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Prediction of Fe-Co-Mn/MgO Catalytic Activity in Fischer-Tropsch Synthesis Using Nu-support Vector Regression

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Support vector regression (SVR) is a learning method based on the support vector machine (SVM) that can be used for curve fitting and function estimation. In this paper, the ability of the nu-SVR to predict the catalytic activity of the Fischer-Tropsch (FT) reaction is evaluated and the result is compared with two other prediction techniques including: multilayer perceptron (MLP) and subtractive clustering-adaptive neuro-fuzzy inference system (SUB-ANFIS). The Fischer-Tropsch synthesis (FTS) was studied in a fixed bed micro-reactor under different operating conditions. An extensive experimental data set of MgO supported Fe-Co-Mn catalyst was used to predict the FTS. The input variables of three aforesaid models were: reactor temperature, H_2/CO ratio and total pressure, while the CO conversion (catalytic activity) was used as an output variable. Finally, the achieved results from these approaches were compared. The results reveal that the nu-SVR model has more accurate (MSE = 0.0014) than the MLP (MSE = 0.0097) and ANFIS (MSE = 0.0043) approaches.

Keywords: Support vector regression, Fischer-Tropsch (FT) reaction, Multilayer perceptron, Adaptive neuro-fuzzy inference system, Operating conditions

INTRODUCTION

The Fischer-Tropsch synthesis is a chemical process for converting coal-derived syngas (CO and H_2) and natural gas to valuable liquid fuels [1,2]. For this process, the group VIII metals, such as Fe, Co, Ni and Ru are used as a catalyst [1,3]. Mixed-metal catalysts are often used in FTS because of higher activity, selectivity and stability than single component ones [4,5].

Catalyst development and reactor design of the FTS requires a thorough understanding of the behaviors, comprehensive kinetic studies and knowledge of the mechanisms governing this process [6,7]. The rate of synthesis gas consumption depends on the operating conditions, such as temperature, pressure and feed gas composition [2,8].

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Provision of the experimental numerous data requires a significant amount of attempt, time and money. Thus, the experimental work can be improved using some computational methods to interpret the results of studies [9-11]. Powerful computational methods, such as artificial neural networks (ANNs), neuro-fuzzy (NF) systems and support vector machines (SVMs) are common in the modeling of non-linear empirical data with a strong predictive ability [12-14].

A neural network model of a phenomenon (in this research work, the catalytic activity) treats as a 'black-box' without any external information [15]. The common network structure in modeling of complex behaviors is the multilayer perceptron (MLP). The MLP has one or more hidden layers of neurons [16,17]. Several prosperous applications of ANNs in the fields of chemistry and chemical engineering have been reported in the literatures [18-20]. Numerous successful implementations of neural

network modeling on catalyst studies were described by Günay and Yildirim [21,22].

Neural network algorithms have shortcomings, such as difficulty of tuning the network parameters for achieving a proper result, the risk of over-fitting and lack of adaptation [23,24]. Because of these weaknesses, some techniques are developed to improve the neural network model [24].

Among the new methods of modeling, fuzzy systems have a special place. The important point of fuzzy logic is using the human experiment in the modeling. The primary mechanism for doing this model is a list of sentences IF-THEN that are called laws [25,26]. Combined use of fuzzy systems and ANN introduces the adaptive neuro-fuzzy inference system (ANFIS) as a powerful tool for modeling and prediction [26,27].

The SUB-ANFIS combines the ANFIS and the subtractive clustering to improve the learning algorithm. The subtractive clustering considers each data point as a potential cluster center, according to the density of surrounding data points [28,29].

Support vector machines (SVM) are a powerful new technique for solving classification and regression problems. This method was proposed by Vapnik and his co-workers [30-32]. The regression formulation of SVM is based on the structural risk minimization (SRM) principle, so that it has a higher generalization performance than the other conventional algorithms, such as ANN, which implements the empirical risk minimization (ERM) principle in solving many machine learning problems. The SRM minimizes an upper bound on the generalization error while the ERM only minimizes the training error [33-35]. The SVM methods are more flexible than the other conventional algorithms [30]. A review of the basic ideas SVM for regression and function estimation has been given in [36] and the results confirm the preference of SVM. Recently, SVMs [14,37] have been applied to solve nonlinear predicting problems in various fields. In [37], the learning method based on SVM has been applied for predictive modeling in heterogeneous catalysis.

Support vector regression (SVR) is a new learning method based on SVM that can be used for curve fitting and function estimation [38].

The successful applying of ANN, ANFIS, and SVR approaches in modeling, persuaded/motivated us to use these approaches in modeling and data prediction of FTS. The performance of these approaches in data prediction has been compared in a few studies [39-43].

In this study, the FT reaction is carried out upon MgO supported Fe-Co-Mn ternary catalyst prepared using the fusion procedure over the fixed bed micro-reactor. The obtained experimental data of this process are used for modeling the system based on ANN, ANFIS and SVR approaches. In this paper, the ability of the nu-SVR model for prediction of the catalytic activity of the FT reaction is evaluated and the obtained result is compared with two other prediction techniques, MLP and SUB-ANFIS.

In the present research work, at first, the method achieving the kinetic data are explained. Then, the SVR model and data processing are introduced. Finally, the obtained results from SVR model are compared with the other approaches.

EXPERIMENTAL

Catalyst Preparation

The 33% Fe/ 33% Co/ 33% Mn/ 10% wt. MgO catalyst used in this study was prepared using fusion procedure, according to our previous work [44].

Catalyst Testing

The experiments were carried out in a fixed bed stainless steel micro-reactor with a composite catalyst of 1.0 g. A complete description of the reactor setup and analysis method has been reported in our previous works [1,45].

