Modeling the Electrical Conductivity of Anode for Solid Oxide Fuel Cell using Support Vector Regression Machine

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Abstract. The electrical conductivity of Solid Oxide Fuel Cell (SOFC) anode is one of the most important indexes effect the efficiency of SOFC. In order to improve performance of fuel cell systems, it is necessary to have model which modeling the electrical conductivity. In this paper, a model using Support Vector Regression Machine (SVRM) was established to modeling the electrical conductivity of La$_{0.75}$Sr$_{0.25}$Cr$_{0.5}$Mn$_{0.5}$O$_{3-δ}$xCuO (LSCM-xCu) composite anode under two influence factors, including operating temperature ($T$) and Cu content ($x$) in LSCM-xCu composites anode. The test result by SVRM support that the generalization ability of SVRM model is with high accuracy. The mean absolute error (MAE) of 4 test samples is 0.32, mean absolute percentage error (MAPE) is 1.05%, multiple correlation coefficients ($R^2$) is 1.00, which is quite satisfied with the engineering demand. This investigation suggests that SVRM is a powerful tool to be used for optimal designing or controlling the technological process of fuel cell system.

1. Introduction

Solid Oxide Fuel Cell (SOFC) is an environment friendly and higher efficiency electrochemical device. It can directly convert the chemical energy to electrical energy and thermal energy without burning. Due to have virtues such as completely solid component, no causticity, no leak, simple equipment and fuel adaptability, SOFC become a worldwide attention energy source with progressive increase in electrical energy demand and environment consciousness [1-3].

In the last several decades, Artificial Neural Network (ANN) has been used to derive a SOFC model from the experimental data to modeling the performance of SOFC. The ANN has the ability to learn and approach the nonlinear function, and has been considered as a powerful computing tool for establishing the mathematical relationship of the nonlinear system based on the input-output data. But, ANN has the following insurmountable shortcomings: lack of a unified mathematical theory; easy to enmesh local minimization; weakly generalization ability for the small-sample dataset; prone to over-fitting, etc.

As a machine learning method, Support Vector Regression Machine (SVRM), proposed by Vapnik and co-workers in 1995, base on Structural Risk Minimization (SRM) and Vapnik-Chevronenks dimensions principle [4-5]. Research shows that SVRM with many excellences, such as fast-learning, global optimization and excellent generalization ability for the small-sample dataset, are generally superior to ANN model. At the present time, SVRM has been successfully applied to solve modeling problems in numerous fields [6-8].

In this paper, the SVRM model was set up to modeling the electrical conductivity of La$_{0.75}$Sr$_{0.25}$Cr$_{0.5}$Mn$_{0.5}$O$_{3-δ}$xCuO (LSCM-xCu) anode according to the SOFC electrical conductivity.
dataset which was measured under different operating temperature and Cu content in LSCM-xCu composites anode by Z Y Zhang[9].

2. Methods and Materials

2.1. Brief theory of SVRM

In SVRM, the basic idea is to map X from the input space into a higher-dimensional feature space F via a nonlinear mapping function \( \Phi(x) \), and then to conduct linear regression in F space. Therefore, SVRM is to find the linear relation equation (1) based on a given dataset \((x_1, y_1), \ldots, (x_n, y_n)\) [10].

\[
    f(x) = w \cdot \Phi(x) + b, \quad \Phi : R^n \rightarrow F, \quad w \in F.
\]

Where \( w \) is a vector for regression coefficients, \( b \) is a bias. They are estimated by minimizing the regularized risk function \( R(C) \), namely:

\[
    \text{minimize } R(C) = \frac{1}{2} \|w\|^2 + C \sum_{i=1}^{n} L_i(f(x_i) - y_i),
\]

\[
    L_i(f(x_i) - y_i) = \begin{cases} 
    0, & \text{if } |f(x_i) - y_i| < \varepsilon, \\
    |f(x_i) - y_i| - \varepsilon, & \text{if } |f(x_i) - y_i| \geq \varepsilon.
    \end{cases}
\]

Where \( C \) is a regularized factor, \( n \) is the number of training samples, \( \varepsilon \) is a prescribed parameter controlling the tolerance to error, \( (1/2)\|w\|^2 \) is used as a measurement of function flatness. After solved, the regression function (1) has the following explicit form:

\[
    f(x) = \sum_{i=1}^{l} (\alpha_i - \alpha_i^*) k(x, x_i) + b,
\]

(4)

In equation (4), \( k(x, x_i) = \Phi(x) \cdot \Phi(x_i) \) is a kernel function, \( \alpha_i \) and \( \alpha_i^* \) are Lagrange multipliers. Choosing different kernel function can generate different SVRM models. There are four commonly used kernel functions, i.e., radial basis kernel, sigmoid kernel, polynomial kernel, linear kernel, etc. In this paper, the radial basis kernel (5) was utilized:

\[
    k(x, x_i) = \exp(-\gamma \|x - x_i\|^2),
\]

(5)

2.2. Description of the SOFC

The typical structure of a single SOFC is consists of anode, electrolyte membrane and cathode. It is shown in Figure 1[11].

