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Short communication

Nonlinear modeling of a SOFC stack based on a least squares support vector machine

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Abstract

This paper reports a nonlinear modeling study of a solid oxide fuel cell (SOFC) stack using a least squares support vector machine (LS-SVM). SOFC is a nonlinear, multi-input and multi-output system that is hard to model by traditional methodologies. So far, most of the existing models are based on conversion laws, which are very useful for cell design. However, they are too complicated to be applied to control system design. To facilitate a valid control strategy design, this paper tries to avoid the internal complexities and presents a black-box model of the SOFC based on LS-SVM. The simulation tests reveal that it is feasible to establish the model using LS-SVM. At the same time, the experimental comparisons between the LS-SVM model and radial basis function neural network (RBFNN) model demonstrate that the LS-SVM is superior to the conventional RBFNN in predicting stack voltage with different fuel utilizations. Furthermore, based on this black-box LS-SVM model, valid control strategy studies such as predictive control, robust control can be developed.

Keywords: Solid oxide fuel cell (SOFC); Least squares support vector machine (LS-SVM); Radial basis function neural network (RBFNN); Fuel cell modeling

1. Introduction

The solid oxide fuel cell (SOFC) is an energy conversion device that produces electricity by electrochemically combining fuel (e.g. hydrogen) with oxidant (e.g. oxygen) gases across an ionic conducting oxide [1]. SOFC provides many advantages over traditional energy conversion systems including high efficiency, modularity, fuel adaptability and very low levels of NO_x emission. An important tool in fuel cell development is mathematical modeling, which is particularly appropriate for SOFCs, where localized experimental measurements are difficult due to the high operating temperature [2]. The results obtained from a reliable and effective model can be very useful to guide future research for fuel cell improvements and optimization.

It is well known that the SOFC system is sealed, and works in a complicated high-temperature (600–1000 °C) environment. As a nonlinear multi-input and multi-output system, SOFC is hard to model using traditional methodologies. In the last several decades, fruitful results from SOFC stack modeling have been obtained [3–5]. However, most of the existing models that have been developed emphasized the detailed description of cell internal processes, such as mass balances, energy balances and electrochemical kinetics. These models are very useful for cell design, but they are too complicated to be used for a control system design.

To meet the demands of developing valid control strategies, some researchers have attempted to establish novel SOFC models. A black-box identification technique such as the artificial neural network (ANN) has been used to derive a SOFC model from the experimental data quickly [6]. Although this ANN model shows a high accuracy and is much faster and easier to use, its practical design suffers from drawbacks such as the existence of local minima and over-fitting, choice of the number of hidden units, etc. So a new modeling approach is needed to provide a better solution. In this work, a least squares support vector machine (LS-SVM) is presented to establish a black-box model for the SOFC.

LS-SVM proposed by Suykens and Vandewalle [7] is a modification of the standard SVM. Unlike ANN, LS-SVM possesses prominent advantages: over-fitting is unlikely to occur by adopting the structural risk minimization (SRM) principle, and the global optimal solution can be uniquely obtained by solving a

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Nomenclature

b	bias term
e	predictive error
$f(\cdot)$	nonlinear function
I	stack current
$K(x, x_i)$	kernel function
m	lag of the fuel utilization
n	lag of the output voltage
N_0	number of cells in the stack
P	stack dc output power
q_{H_2}	input hydrogen flow rate
q_{O_2}	input oxygen flow rate
T	stack operating temperature
u	fuel utilization
V	stack output voltage
$\hat{V}$	predictive output voltage
w	weight vector
x_i	ith original training datum
x_{max}	maximum of the training data
x_{min}	minimum of the training data
x'	normalized result

Greek letters

α_i	Lagrange multipliers
γ	regularization parameter
σ	kernel width

set of linear equations. A number of structures and algorithms for modeling using LS-SVM have been proposed [8–10]. However, the concrete study of modeling SOFC with LS-SVM cannot be found in prior papers.

This paper is organized as follows. In Section 2, a brief analysis of the characteristics of a SOFC stack is presented. In Section 3, LS-SVM for nonlinear system modeling is explained. In Section 4, Identification structure of a SOFC stack and the detailed processes of training and testing the LS-SVM model are given. In Section 5, conclusions and suggestions for future work are summarized.

2. Description and analysis of SOFC stack

A brief description and analysis of the SOFC stack is given in this section. The reason for establishing a cell voltage–fuel utilization model under different cell currents is also explained.