Kinetic Experimental Data

The Fischer-Tropsch reaction was carried out in a fixed bed micro-reactor containing the required amount of MgO supported Fe/Co/Mn catalyst. Prior to synthesis gas exposure, the catalyst was kept in situ pre-reduced at atmospheric pressure using H_2 (30 ml min^{-1}) and N_2 (30 ml min^{-1}) gas mixture at 350 ºC for 14 h. After the reduction, purified H_2, CO and N_2 gases were fed into the reactor. The partial pressures of CO and H_2 were varied. In each test, 1.0 g catalyst was loaded in the middle of reactor and the reactor operated about 12 h to ensure steady state operations were attained. The feed and products were analyzed using an on-line gas chromatography (Thermo ONIX UNICAM

Table 1. The Experimental Conditions and the Obtained Kinetic Results

Run number	T (K)	H_2/CO (molar ratio)	P_{tot} (bar)	X_{co} (%)	Run number	T (K)	H_2/CO (molar ratio)	P_{tot} (bar)	X_{co} (%)
1	523.15	2	10	14.23	37	503.15	2	10	6.47
2	523.15	2	8	14.12	38	503.15	2	8	5.63
3	523.15	2	6	13.02	39	503.15	2	6	11.12
4	523.15	2	4	13.42	40	503.15	2	4	10.23
5	523.15	2	2	8.93	41	503.15	2	2	9.54
6	523.15	2	1	10.24	42	503.15	2	1	6.98
7	523.15	1.5	10	11.37	43	503.15	1.5	10	5.06
8	523.15	1.5	8	11.51	44	503.15	1.5	8	9.23
9	523.15	1.5	6	11.10	45	503.15	1.5	6	10.12
10	523.15	1.5	4	10.67	46	503.15	1.5	4	8.01
11	523.15	1.5	2	10.36	47	503.15	1.5	2	7.67
12	523.15	1.5	1	8.61	48	503.15	1.5	1	5.23
13	523.15	1	10	7.56	49	503.15	1	10	7.26
14	523.15	1	8	8.65	50	503.15	1	8	4.07
15	523.15	1	6	7.98	51	503.15	1	6	7.76
16	523.15	1	4	6.86	52	503.15	1	4	3.78
17	523.15	1	2	6.59	53	503.15	1	2	3.34
18	523.15	1	1	3.51	54	503.15	1	1	2.39
19	513.15	2	10	9.54	55	493.15	2	10	6.13
20	513.15	2	8	14.03	56	493.15	2	8	5.71
21	513.15	2	6	8.63	57	493.15	2	6	4.16
22	513.15	2	4	12.18	58	493.15	2	4	3.21
23	513.15	2	2	8.13	59	493.15	2	2	2.85
24	513.15	2	1	7.86	60	493.15	2	1	2.33
25	513.15	1.5	10	11.72	61	493.15	1.5	10	3.72
26	513.15	1.5	8	10.63	62	493.15	1.5	8	3.31
27	513.15	1.5	6	9.61	63	493.15	1.5	6	3.03
28	513.15	1.5	4	8.84	64	493.15	1.5	4	2.77
29	513.15	1.5	2	7.26	65	493.15	1.5	2	2.51
30	513.15	1.5	1	6.75	66	493.15	1.5	1	2.16
31	513.15	1	10	8.27	67	493.15	1	10	1.87
32	513.15	1	8	7.82	68	493.15	1	8	2.18
33	513.15	1	6	6.72	69	493.15	1	6	1.69
34	513.15	1	4	5.96	70	493.15	1	4	1.48
35	513.15	1	2	6.45	71	493.15	1	2	1.14
36	513.15	1	1	2.72	72	493.15	1	1	0.69

PROGC+) to obtain the kinetic data.

As shown in Table 1, the experimental conditions are ranged from 220-250 ºC for temperature; 1-10 bar for total pressure and 1-2 for H_2/CO ratio. All experiments were carried out at a constant GHSV of 6600 h^{-1} and the catalyst particle size was lower than 0.297 mm.

The catalytic activity is defined as the ability of catalyst to convert input feed to product and is generally expressed by CO conversion in FTS.

METHODOLOGY

Support Vector Regression

Support vector regression (SVR) is an application of SVMs [30,39]. In other words, SVM can be extended to the task of regression with the introduction of an ε-insensitive loss function, called SVR. The ε-insensitive SVR formulation was proposed by Vapnik *et al.* [38]. In contrary to the neural network that tries to define the complex functions of the input space, the initial aim of SVR is the non-linear mapping of data into a higher dimensional feature space using the kernel functions and then using the simple linear functions to make linear decision boundaries in the new space [46]. Assume that a data set of m training samples $\{(x_i, y_i)\}_{i=1,2,...,m}$ is given, where for each input data $x_i \in R^m$, let $y_i \in R$ be the desired output value. The SVR method with the ε-insensitive loss function yields the regression function, $y = f(x)$, which exactly predicts an output value corresponding to a new set of data points. The prediction functions $f(x_i)$ are expanded on a subset of the training data, namely the support vectors (SVs) [39]. According to Fig. 1, the Eq. (1) is assigned to the ε-insensitive loss function. Therefore, the value of $|y - f(x)|_\varepsilon$ for all data should be minimized:

$$|y - f(x)|_\varepsilon = \begin{cases} |y - f(x)| - \varepsilon, & \text{if } |y - f(x)| \geq \varepsilon \\ 0, & \text{otherwise} \end{cases} \quad (1)$$

where ε is the tolerance of error.

