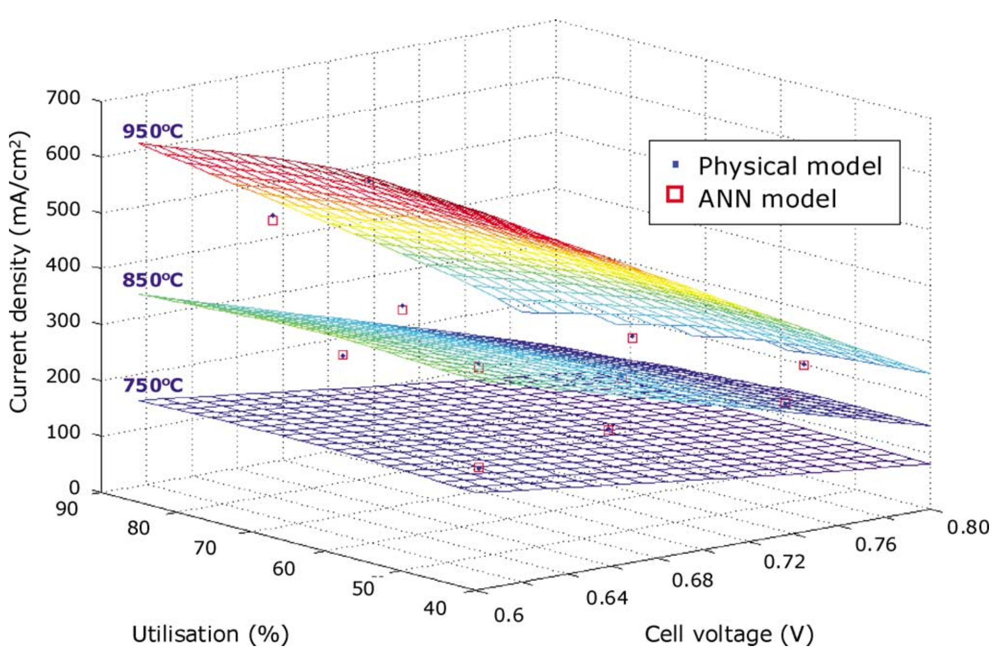

Fig. 10. Prediction of arbitrary operation points by ANN, using CH_4 as fuel at 5 bar.

Table 1
Distribution of error for the different output parameters

	Average error ANN for H_2 (%)	Maximum error ANN for H_2 (%)	Average error ANN for CH_4 (%)	Maximum error ANN for CH_4 (%)
Air flow	0.61	2.82	0.58	3.84
Current density	0.21	0.90	0.17	0.99
Reversible voltage	0.03	0.10	0.02	0.08
Air outlet temperature	0.03	0.20	0.05	0.23
Fuel outlet temperature	0.10	0.42	0.05	0.55
Mean solid temperature	0.09	0.37	0.04	0.15

is set to be constant, 150 °C above the gas inlet temperature. The fuels used when modelling the cell were: (a) hydrogen with 90% by mole H_2 and 10% by mole H_2O and (b) reformed methane with the composition 17.1% by mole CH_4, 26.26% by mole H_2, 49.34% by mole H_2O, 2.94% by mole and 4.36% by mole CO_2. These fuels are further on referred to as H_2 and CH_4, respectively.

3.3. The training process

To be able to produce the correct output data, the network was trained with an improved version of the BP algorithm, i.e. the Levenberg–Marquardt algorithm. Half of the operational points were used to train the ANN, while the other half was used for the validation. During the learning process the error function was minimised with an increasing number of training epochs, as shown in Fig. 4. An epoch is a cycle that is finished when all the available training input patterns have been presented to the network once.

Once the ANN provided a satisfactory output on the validation data set, cross-validation was carried out with a test set (*unseen* data, i.e. new operational points with arbitrary fuel utilisation, voltage and gas inlet temperature). After this final test, the network was ready to generate *I–V* characteristics for a broad range of conditions.

4. Results

The *I–V* characteristics generated by the ANN model showed good consistency with the physical model, as can be seen in Figs. 5–8.

Figs. 5 and 6 show *I–V* characteristics for H_2 and CH_4, respectively, when fuel utilisation is 85%.

When the fuel utilisation is added as an extra variable, three-dimensional *I–V* charts are obtained, showing more complete performance maps of the SOFC. In Figs. 7 and 8, the training and validation points are denoted as black dots, while the result generated by the ANN model is shown as isothermal surfaces. The concordance between both models is clear.

The result of the test with the unseen operational data points is shown in Figs. 9 and 10 later on. It can be stated that the ANN is able to capture the generic relationship between inputs and outputs, even for these arbitrary points.

In addition to the figures given earlier, the average and the maximum discrepancies between the physical model and the ANN model are summarised in Table 1. As can be seen, the most difficult parameter to predict is the air flow, which has a maximum error of 3–4%. The remaining parameters have a maximum error of less than 1%. On the other hand, the average values are all well below 1%.

5. Conclusions

The SOFC model based on an artificial neural network showed a good congruence with the physical model, which was used to generate the training, validation and test data. The average values of the errors are well below 1%, and the maximum errors are below 4%. Besides the numerical accuracy, the ANN model is much faster and easier to use, which makes it suitable for the generation of performance maps. The ANN model showed to be generic to other operational conditions as well.

In the future, this type of statistical model could be trained with data from an experimental set up, and the ANN could be used to predict the different parameters of the SOFC with good accuracy, reducing development costs and the need for extensive experiments.

References

[1] E. Achenbach, SOFC Stack Modelling, IEA Report, 1996.
[2] A. Selimovic, Solid oxide fuel cell modelling for SOFC/gas turbine combined cycle simulations, Thesis for degree of Licentiate in Engineering, ISRN/LUTMDN/TMVK-7039, Lund University, Sweden, 2000.
[3] C.M. Bishop, Neural Networks for Pattern Recognition, Oxford University Press, Oxford, 1995.
[4] Haykin, S., Neural Networks—A Comprehensive Foundation, 2nd Edition, Prentice-Hall, Englewood Cliffs, NJ, 1999.
[5] D. Rumelhart, G. Hinton, R. Williams, Learning internal representations by error propagation, in: D. Rumelhart, J. McClelland (Eds.), Parallel Distributed Processing: Explorations in the Microstructure of Cognition, Vol. 1, MIT Press, Cambridge, MA, 1986, pp. 318–362.
[6] D. Massie, Neural network fundamentals for scientists and engineers, in: Proceedings of ECOS'01, Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems, First International Conference on Applied Thermodynamics, Istanbul, 2001.
[7] S. Russell, P. Norvig, Artificial Intelligence: A Modern Approach, Prentice-Hall, Englewood Cliffs, NJ, 1995.