A SOFC consists of an interconnected structure and a three-layer region composed of two ceramic electrodes, anode and cathode, separated by a dense ceramic electrolyte (often referred to as the PEN, Positive-electrode/Electrolyte/Negative-electrode). In this cell, the oxygen ions formed at the cathode migrate through the ion-conducting solid ceramic electrolyte to the anode/electrolyte interface where they react with the hydrogen and carbon monoxide contained in (and/or produced by) the fuel, producing water and carbon dioxide while liberating electrons that flow back to the cathode/electrolyte interface via

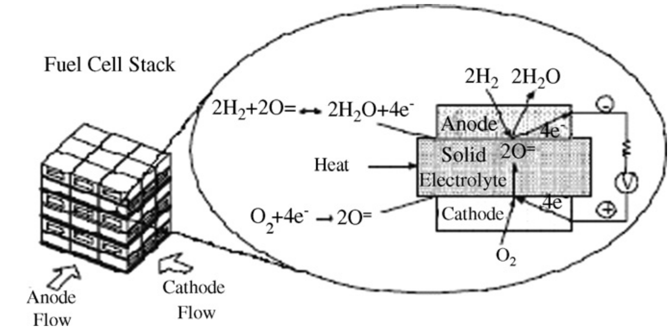

Fig. 1. Single cell and stack of SOFC.

an external circuit [11]. The typical hydrogen fed cross-flow configuration of a SOFC is shown in Fig. 1 [12].

A single cell produces an open-circuit voltage of approximately 1 V. Cells have to be connected together in a series arrangement to form a cell stack that delivers the higher voltages suited to static converters [13].

As we know, cell voltage calculation is the core of any fuel cell modeling. For a given SOFC stack, the output voltage is influenced by many operating parameters such as temperature, pressure, fuel utilization, flow rate, etc. However, due to the high number of operating variables, a complete experimental database of SOFC under the different operating conditions is difficult to obtain and no data are available in the open literature yet [14]. Up to now, almost no model has ever been able to accommodate all these operating variables. Our LS-SVM model is no exception. Fuel utilization is one of the most important operating parameters for a fuel cell and has significant effects on the cell voltage. In order to analyze the effects of different fuel utilizations on output voltage, we chose current, which is determined by the external load, and fuel utilization as variables, while holding other operating parameters constant. Based on the LS-SVM approach, we present a voltage–fuel utilization model under different currents in this paper. Furthermore, like the standard SVM, LS-SVM also has better generalization performance and this ability is independent of the dimensionality of the input data. So our LS-SVM model, obtained with the two variables, can predict stack voltage as precisely as a model considering more variables. Besides, by adding more variables to our LS-SVM model and training it again, the new multi-dimensional model can be obtained easily.

3. LS-SVM for nonlinear system modeling

In the following, we briefly introduce LS-SVM algorithm for nonlinear system modeling, based on [7,15].

Assume a set of training data is given:

$$(x_1, y_1), \ldots, (x_N, y_N) \in R^n \times R \tag{1}$$

The nonlinear function $\psi(\cdot)$ is employed to map the original input space R^n to high dimensional feature space $\psi(x) = (\varphi(x_1), \varphi(x_2), \ldots, \varphi(x_N))$. Then the linear decision function $y(x_i) = w^{\mathrm{T}}\varphi(x_i) + b$ is constructed in this high dimensional feature space. Thus nonlinear function estimation in original space becomes linear function estimation in feature space.

The quadratic loss function is selected in LS-SVM. Then the optimization problem of LS-SVM is formulated as:

$$\min_{w,b,e} J(w, e) = \frac{1}{2}w^{\mathrm{T}}w + \gamma\frac{1}{2}\sum_{i=1}^{N}e_i^2, \quad \gamma > 0 \tag{2}$$

subject to the equality constraints

$$y_i = w^{\mathrm{T}}\varphi(x_i) + b + e_i, \quad i = 1, \ldots, N \tag{3}$$

We construct the Lagrangian as

$$L(w, b, e, \alpha) = J(w, e) - \sum_{i=1}^{N}\alpha_i\{w^{\mathrm{T}}\varphi(x_i) + b + e_i - y_i\} \tag{4}$$

where α_i ($i = 1, \ldots, N$) are the Lagrange multipliers. The conditions for optimality are given by

$$\frac{\partial L}{\partial w} = 0 \to w = \sum_{i=1}^{N}\alpha_i\varphi(x_i), \qquad \frac{\partial L}{\partial b} = 0 \to \sum_{i=1}^{N}\alpha_i = 0,$$

$$\frac{\partial L}{\partial e_i} = 0 \to \alpha_i = \gamma e_i, \quad i = 1, \ldots, N,$$

$$\frac{\partial L}{\partial \alpha_i} = 0 \to y_i = w^{\mathrm{T}}\varphi(x_i) + b + e_i, \quad i = 1, \ldots, N \tag{5}$$

