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Solubility Prediction of Supercritical Carbon Dioxide in 10 Polymers using Radial Basis Function Artificial Neural Network based on Chaotic Self-adaptive Particle Swarm Optimization and K-harmonic Means

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ABSTRACT: A novel model combined with chaos theory, self-adaptive particle swarm optimization (PSO) algorithm, K-harmonic means (KHM) clustering and radial basis function artificial neural network (RBF ANN) is proposed, hereafter called CSPSO-KHM RBF ANN. Traditional PSO algorithm is modified by chaos theory and self-adaptive inertia weight factor in order to reduce premature convergence problem. The modified PSO algorithm is employed to trim the RBF ANN connection weights and biases, whereas KHM is used to tune the hidden centers and spreads. The CSPSO-KHM RBF ANN model was employed to investigate the solubility of supercritical carbon dioxide in 10 polymers. Compared with other methods, such as RBF ANN, adaptive neuro-fuzzy inference system and PSO ANN, the proposed model displays optimal prediction performance. Results discover that the CSPSO-KHM RBF ANN model is an effective method for solubility prediction with high accuracy, and is a practicable method for chemical process analyzing and designing.

1. INTRODUCTION

Supercritical carbon dioxide (SCCO₂) has been used successfully as solvent, anti-solvent or plasticizer in material processing, such as material modification, material composites, material blending, microcellular foaming particle production, and material synthesis [1-4]. It is non-toxic, non-flammable, chemically inert and inexpensive, and its supercritical conditions are easily attained ($T_c=304$ K, $P_c=7.38$ Mpa) [5, 6]. Scrutiny of the literature evinces the considerable attention that lots of researchers have given to topics related to solubility of SCCO₂ in polymers [7-12]. The solubility is one of the most important thermophysical property that determines the compatibility of components of a blending system. To design optimized supercritical processes, solubility data of the considered compounds are needed. However, experimental studies such as pressure decay, gravimetric, phase separation, volumetric and chromatographic method are very expensive and time consuming [13-17], many researchers have tried to predict the thermodynamic properties by theoretical methods [18-21]. Because of the nonlinear nature of solubility, the conventional theoretical methods cannot predict the solubility of highly polar substances correctly and its predictions have a large inaccuracy while artificial neural network (ANN) could be considered as an alternative tool for solubility prediction [22, 23]. The ANN models have lower inaccuracy, cost, and time-consumption [24, 25].

Thus far, numerous ANN models for predicting physicochemical properties have been proposed [26, 27]. A comparison between equations of state and ANN is presented by Bakhbakhhi, Y [28] and it indicated that the ANN is a powerful model with better accuracy. Pahlavanzadeh, H.[29] proposed an ANN model for solubility prediction of CO₂ in AMP (2-amino-2-methyl-1-propanol) and demonstrated that the ANN model provides better prediction capability. Mehdizadeh, B.[30] and Gharagheizi, F.[31] proposed ANN method for solubility prediction of different compounds in SCCO₂ and discovered that ANN show better performance. Currently, Radial basis function artificial neural networks (RBF ANN) have received considerable attention due to their potential to approximate nonlinear behavior. Khajeh, A.[32] proposed both adaptive neuro-fuzzy inference system (ANFIS) and RBF ANN method for prediction of gas solubility in

polystyrene, and indicated that the ANFIS shows the best prediction performances.

As far as the solubility of SCCO₂ in polymers is concerned, it depends on many factors such as temperature and pressure as well as, weak interactions with the chain groups in the polymer. Due to the nonlinear nature among these factors, RBF ANN without parameter optimization cannot achieve the desired performance. To dwarf this problem, many intelligent algorithms, such as genetic algorithm [33-36], ant colony algorithm, simulated annealing algorithm, cuckoo search[37], Tabu Search and particle swarm optimization algorithm (PSO) [38-40] have been employed for the parameter optimization of ANN. The PSO algorithm is a global and advanced algorithm with a strong ability to search the global optimum. Compared with the other algorithms, PSO is easy to implement and there are few parameters to adjust. Liu, X. G. [41] presented a fuzzy ANN model based on PSO algorithm and online correction strategy for melt index prediction. Lazzus, J. A. [42] introduced a hybrid model based on ANN and PSO for estimation of solid vapor pressures of pure compounds at different temperatures. Over the past few years, researchers have demonstrated that the PSO is a powerful approach for ANN training [43]. Although PSO ANN shows high performance, it is easily trapped into a local minimum. Li, M.S.[44-47] developed a hybrid ANN model for prediction of gas solubility in polymers, and demonstrated that the performance of the hybrid ANN model is similarly excellent.

