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Modeling the Electrical Conductivity of $Ni_{1-x}Fe_x$-SDC Composite Anode by Using PSO-SVR

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Abstract. Studies have shown that numerous indexes affecting the electrical conductivity of Solid Oxide Fuel Cell (SOFC) anode. In order to improve performance of SOFC, it is advantageous to have a model with which one can modeling the electrical conductivity at different operating conditions. In this study, a model utilizing support vector regression (SVR) approach combined with particle swarm optimization (PSO), was proposed to modeling the electrical conductivity of $Ni_{1-x}Fe_x(0\leqslant x\leqslant 0.25)$-$Ce_{0.85}Sm_{0.15}O_{2-\delta}$(SDC) composite anode. The test result by PSO-SVR show that the root mean square error (*RMSE*) of test samples is 3.79, mean absolute percentage error (*MAPE*) of test samples is 0.82%, multiplecorrelation correlation coefficients (R^2) of test samples is 1.00, which is satisfied with the engineering demand. The result of this investigation provides that PSO-SVR is an effective tool for modeling the electrical conductivity of $Ni_{1-x}Fe_x$-SDC composite anode.

1. Introduction

Solid Oxide Fuel Cell (SOFC) is a class of fuel cells. It can produces electricity directly from oxidizing a fuel. Advantages of this class of fuel cells include high efficiency, low emissions, completely solid component, fuel adaptability, and relatively low cost [1]. Studies have shown that numerous indexes affecting the electrical conductivity of SOFC anode. In order to improve performance of SOFC, it is advantageous to have a model with which one can modeling the electrical conductivity of SOFC anode at different operating conditions.

As a supervised learning method, Support Vector Regression (SVR) proposed by Vapnik and co-workers. Unlike most of the traditional methods, SVR is a new method of soft sensor modelling based on Statistical Learning Theory (SLT) [2]. Research shows that SVR with many remarkable characteristics, such as fast-learning, resistant to the over-fitting problem, and excellent generalization performance for the small-sample dataset. In the last few years, SVR has been successfully applied to solve modeling problems in fuel cell fields [3, 4].

In this study, the SVR model was proposed to modeling the electrical conductivity of $Ni_{1-x}Fe_x(0\leqslant x\leqslant 0.25)$-$Ce_{0.85}Sm_{0.15}O_{2-\delta}$(SDC) composite anode according to the SOFC electrical conductivity dataset which was measured under different operating temperature and Fe content in $Ni_{1-x}Fe_x$-SDC composite anode by J. P Niu. Particle Swarm Optimization (PSO) is used in this study for searching the best parameter set of SVR for improving the accuracy of the SVR model.

2. Material and methods

2.1. 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[5].

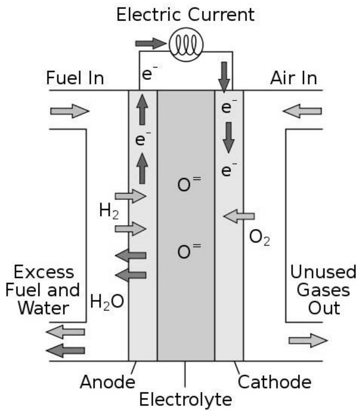

Figure1. Schematic of an Individual SOFC

The electrochemical reactions at the anode in a single SOFC are below:

Anode reactions: $2O^{2-} + 2H_2 - 4e^- \rightarrow 2H_2O$

OR: $4O^{2-} + CH_4 - 8e^- \rightarrow 2H_2O + CO_2$

$O^{2-} + CO - 2e^- \rightarrow CO_2$

2.2. SVR theory [6]

For SVR, 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, SVR is to find the linear relation equation (1) based on a given dataset (x_1, y_1), …, (x_n, y_n).

$$f(\boldsymbol{x}) = \boldsymbol{w} \cdot \boldsymbol{\Phi}(\boldsymbol{x}) + b, \ \boldsymbol{\Phi} : \boldsymbol{R}^n \rightarrow \boldsymbol{F}, \ \boldsymbol{w} \in \boldsymbol{F}. \tag{1}$$

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

$$\text{minimize } R(C) = 1/2\|\boldsymbol{w}\|^2 + C \sum_{i=1}^{n} L_{\varepsilon}(f(\boldsymbol{x}_i) - y_i), \tag{2}$$

$$L_\varepsilon(f(\boldsymbol{x}_i) - y_i) = \begin{cases} 0, & \text{if } |f(\boldsymbol{x}_i) - y_i| < \varepsilon, \\ |f(\boldsymbol{x}_i) - y_i| - \varepsilon, & \text{if } |f(\boldsymbol{x}_i) - y_i| \geq \varepsilon. \end{cases} \tag{3}$$

where C is a regularized factor, n is the number of training samples, ε is a prescribed parameter controlling the tolerance to error. After solved the regression function (1) has the following explicit form:

$$f(\boldsymbol{x}) = \sum_{i=1}^{l} (\alpha_i - \alpha_i^*) k(\boldsymbol{x}, \boldsymbol{x}_i) + b, \tag{4}$$