With solution

$$\begin{bmatrix} 0 & 1 & \cdots & 1 \\ 1 & K(x_1, x_1) + 1/\gamma & \cdots & K(x_1, x_N) \\ \vdots & \vdots & \ddots & \vdots \\ 1 & K(x_N, x_1) & \cdots & K(x_N, x_N) + 1/\gamma \end{bmatrix} \begin{bmatrix} b \\ \alpha_1 \\ \vdots \\ \alpha_N \end{bmatrix} = \begin{bmatrix} 0 \\ y_1 \\ \vdots \\ y_N \end{bmatrix} \tag{6}$$

The resulting LS-SVM model for nonlinear system becomes

$$y(x) = \sum_{i=1}^{N}\alpha_i K(x, x_i) + b \tag{7}$$

where α_i, b are the solution to the linear system. Using the normal linear equations program method, we can get the parameters α_i of (6). By the Karush–Kuhn–Tucker (KKT) conditions, the parameter b can be calculated, so the LS-SVM model for nonlinear system can be obtained.

The kernel function $K(x, x_i)$ is any symmetric function that satisfies Mercer's condition. The typical examples of kernel function include linear, polynomial, radial basis function (RBF) kernel.

$$\text{Linear}: \quad K(x_1, x_2) = x_1^{\mathrm{T}}x_2 \tag{8}$$

$$\text{Polynomial}: \quad K(x_1, x_2) = (x_1^{\mathrm{T}}x_2 + 1)^p, \quad p \in N \tag{9}$$

$$\text{RBF}: \quad K(x_1, x_2) = \exp\left(\frac{-||x_1 - x_2||^2}{2\sigma^2}\right) \tag{10}$$

The selection of kernel function needs some knowledge in advance, there is no common conclusion currently. In this paper, the RBF function is used as the kernel function of LS-SVM because RBF kernels tend to give good performance under general smoothness assumptions.

4. Modeling SOFC based on LS-SVM

A LS-SVM can be regarded as a black-box which can produce certain output data as a response to the specific input data. In this modeling procedure, the relationship between input and output of SOFC can be emphasized while the sophisticated inner structure is ignored. In order to establish the expected nonlinear model of SOFC, we choose fuel utilization and cell current as the model inputs, and cell voltage as the output. In the following, identification structure of SOFC stack based on LS-SVM is given firstly, and then the processes of training and testing the LS-SVM model are presented.

4.1. Identification structure of SOFC stack based on LS-SVM

In general, a wide class of nonlinear systems can be described by nonlinear autoregressive model with exogenous inputs (NARX). So in this paper the SOFC nonlinear system with two inputs and one output can be described as follows:

$$V(k + 1) = f[V(k), V(k - 1), \ldots,$$
$$V(k - n), u(k), u(k - 1), \ldots, u(k - m), I(k)] \tag{11}$$

Supposing there is a series of inputs $u(k-m), u(k-m+1), \ldots, u(k), I(k)$ and outputs $V(k-n), V(k-n+1), \ldots, V(k)$, then the corresponding output $V(k+1)$ can be obtained from (11). And providing that

$$X(k) = (V(k), V(k - 1), \ldots, V(k - n), u(k),$$
$$u(k - 1), \ldots, u(k - m), I(k)), \quad k = 1, 2, \ldots, N \tag{12}$$

then

$$V(k + 1) = f(X(k)) \tag{13}$$

We firstly construct the training sample set ($X(k)$, $V(k+1)$), and then the nonlinear sample data can be mapped as the linear outputs in high dimensional feature space by using LS-SVM.

Namely

$$\hat{V}(k + 1) = \sum_{i=1}^{N}\alpha_i K(X(k), X(i)) + b \tag{14}$$

The identification structure of SOFC stack based on LS-SVM is shown in Fig. 2, where TDL is the tapped delay line, and the predictive error $e(k + 1) = V(k + 1) - \hat{V}(k + 1)$.