![Figure 1. Schematic of an Individual SOFC](image-url)
The electrochemical reactions at the anode and cathode in a single SOFC are below:

Anode reactions:

\[ 2O_2^- + 2H_2 + 4e^- \rightarrow 2H_2O \]

OR: \[ 4O_2^- + CH_4 + 8e^- \rightarrow 2H_2O + CO_2 \]

\[ O_2^- + CO + 2e^- \rightarrow CO_2 \]

Cathode reactions:

\[ O_2 + 4e^- \rightarrow 2O_2^- \]

Overall reactions:

OR: \[ 2O_2^- + CH_4 \rightarrow 2H_2O + CO_2 \]

\[ O + 2CO \rightarrow 2CO_2 \]

2.3. Dataset

The dataset used in this study was generated by Z Y Zhang. (Reference 9) and is tabulated in Table 1. This dataset includes the electrical conductivity of LSCM-xCu composite anode data for 36 samples in different operating temperatures \( (T \, (^\circ\,C)) \) and Cu contents \( (x = 10, 20, 30, 40 \, (wt\%)) \).

| \( T \, (^\circ\,C) \) | Sample |
|-----------------|--------|
|                 | LSCM-10Cu | LSCM-20Cu | LSCM-30Cu | LSCM-40Cu |
| 400             | 0.0609   | 55.601    | 262.5286  | 1224.223  |
| 450             | 0.0869   | 52.3414   | 246.5688  | 1145.267  |
| 500             | 0.1104   | 48.6229   | 229.5001  | 1069.878  |
| 550             | 0.1506   | 46.0421   | 216.1346  | 1001.864  |
| 600             | 0.2172   | 42.3817   | 201.2089  | 943.8957  |
| 650             | 0.2857   | 40.3967   | 191.0472  | 892.7194  |
| 700             | 0.375    | 38.7124   | 181.8775  | 844.1343  |
| 750             | 0.4798   | 37.1665   | 174.3879  | 808.4111  |
| 800             | 0.5934   | 36.9213   | 173.8623  | 788.618   |

2.4. Modeling and Results

In the SVRM model, the operating temperature and Cu content were employed as input variables, while as the electrical conductivity of LSCM-xCu composite anode as output variable.

Thirty-two samples were randomly selected as training samples, the other four samples numbered acted as the validation samples.
### Table 2. Lists the modeling results by SVRM.

| NO | Input | Output | percentage |
|----|-------|--------|------------|
|    | operating temperature (°C) | Cu contents (wt%) | electrical conductivity (S·cm⁻¹) | modeling results (S·cm⁻¹) | error (%) |
| 1  | 400   | 10     | 0.0609     | 0.060310 | -0.969351   |
| 2  | 400   | 20     | 55.601     | 55.592180| -0.015864   |
| 3  | 400   | 30     | 262.5286   | 262.534083| 0.001936    |
| 4  | 400   | 40     | 1224.223   | 1224.211565| -0.000689   |
| 5  | 450   | 10     | 0.0869     | 0.086393 | -0.813190   |
| 6* | 450   | 20     | 52.3414    | 52.406455| 0.124289    |
| 7  | 450   | 30     | 246.5688   | 246.061492| -0.205828   |
| 8  | 450   | 40     | 1145.267   | 1145.572610| 0.026423   |
| 9  | 500   | 20     | 48.6229    | 48.617810| -0.010468   |
| 10 | 500   | 30     | 1069.878   | 1068.838049| -0.097390   |
| 11 | 500   | 40     | 229.5001   | 229.500935| 0.000407    |
| 12 | 500   | 40     | 1069.878   | 1068.838049| -0.097390   |
| 13*| 550   | 10     | 0.1506     | 0.145001 | -3.717806   |
| 14 | 550   | 20     | 46.0421    | 45.068276| -2.115072   |
| 15 | 550   | 30     | 216.1346   | 214.535319| -0.740130   |
| 16 | 550   | 40     | 1145.267   | 1145.572610| 0.026423   |
| 17 | 500   | 10     | 0.2172     | 0.217249 | -0.000392   |
| 18 | 500   | 20     | 42.3817    | 42.372971| -0.020597   |
| 19 | 500   | 30     | 201.2089   | 201.904130| 0.345477    |
| 20 | 500   | 30     | 229.5001   | 229.500935| 0.000407    |
| 21 | 500   | 40     | 1069.878   | 1068.838049| -0.097390   |
| 22 | 500   | 40     | 943.8957   | 943.892303| -0.000392   |
| 23 | 500   | 40     | 42.3817    | 42.372971| -0.020597   |
| 24 | 500   | 40     | 201.2089   | 201.904130| 0.345477    |
| 25 | 500   | 40     | 844.1343   | 844.132509| -0.000177   |
| 26 | 500   | 40     | 844.1343   | 844.132509| -0.000177   |
| 27*| 700   | 30     | 181.8775   | 181.415941| -0.254049   |
| 28 | 700   | 30     | 181.8775   | 181.415941| -0.254049   |
| 29 | 700   | 30     | 174.3879   | 174.385849| -0.001233   |
| 30 | 700   | 30     | 807.673015 | 807.673015| -0.091288   |
| 31 | 700   | 30     | 807.673015 | 807.673015| -0.091288   |
| 32*| 700   | 30     | 807.673015 | 807.673015| -0.091288   |
| 33 | 800   | 10     | 0.5934     | 0.596312 | 0.490704    |
| 34 | 800   | 20     | 36.9213    | 36.912050| -0.025053   |
| 35 | 800   | 30     | 173.8623   | 173.862195| 0.000112    |
| 36 | 800   | 40     | 788.6168   | 788.611888| -0.000775   |