Assume that the non-linear regression estimation function $f \to R^n \to R$, is as follows:

$$f(x) = w^t \phi_i(x) + b, \quad (2)$$

where $\phi_i(x)$, w and b are input features, weight vector in the feature space and scalar threshold, respectively. The ε-insensitive SVR formulation is used to calculate w and b coefficients as the solution of the following quadratic programming (QP) problem [30,34,47,48]:

$$\min_{w,b,\varepsilon,\xi_i} = \frac{1}{2} w^t w + C \sum_{i=1}^{m} (\xi_i + \xi_i^*) \quad (3)$$

$$\text{subject to} \quad \begin{cases} w^t \phi(x_i) + b - y_i \leq \varepsilon + \xi_i, \\ y_i - w^t \phi(x_i) - b \leq \varepsilon + \xi_i^*, \\ \xi_i, \xi_i^* \geq 0, \qquad i = 1, 2, ...m \end{cases} \quad (4)$$

where ξ_i and ξ_i^* are slack variables, as illustrated in Fig. 1, and C > 0 and ε > 0 are input parameters. By introducing Lagrange multipliers and exploiting the optimality constraints, the optimization problem in Eq. (3) can be rewritten as [49]:

$$f(x, \alpha_i, \alpha_i^*) = \sum_{i=1}^{m} (\alpha_i - \alpha_i^*) K(x, x_i) + b \quad (5)$$
$$0 \leq \alpha_i^*, \ \alpha_i \leq C, \ i = 1,2,...m$$

where $K(x, x_i)$ is the kernel function, and α_i and α_i^* are Lagrange multipliers which can be calculated by maximizing the dual function of Eq. (5) as follows:

maximize

$$\sum_{i=1}^{m} (\alpha_i - \alpha_i^*) y_i - \varepsilon \sum_{i=1}^{m} (\alpha_i + \alpha_i^*) - \frac{1}{2} \sum_{i,j=1}^{m} (\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*) K(x_i, x_j) \quad (6)$$

under the constraints, $\sum_{i=1}^{m} (\alpha_i - \alpha_i^*) = 0$; $0 \leq \alpha_i \leq C$, i =1,2,…,*m*; $0 \leq \alpha_i^* \leq C$, i =1,2,…,*m*.

Eventually, the estimate of the regression function can be obtained as:

$$f(x) = \sum (\alpha_i - \alpha_i^*) K(x_i, x_j) + b, \text{ for any } x \in R^n \quad (7)$$

Since the mapping ϕ is usually non-linear and unknown, the kernel function, *K*, is used to calculate the legitimate inner product of the two vectors x_i and x_j, in the feature space $\phi(x_i)$ and $\phi(x_j)$, so $K(x_i, x_j) = \phi(x_i) \times \phi(x_j)$.

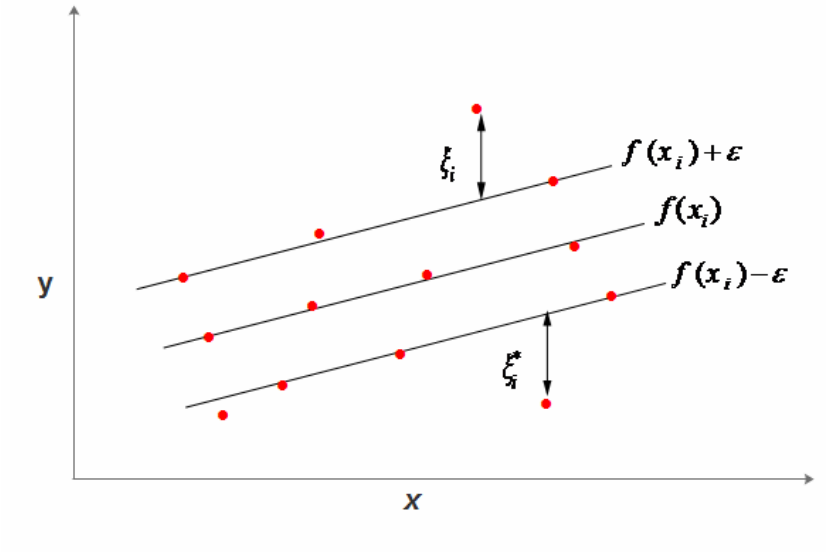

Fig. 1. Graphical depiction of an ε-insensitive loss function and slack variable.

Generally, any valid function satisfying Mercer's condition [49] can be used as the kernel function. Between the kernel functions, Gaussian radial basis function (RBF) is the most commonly used [50]. This function is defined as:
Radial Basis Function (RBF):

$$R(x_i, x_j) = \exp(-\sigma \left\| x_i - x_j \right\|^2) \tag{8}$$

where σ is kernel parameter.

To build an SVR model efficiently, we need to select the regulation parameter *C*, the width of the tube ε and the parameter of the chosen kernel function [42].

In the classical SVR, finding a proper value for the parameter ε to achieve a good performance is a challenge. Nu-support vector regression (nu-SVR), introduced by Schölkopf, is a new class of support vector machine (SVM) [51]. In nu-support vector regression, the problem of finding ε is partially resolved so that ε also becomes a variable in the optimization process and is controlled by the extra term $\nu \in (0,1]$, which tries to minimize ε [39,51]. ν is the upper bound on the fraction of error points and a lower bound on the fraction of points inside the ε -insensitive tube. Thus, a proper ε can be automatically found by selecting ν [36,51]. In this method, the Eq. (3) is modified as follows:

$$\min_{w,b,\varepsilon,\xi_i} = \frac{1}{2} w^t w + C(\nu\varepsilon + \frac{1}{m}\sum_{i=1}^{m}(\xi_i + \xi_i^*)) \tag{9}$$

$$\text{subject to} \quad \begin{cases} w^t\phi(x_i) + b - y_i \le \varepsilon + \xi_i, \\ y_i - w^t\phi(x_i) - b \le \varepsilon + \xi_i^*, \\ \varepsilon, \xi_i, \xi_i^* \ge 0, \quad i = 1,2,...m \end{cases} \tag{10}$$

where $0 \le \nu \le 1$ and C > 0.