In equation (4), $k(\boldsymbol{x}, \boldsymbol{x}_i) = \Phi(\boldsymbol{x}) \cdot \Phi(\boldsymbol{x}_i)$ is a kernel function, α_i and α_i^* are Lagrange multipliers. Choosing different kernel function can generate different SVR models. In this paper, the radial basis kernel (5) was utilized:

$$k(\boldsymbol{x}, \boldsymbol{x}_i) = \exp(-\gamma \|\boldsymbol{x} - \boldsymbol{x}_i\|^2), \tag{5}$$

2.3. Choosing of SVR parameters by PSO

PSO is an evolutionary computing technology designed by Kennedy and Eberhart in 1995[7]. It has been applied successfully to various optimization problems.

In this study, PSO was introduced to search the optimal subset (ε, C, γ) of SVR [8]. PSO searches the best parameter subset (ε, C, γ) of SVR by regulating velocity and location of particles. Each particle is made up of a parameter vector (ε, C, γ). The ith particle is looked as a point in the 3D space and represented as $\boldsymbol{u}_i = (u_{i1}, u_{i2}, u_{i3})^T$, its velocity is represented as $\boldsymbol{v}_i = (v_{i1}, v_{i2}, v_{i3})^T$, the position of each particle with its best-fit value that is its local best, is remembered and denoted as $\boldsymbol{p}_{\mathrm{ibest}}$, its global best, which is the position with the best-fit value of all particles, is also recorded as $\boldsymbol{g}_{\mathrm{best}}$. At each iterative process, the velocity and position of each particle was adjusted by tracking its local best value, global best value and its present velocity, their iterative equations are as follows:

$$\begin{aligned}\boldsymbol{v}_i(t+1) = \omega \cdot \boldsymbol{v}_i(t) + c_1 \cdot \mathrm{rand}() \cdot (\boldsymbol{p}_{\mathrm{ibest}} - \boldsymbol{u}_i(t)) + \\ c_2 \cdot \mathrm{rand}() \cdot (\boldsymbol{g}_{\mathrm{best}} - \boldsymbol{u}_i(t))\end{aligned} \tag{6}$$

$$\boldsymbol{u}_i(t+1) = \boldsymbol{u}_i(t) + \boldsymbol{v}_i(t+1) \tag{7}$$

where $\boldsymbol{v}(t)$, $\boldsymbol{v}(t+1)$, $\boldsymbol{u}(t)$, $\boldsymbol{u}(t+1)$ are respectively the speed and position of present moment and the next moment; rand() is a random value between 0 and 1; c_1 and c_2 are both learning factors; ω is a weighting factor to accelerate the convergence rate, its value should be automatically regulated with the iterative time of algorithm extending, defined generally as:

$$\omega = \omega_{\min} + (iter_{\max} - iter) \cdot (\omega_{\max} - \omega_{\min}) / iter_{\max} \tag{8}$$

where $\omega_{\max}$ and $\omega_{\min}$ are the biggest and smallest weighting factors respectively, $iter$ is the number of current iteration. $iter_{\max}$ is the total number of iterations.

2.4. Dataset

The dataset used in this study was generated by J. P Niu [9] and is tabulated in Table 1. This dataset includes the electrical conductivity of $Ni_{1-x}Fe_x$-SDC composite anode for 42 samples in different operating temperatures (T (°C)) and Fe contents (x = 0, 0.05, 0.10, 0.15, 0.20, 0.25). The atomic mole ratio of Ni and Fe is 1:0, 0.95:0.05.0.90:0.10, 0.85:0.15, 0.80:0.20, 0.75:0.25, labeled F0, F1, F2, F3, F4,F5.

Table 1 The electrical conductivity of $Ni_{1-x}Fe_x$-SDC composite anode at different operating temperatures.

T (°C)	Sample					
	F0 δ(S· cm^{-1})	F1 δ(S· cm^{-1})	F2 δ(S· cm^{-1})	F3 δ(S· cm^{-1})	F4 δ(S· cm^{-1})	F5 δ(S· cm^{-1})
500	1448.579	1770.277	1057.153	810.173	858.632	639.792
550	1384.018	1705.553	1022.898	713.234	752.388	569.120
600	1306.730	1644.067	995.233	680.070	679.976	505.219
650	1268.693	1587.272	959.262	659.398	657.491	478.010
700	1213.537	1527.940	930.118	642.612	642.972	468.367
750	1170.925	1485.234	904.463	628.380	631.479	462.814
800	1142.038	1452.910	884.672	617.844	621.775	462.724

2.5. Modeling and results

In the SVR model, the operating temperature and Fe content were employed as input variables, while as the electrical conductivity of $Ni_{1-x}Fe_x$-SDC composite anode as output variable.