* Test sample

#### 2.5. Evaluation of Model's Performance

Three indices, mean absolute error (MAE), mean absolute percentage error (MAPE) and multiple correlation coefficients ($R^2$) were adopted for performance evaluation. They are formulated by equations (6), (7) and (8) respectively[12]:

$$MAE = \frac{1}{m} \sum_{j=1}^{m} |\hat{y}_j - y_j|$$

(6)
MAPE = \frac{1}{m} \sum_{j=1}^{m} \frac{\hat{y}_j - y_j}{y_j} \quad (7)

\begin{align*}
R^2 &= \left[ \frac{\sum_{j=1}^{m} (y_j - \bar{y})(\hat{y}_j - \bar{y})}{\sum_{j=1}^{m} (y_j - \bar{y})^2 \cdot \sum_{j=1}^{m} (\hat{y}_j - \bar{y})^2} \right]^2 \quad (8)
\end{align*}

Where \( m \) denotes the number of test samples, \( y_j \) represents the \( j \)th target value, \( \hat{y}_j \) stands for the predicted value for the \( j \)th test sample, \( \bar{y} \) is the mean value of the predicted values \( \hat{y}_j \) (\( j=1 \sim m \)) for test samples.

| Table 3. Performance of SVRM model. |
|--------------------------------------|
| MAE | MAPE (%) | \( R^2 \) |
|--------------------------------------|
| Training samples | 0.21 | 0.33 | 1.00 |
| Test sample | 0.32 | 1.05 | 1.00 |

2.6. Analysis and Discussions

From Table 2, it can be observed that, the maximum percentage error for the 32 training sample's electrical conductivity of LSCM-xCu composite anode(#25) is 3.20%. The number of the training samples, whose percentage error no more than 1% are 30. There are only 2 training sample's percentage error exceed 1%. The maximum percentage error for the 4 test sample's electrical conductivity of LSCM-xCu composite anode(#13) is 3.72%, the rest of test samples under 0.3%.

Table 3 reveals that the MAP of 32 training samples comes up to 0.21, the MAPE is 0.33%, \( R^2 \) as high as 1.00. The MAP of 4 test samples comes up to 0.21, the MAPE is 0.33%, \( R^2 \) reach 1.00 too.

All these results indicate, the performance of SVRM is excellent, it enough to meet the engineering demand.

3. Conclusions

In this study, the SVRM model was established to modeling the electrical conductivity of \( \text{La}_{0.75}\text{Sr}_{0.25}\text{Cr}_{0.5}\text{Mn}_{0.5}\text{O}_3-\delta-x\text{CuO} \) composite anode under two influence factors, including operating temperature (\( T \)) and Cu content (\( x \)) in LSCM-xCu composites anode. The result is revealed that:

(1) For the electrical conductivity of LSCM-xCu composites anode, the effect of operating temperature and Cu content in LSCM-xCu composites anode is complicated.

(2) The SVRM model possesses strong modeling ability. It can predict the electrical conductivity of LSCM-xCu composites anode accurately.

(3) The accuracy of SVRM model is higher enough to meet the demand of engineering.

This study suggests that the SVRM approach is a promising and practical methodology to modeling and simulate the fuel cell system.

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