By introducing Lagrange multipliers, α_i^*, η_i^* and $\beta \ge 0$, it can be proved that the dual problem changes as follows:
maximize

$$\sum_{i=1}^{m}(\alpha_i^* - \alpha_i)y_i - \frac{1}{2}\sum_{i,j}^{m}(\alpha_i^* - \alpha_i)(\alpha_j^* - \alpha_j)K(x_i, x_j) \tag{11}$$

under the constraints,

$$\begin{cases} \sum_{i=1}^{m}(\alpha_i^* - \alpha_i) = 0, \\ \sum_{i=1}^{m}(\alpha_i + \alpha_i^*) \le C\nu, \\ 0 \le \alpha_i^* \quad , \alpha_i \le \dfrac{C}{m} \quad , i = 1,2,...m \end{cases} \tag{12}$$

where $K(x_i, x_j)$ denotes the matrix of kernel functions

with $K(x_i, x_j) = \phi(x_i)\phi(x_j)$ as kernel function [50]. Finally, the regression estimate can be obtained to take the form

$$f(x) = \sum_{i=1}^{m} (\alpha_i^* - \alpha_i) K(x_i, x) + b \quad (13)$$

Here *b* can be computed by exploiting Karush-Kuhn-Tucker (KKT) conditions [36,52]. This equation is the so-called support vector expansion [34,53].

Data Acquisition and Processing

As mentioned before, the FT reaction performed on the MgO-supported Fe/Co/Mn catalyst under different operating conditions and the obtained data are shown in Table 1. The whole data in FTS were obtained in the physical chemistry and chemical engineering lab.

In this study, an extensive experimental data set of MgO supported Fe/Co/Mn catalyst has been used to develop three approaches, consisting of nu-SVR, ANFIS and MLP, in modeling of FT reaction. The input variables of three approaches are reactor temperature, H_2/CO ratio and total pressure, while the CO conversion (catalytic activity) is used as the output variable. Four data sets, including 72 data in each set are used as the input/output variables of all these approaches. In these modeling approaches, the whole set is separated randomly into training and testing sets, so that 58 (80%) of the whole set of cases and the remaining 14 (20%) are used as training data and testing data, respectively. The testing set is held out during training stage, but it is used to compare the different models [54]. For this purpose, all the input/output variables are normalized in the range of [0.1, 0.9] using the following formula:

$$X_{norm} = 0.8\left(\frac{X_i - X_{\min}}{X_{\max} - X_{\min}}\right) + 0.1 \quad (14)$$

where X_i is the input or output variable X, and X_{min} and X_{max} are the minimum and maximum values of the variable X [55].

All models are created by writing computer codes in MATLAB 8.0.

Evaluation Criteria for Models Performance

Three statistical parameters are used to verify the accuracy o f the models, including coefficient t correlation (R^2), mean square error (MSE), and root-mean-square error (RMSE). The model predictions are in optimum points if the values of R^2 are close to their maximum, as well as MSE and RMSE are close to their minimum. The R^2, MSE and RMSE are calculated from the following equations:

$$\text{Coefficient Correlation } (R^2) = 1 - \frac{\sum_{i=1}^{N} (X_{i,pred} - X_{i,\exp})^2}{\sum_{i=1}^{N} (X_{i,pred} - \bar{X})^2} \quad (15)$$

$$\text{Mean Square Error (MSE)} = \frac{\sum_{i=1}^{N} (X_{i,pred} - X_{i,\exp})^2}{N} \quad (16)$$

$$\text{Root Mean Square Error (RMSE)} = \sqrt{\frac{\sum_{i=1}^{N} (X_{i,pred} - X_{i,\exp})^2}{N}} \quad (17)$$

RESULTS AND DISCUSSION

Computational Results

Support vector regression (SVR) for prediction of CO conversion. The SVR model is used to develop the prediction of catalytic behavior in the FT reaction. First, input data, consisting of T, P_{tot}, and H_2/CO ratio, are fed to the training model. These input data are mapped into a feature space by the map function ϕ. Then, using the kernel function dot products are computed with the images of the training samples under the map ϕ. The weights in the SVR represent the knowledge acquired from the data [43]. The final prediction (output variable) is obtained from Eq. (13). Figure 2 shows the general architecture of SVR model used in this study [43].

The SVR model is prepared with the package LIBSVM [56]. Type of kernel function has a significant effect on the accuracy of the model. In this work, the SVR modeling is accomplished using Laplacian and inverse distance kernel functions [57] through the routine nu-SVR. These functions used are defined as follows:

Laplacian: $$R(x_i, x_j) = \exp(-\sqrt{\sigma} \times \left\| x_i - x_j \right\|) \quad (18)$$

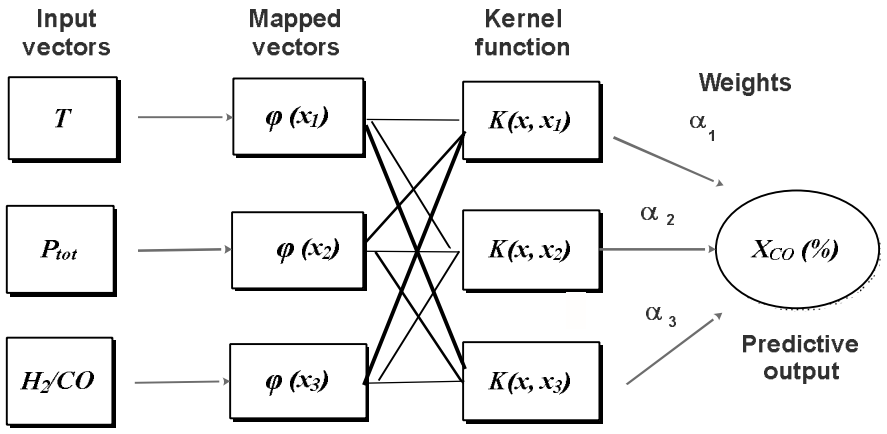

Fig. 2. Training scheme of the SVR model [43].