Forty samples were selected as training samples, the other two samples numbered acted as the test samples.

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Table 2. The modeling results by PSO-SVR.

NO	Input		Output		
	operating temperature (°C)	Fe contents	electrical conductivity ($S\cdot cm^{-1}$)	modeling results ($S\cdot cm^{-1}$)	percentage error (%)
1	500	0.00	1448.579	1448.5790	0
2	550	0.00	1384.018	1384.0190	0
3	600	0.00	1306.730	1306.7300	0
4	650	0.00	1268.693	1268.6940	0
5	700	0.00	1213.537	1213.5370	0
6	750	0.00	1170.925	1170.9250	0
7	800	0.00	1142.038	1142.0390	0
8	500	0.05	1770.277	1770.2760	0
9	550	0.05	1705.553	1705.5530	0
10	600	0.05	1644.067	1644.0670	0
11	650	0.05	1587.272	1587.2720	0
12	700	0.05	1527.940	1527.9390	0
13	750	0.05	1485.234	1485.2340	0
14	800	0.05	1452.910	1452.9100	0
15	500	0.10	1057.153	1057.1540	0
16	550	0.10	1022.898	1022.8990	0
17	600	0.10	995.233	995.2342	0
18	650	0.10	959.262	959.2632	0
19	700	0.10	930.118	930.1190	0
20	750	0.10	904.463	904.4643	0
21	800	0.10	884.672	884.6732	0
22	500	0.15	810.173	810.1731	0
23	550	0.15	713.234	713.2339	0
24	600	0.15	680.070	680.0700	0
25	650	0.15	659.398	659.3980	0
26	700	0.15	642.612	642.6120	0
27	750	0.15	628.380	628.3803	0
28	800	0.15	617.844	617.8439	0
29	500	0.20	858.632	858.6325	0
30	550	0.20	752.388	752.3883	0
31	600	0.20	679.976	679.9764	0
32	650	0.20	657.491	657.4918	0
33	700	0.20	642.972	642.9728	0
34	750	0.20	631.479	631.4793	0
35	800	0.20	621.775	621.7758	0
36	500	0.25	639.792	639.7921	0
37	550	0.25	569.120	569.1200	0
38	600	0.25	505.219	505.2190	0
39	650	0.25	478.010	478.0104	0
40	700	0.25	468.367	468.3676	0
41*	750	0.25	462.814	466.6071	0.82
42*	800	0.25	462.724	458.9360	-0.82

* Test sample

2.6. Evaluation of model's performance

Three indices, root mean square error (*RMSE*), mean absolute percentage error (*MAPE*) and multiplecorrelation coefficients (R^2) were adopted for performance evaluation. They are formulated by equations. (9), (10) and (11) respectively:

$$RMSE = \sqrt{\frac{1}{m}\sum_{i=1}^{m}(\hat{y}_i - y_i)^2} \tag{9}$$

$$MAPE = \frac{1}{m}\sum_{j=1}^{m}\left|\frac{\hat{y}_j - y_j}{y_j}\right| \tag{10}$$

$$R^2 = \left[\sum_{j=1}^{m}(y_j - \bar{y})(\hat{y}_j - \bar{\hat{y}})\right]^2 \Big/ \sum_{j=1}^{m}(y_j - \bar{y})^2 \cdot \sum_{j=1}^{m}(\hat{y}_j - \bar{\hat{y}})^2 \tag{11}$$

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

Table 3. Performance of PSO-SVR model.

	RMSE	*MAPE* (%)	R^2
Training samples	0.00	0.00	1.00
Test sample	3.79	0.82	1.00

2.7. Analysis and discussions

In this study, the optimal parameter subset (ε, C, γ) of PSO-SVR model were (0.000002, 4238671.400509, 94.790245).

From Table 2, it can be observed that, all the percentage error for the 40 training sample's electrical conductivity of $Ni_{1-x}Fe_x$-SDC composite anode is 0. The percentage error for the 2 test sample's electrical conductivity of $Ni_{1-x}Fe_x$-SDC composite anode is no more than ±1%.

Table 3 reveals that the *RMSE* of 40 training samples is 0, the *MAPE* is 0, R^2 as high as 1.00. The *RMSE* of 2 test samples comes up to 3.79, the *MAPE* is 0.82%, R^2 reach 1.00 too.

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

3. Conclusions

In this study, the PSO-SVR model was established to modeling the electrical conductivity of $Ni_{1-x}Fe_x$-SDC composite anode under two influence factors, including operating temperature (T) and Fe content in $Ni_{1-x}Fe_x$-SDC composites anode. The result is revealed that: the generalization ability of PSO-SVR model is high enough. The PSO-SVR is a promising and practical methodology to modeling the electrical conductivity of $Ni_{1-x}Fe_x$-SDC composite anode.

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