4.2. Training process of LS-SVM

In general, steps used in training LS-SVM include: training data choosing and preprocessing, selection of the optimal

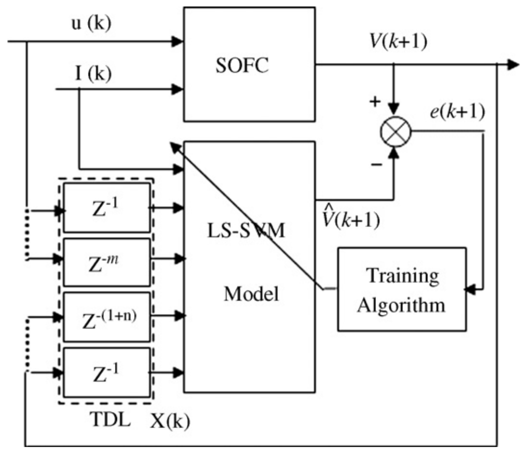

Fig. 2. Identification structure of SOFC stack based on LS-SVM.

LS-SVM parameters, testing data choosing and preprocessing.

4.2.1. Training data choosing and preprocessing

In our study, a mathematical model in [16] is used to generate the data required for the training of the LS-SVM model. The mathematical model has been developed to research the steady-state feasible operating regime of the SOFC. Here three groups of fuel utilization and cell voltage data at 100, 200, and 300 A are chosen as training data, and each group has 101 pairs of data. Main operational parameters of SOFC are varied, such as fuel utilization (0.4–0.9), stack current (100–300 A) and voltage in ranges that correspond to the fuel utilization and stack current as shown in Fig. 3. Some parameters of the SOFC stack used in the LS-SVM modeling are shown in Table 1.

In most cases, all given training data are normalized to [0, 1] or [−1, 1] in order to increase the training speed, facilitate modeling and predicting. In this paper, we normalize each group of training data, including fuel utilization, stack current and voltage, to [0, 1] by

$$x' = \frac{x_i - x_{\min}}{x_{\max} - x_{\min}} \tag{15}$$

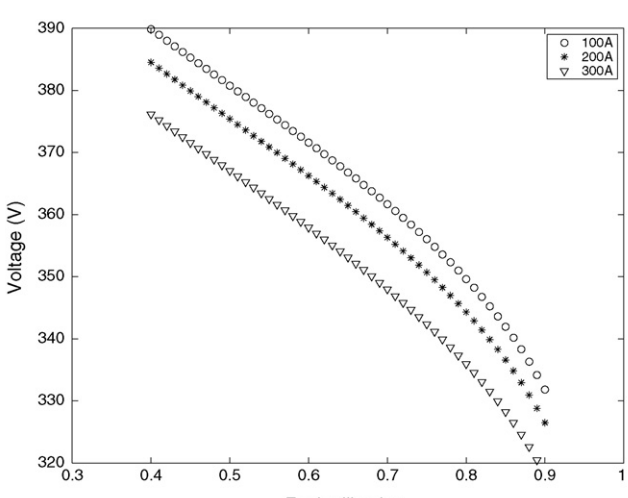

Fig. 3. Training data: stack voltage (V) vs. fuel utilization (u) at 100, 200 and 300 A.

Table 1
Parameters of the SOFC stack used in the LS-SVM modeling

Item	Value
N_0	384
T	1273 K
P	100 kW
I	100–300 A
V	Variable
u	0.4–0.9
q_{H_2}	1.2e−3 kmol/s
q_{O_2}	2.4e−3 kmol/s

4.2.2. Selection of the optimal LS-SVM parameter

The precision and convergence of LS-SVM are affected by regularization parameter γ and kernel width σ. So in order to obtain high level SOFC model, γ and σ in the LS-SVM have to be tuned.

(1) γ, which determines the trade-off between minimizing training errors and minimizing model complexity, is important to increase the generalization performance of LS-SVM model.
(2) σ influences directly the number of initial eigenvalues/eigenvectors. Small values of σ yield a large number of regressors, and eventually it can lead to over-fitting. On the contrary, a large value of σ can lead to a reduced number of regressors, making the model more parsimonious, but eventually not so accurate [17].

Several researchers have presented some methods for determining these two parameters, such as bootstrapping, Bayesian methods and so on. However, most of the available methods can be very expensive in terms of computation time and/or training data. For the industrial application of LS-SVM, there is a need for a fast and robust method to estimate these two parameters. Fortunately, we can rapidly tune these two parameters with a 10-fold cross-validation procedure and a grid search mechanism by LS-SVM toolbox [18]. In the final optimal LS-SVM parameters are: $\gamma = 419.0603$, $\sigma = 0.4080358$.