Table 2. Optimal Parameters for nu-SVR Model

Kernel function	C	*v*	σ
Laplacian	30	0.7	3.536
Inverse Distance	30	0.7	3.608

Inverse Distance: $R(x_i, x_j) = \frac{1}{(\sqrt{\sigma}\|x_i - x_j\| + 1)}$ (19)

where σ is the kernel parameter. Three optimal parameters *v*, C and σ, of this model are given in Table 2.

Performances of nu-SVR model for prediction of experimental CO conversion values in training and testing stages are depicted in Figs. 3 and 4, respectively. The obtained results from the nu-SVR model are shown in Table 3. The MSE values for training and testing stages represent a high correlation between experimental and predicted results.

Multilayer perceptron (MLP) neural network for prediction of CO conversion. In this section, a feed forward neural network (with two hidden layers) based on the back propagation learning rule is used to predict the CO conversion (X_{co}) in FTS. As well as SVR model, the MLP neural network has three input neurons (temperature, H_2/CO ratio and pressure) and one output neuron (CO conversion). The number of neurons in the two hidden layers is adjusted to create the best fit. Using trial and error method [58], and changing the initial parameters, an MLP model architecture with 8 and 6 neurons in hidden layers provides the best prediction of the CO conversion in terms of MSE. In this network, the hyperbolic tangent transfer function (tansig) at two hidden layers and linear transfer function (purelin) at output layer are used as activation function, while the delta rule is employed as the error correcting rule [21,58]. The Levenberg-Marquardt (LM) optimization algorithm is used for network training [59]. The experimental data used for training and testing of the network are presented in Table 1. The training data set including three inputs, and its corresponding experimental output (target) are presented to the network. The learning algorithm adjusts the weights, so that the output responses to input values are close to the target. To evaluate the performance, network outputs are

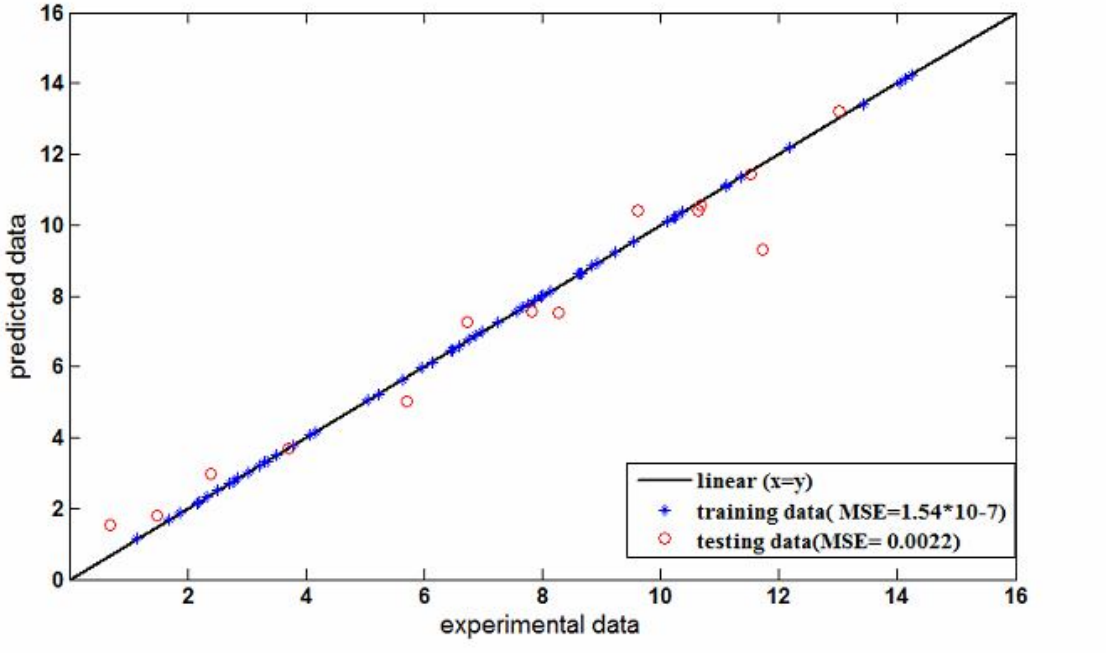

Fig. 3. Experimental *vs.* predicted CO conversions obtained by the nu-SVR model with Laplacian kernel function for training and testing stages.

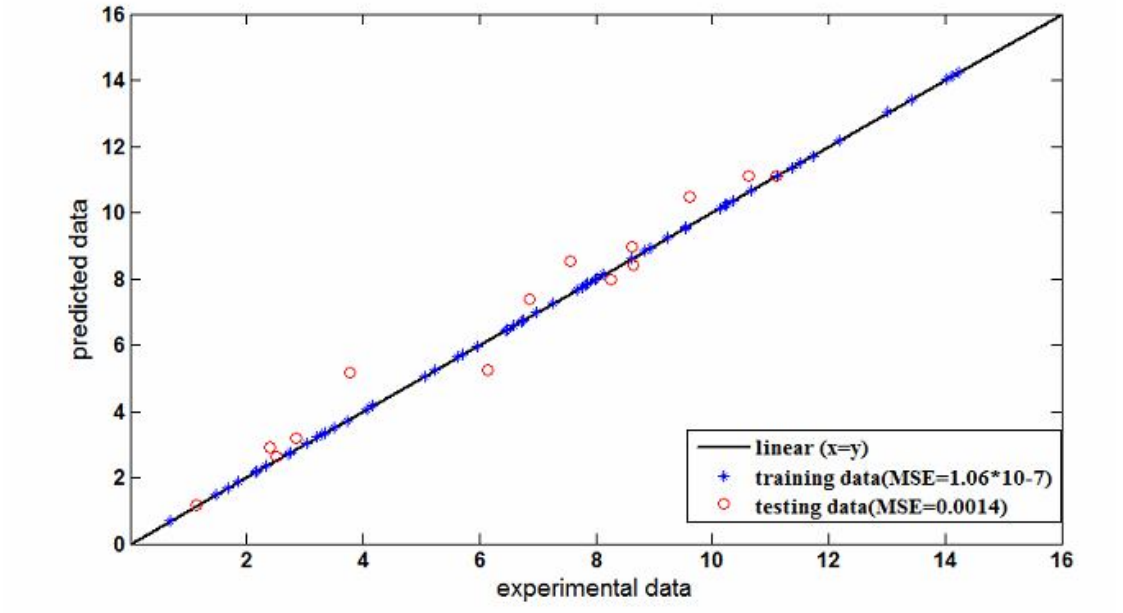

Fig. 4. Experimental *vs.* predicted CO conversions obtained by the nu-SVR model with Inverse Distance kernel function for training and testing stages.

Table 3. Obtained Results from nu-SVR Model for Prediction of CO Conversion

Approach	Kernel function	Training set			Testing set		
		MSE	RMSE	R^2	MSE	RMSE	R^2
nu-SVR	Laplacian	1.54×10^{-7}	3.9×10^{-4}	1.0	0.0022	0.047	0.96
	Inverse Distance	1.06×10^{-7}	3.2×10^{-4}	1.0	0.0014	0.037	0.97

Table 4. Obtained Results from ANN Model for Prediction of CO Conversion

Approach	Training set			Testing set		
	MSE	RMSE	R^2	MSE	RMSE	R^2
ANN	0.0074	0.086	0.85	0.0097	0.098	0.81

Table 5. Obtained Results from ANFIS Model for Prediction of CO Conversion

Approach	Training set			Testing set		
	MSE	RMSE	R^2	MSE	RMSE	R^2
ANFIS	6.89×10^{-32}	2.62×10^{-16}	1.0	0.0043	0.065	0.88

compared with the targets. The results for training and testing data are presented in Table 4. The MSE values for training and testing stages are 0.0074 and 0.0097, respectively. Also, scatter diagram of MLP predicted data *vs*. experimental data for training and testing stages is shown in Fig. 5. It shows that the predictions of the MLP model fit relatively well with the experimental data.

Adaptive neuro-fuzzy inference system (ANFIS) for prediction of CO conversion. In this section, ANFIS network is used to predict the CO conversion (X_{co}) in FTS. ANFIS performances depend intensively on the choice of the available data set including input/output variables, and the domain used for training purposes [60].

The structure of ANFIS network contains three input variables and one output variable of the FT reaction. The fuzzy interference system (FIS) is created using sub-clustering technique (is called SUB-ANFIS) [29]. The SUB-ANFIS model is made using 58 rules and cluster radius is 0.15. The hybrid learning algorithm, that is a combination of the least-squares method and the back-propagation gradient descent method, is applied to update parameters of ANFIS [61]. Up to 50 epochs are specified for training process to assure the gaining of the minimum error tolerance.

The prediction performance of ANFIS model for experimental CO conversion values in training and testing