4.2.3. Testing data choosing and preprocessing

Testing data should be different from the data used for training. If testing data are identical to training data, then the LS-SVM is just interpolating points on a line—which is not what we expect the LS-SVM to do [19]. In our study, the testing data chosen for this work are also provided by the above-mentioned mathematical model in [16]. A group of fuel utilization and stack voltage data at 280 A are chosen as testing data. Preprocessing of testing data is done in the same way as training data.

4.3. Predicting with the LS-SVM model

The criterion of training LS-SVM is to minimize sum squared error (SSE). After training, a LS-SVM model is obtained, which

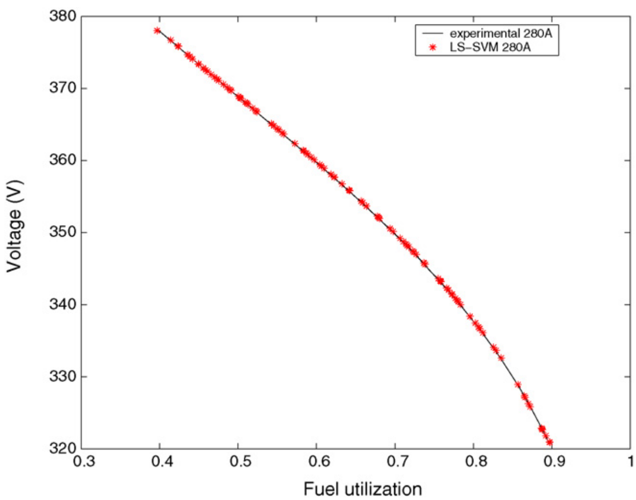

Fig. 4. Voltage–fuel utilization characteristics: predicted by LS-SVM model and experimental at 280 A.

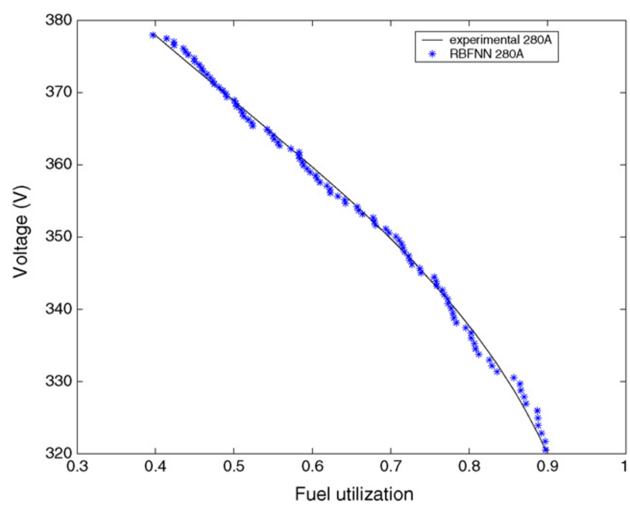

Fig. 5. Voltage–fuel utilization characteristics: predicted by RBFNN model and experimental at 280 A.

can be used to predict new input data. Now the trained LS-SVM model is used to predict stack voltage at 280 A with different fuel utilizations. The comparison of predicted and experimental voltage–fuel utilization curve at 280 A is then made to evaluate the LS-SVM model's prediction precision (as shown in Fig. 4). At the same time, RBFNN model is also used to predict the stack voltage at 280 A, and the predicted result is shown in Fig. 5. From Figs. 4 and 5, we can see the LS-SVM is superior to the conventional RBFNN in predicting stack voltage with different fuel utilizations. These indicate LS-SVM is a powerful tool for modeling SOFC and our LS-SVM model presented in this paper is accurate and valid.

5. Conclusions

To facilitate valid control strategy design, a nonlinear modeling study of SOFC using LS-SVM is reported in this paper. It is shown that the LS-SVM model is more attractive in that it avoids using complicated differential equations to describe the stack, and the input–output characteristics can be achieved quickly by LS-SVM estimation. Besides, the performance of our proposed LS-SVM modeling approach has been tested and compared with the RBFNN approach, and simulation results show that the LS-SVM approach yields higher prediction accuracy compared to the RBFNN approach. These indicate that it is feasible to establish the model of the SOFC by using LS-SVM, and the LS-SVM model presented in this paper is accurate and valid.

In the future, based on this black-box LS-SVM model, some control scheme studies such as predictive control and robust control can be developed. In addition, because better generalization performance of LS-SVM is independent of the dimensionality of the input data, a multi-dimensional LS-SVM model considering other operating parameters can be obtained easily.

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