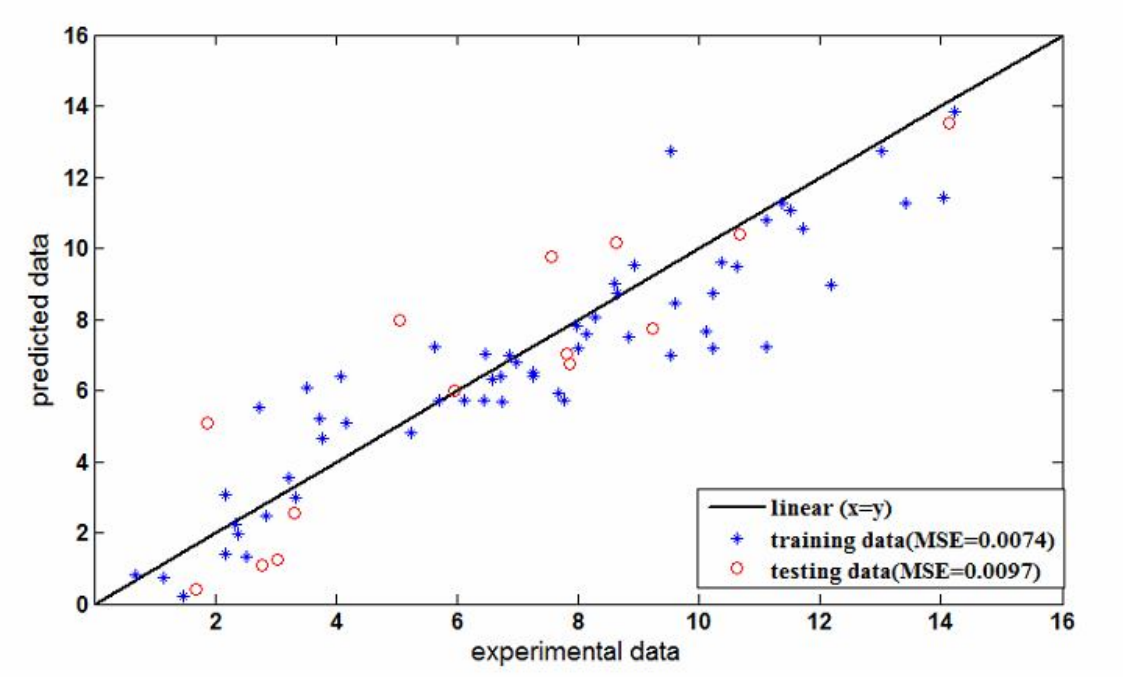

Fig. 5. Experimental *vs.* predicted CO conversions obtained by the MLP model for training and testing stages.

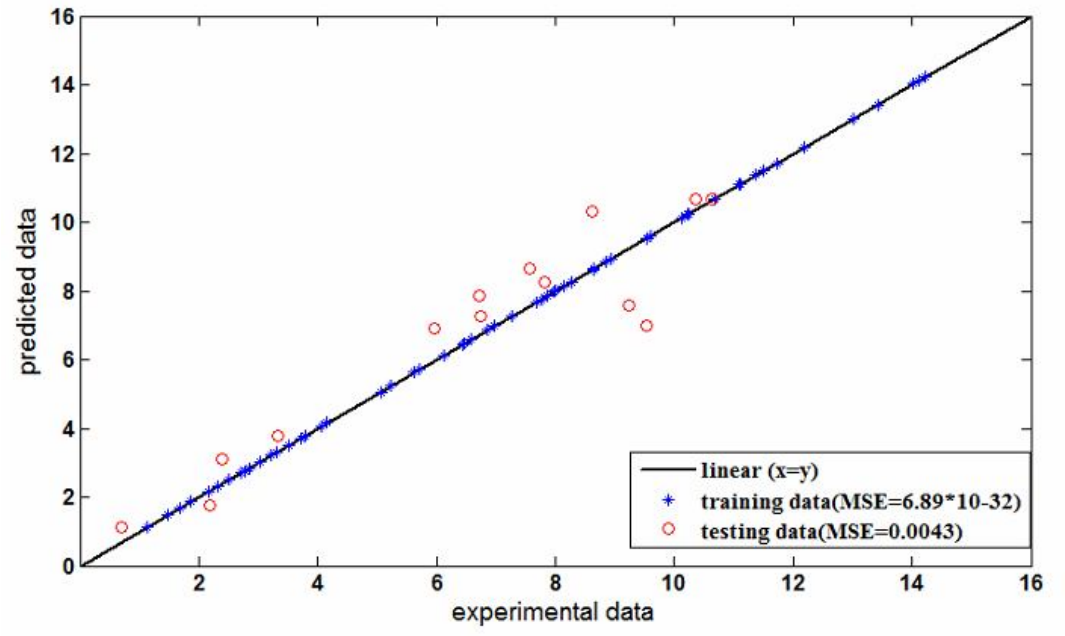

Fig. 6. Experimental *vs.* predicted CO conversions obtained by the ANFIS model for training and testing stages.

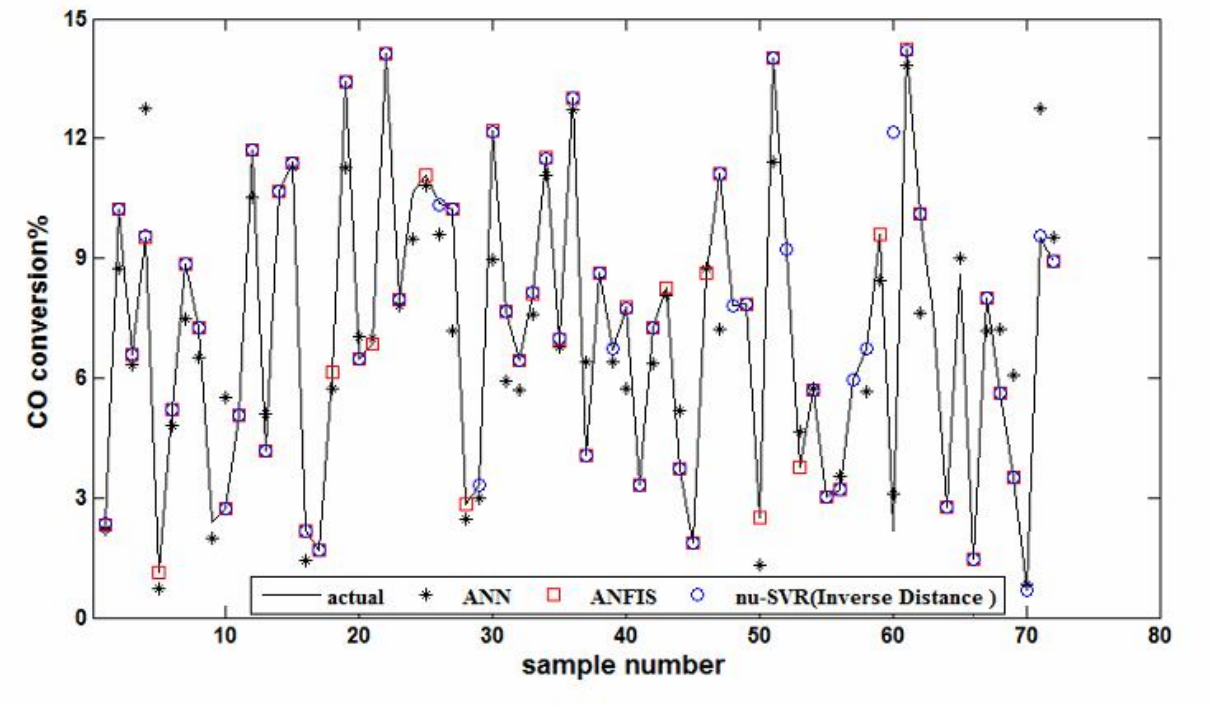

Fig. 7. Experimental results along with predictions of the models for training data.

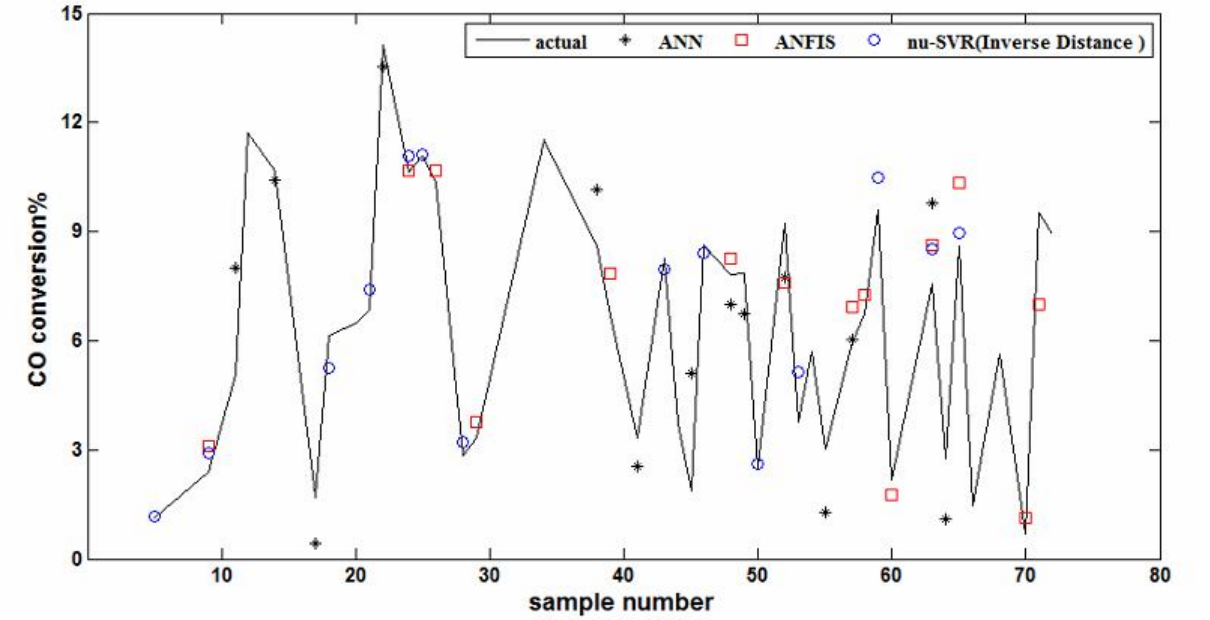

Fig. 8. Experimental results along with predictions of the models for testing data.

stages is shown in Fig. 6. As shown, the obtained values from the training and testing are very close to the experimental results. The performance of the ANFIS model is shown in Table 5. The best MSE values for training and testing stages are 6.89×10^{-32} and 0.0043, respectively. The MSE values show that the proposed ANFIS model has a good accuracy to predict the catalytic behavior in the FTS.

Comparison of nu-SVR with SUB-ANFIS and MLP models. According to the results presented in Tables 3, 4, and 5, it is obvious that the proposed nu-SVR model is more capable than MLP and SUB-ANFIS models in prediction of CO conversion values in Fischer-Tropsch synthesis. The prediction performances of nu-SVR with MLP and SUB-ANFIS models are compared and the results are presented in Figs. 7 and 8 for training and testing stages, respectively.

CONCLUSIONS

The FTS is one of the important processes for fuel production in the world. Finding a method for reducing the cost of processes is a great challenge for researchers. Therefore, many computational methods for modeling and prediction of FT synthesis have been proposed in recent years. In order to develop a theoretical model for data prediction, three approaches namely nu-SVR, MLP and ANFIS have been trained for prediction of CO conversion values in the FTS. In all three approaches, input dimensions are T, P_{tot} and H_2/CO ratio, as well as the CO conversion value as the output. Firstly, nu-SVR model was designed based on the obtained data from FTS. Then MLP and ANFIS were trained using the same data. Finally, the achieved results from these approaches were compared. The results reveal that the nu-SVR model is more accurate (MSE = 0.0014) than MLP (MSE = 0.0097) and ANFIS (MSE = 0.0043) procedures. As a result, although the nu-SVR model is much more complex than the two other models, it has more accurate results. Thus, it can be used for modeling when the experimental testing is very costly in money and time.

NOMENCLATURE

b	Bias
GHSV	Gas hourly space velocity
MSE	Mean square error
N	Total number of data
P_{tot}	Total pressure (bar)
R^2	Correlation coefficient
RMSE	Root mean square error
x_i	Input data
$X_{i,exp}$	Experimental data set
$X_{i,pred}$	Predicted data set
X_{co} (%)	Percentage of CO conversion
$\overline{X}$	Average value of experimental output
W	Weight factor
y_i	Desired output value

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