Motivated and inspired by the research problems of PSO algorithm and RBF ANN mentioned above, greater performance of prediction model are still the first-line goal in academia and the industrial community. In this study, we develop a novel solubility prediction model based on RBF ANN, chaos theory, self-adaptive PSO, and K-harmonic means (KHM) clustering methods. Then, the model is employed to predict the solubility of SCCO₂ in 10 polymers within a wide range of temperature and pressure. To reveal our proposed model outperforms RBF ANN and PSO ANN, a comparison among different models is carried out.

2. COMPUTATIONAL METHODS

This paper elaborates on the use of a novel model in predicting SCCO₂ solubility in polymers. To accomplish this task, the model consisted of K-harmonic means (KHM)

clustering method, chaos theory, PSO algorithm and RBF ANN is proposed, hereafter called CSPSO-KHM RBF ANN.

2.1 KHM clustering

KHM clustering algorithm is a more recent algorithm. The objective in this algorithm is to minimize the harmonic average from all points in the data set to all cluster centers. The KHM clustering addresses the intrinsic problem by replacing the minimum distance from a data point to the centers. Its implementation follows below[48] :

Step 1 Initialize the algorithm. In this work, the cluster centers were initialized based on the basis function centers of RBF ANN.

Step 2 Calculate objective function value according to equation (1).

$$KHM(X, C) = \sum_{i=1}^n \frac{k}{\sum_{j=1}^k \frac{1}{\|x_i - c_j\|^p}} \quad (1)$$

where $X = [x_1, \dots, x_n]$, is the data to be clustered, n is the number of the data to be clustered; $C = [c_1, \dots, c_k]$ is the set of cluster centers, k is the number of the cluster centers.

Step 3 For each x_i , compute its membership $m(c_j / x_i)$ and

weight $w(x_i)$ according to equations (2) and (3).

$$m(c_j / x_i) = \frac{\|x_i - c_j\|^{-p-2}}{\sum_{j=1}^k \|x_i - c_j\|^{-p-2}} \quad (2)$$

$$w(x_i) = \frac{\sum_{j=1}^k \|x_i - c_j\|^{-p-2}}{(\sum_{j=1}^k \|x_i - c_j\|^{-p})^2} \quad (3)$$

where p is an input parameter, and set $p = 2$ in this work.

Step 4 For each center c_j , re-compute its location according to equation (4).

$$c_j = \frac{\sum_{i=1}^n m(c_j / x_i) w(x_i) x_i}{\sum_{i=1}^n m(c_j / x_i) w(x_i)} \quad (4)$$

Step 5 Repeat steps 2–4 predefined number of iterations or until $KHM(X, C)$ does not change significantly.

Step 6 Assign data point x_i to cluster j with the biggest $m(c_j / x_i)$.

2.2 CSPSO algorithm

Particle swarm optimization (PSO) is a heuristic optimization algorithm inspired by social behavior and collective behavior of bird flocking or fish schooling. PSO presents some interesting characteristics, such as easy implementation procedure and high performance which make it widely used. In the standard PSO algorithm, the position and velocity are updated as follows:

$$v_{i,d}^{k+1} = \omega v_{i,d}^k + c_1 (p_{i,d}^k - x_{i,d}^k) + c_2 (p_{g,d}^k - x_{i,d}^k) \quad (5)$$

$$x_{i,d}^{k+1} = x_{i,d}^k + v_{i,d}^{k+1} \quad (6)$$

where $i=1, \dots, m$ (m is the number of particles); $x_{i,d}^k$ and $v_{i,d}^k$ denote the position and velocity of i -th particle at d -dimensional and the k -th iteration, respectively, ω denotes the inertia weight, c_1 and c_2 are the acceleration coefficients, $p_{i,d}^k$ represents the best position of i -th particle in d -dimensional while $p_{g,d}^k$ denotes the global best position.

However, PSO does not to guarantee that the exact optimum solution will be found, and the conventional PSO is easily trapped into local minima [49, 50]. In this study, we propose an improved PSO algorithm, called CSPSO, to avoid premature convergence and accelerate the converging speed. Two differences between conventional PSO and CSPSO are as follows: one is that the self-adaptive strategy is proposed to tune the inertia weight factor for the balance between exploration and exploitation; and the other is that the acceleration coefficients (c_1 and c_2) are adapted by chaotic sequences generated by chaos theory. The self-adaptive inertia weight factor is defined as follow:

$$\omega = \omega_{max} - Pgbest(k) / Plbest_{ave} - (\omega_{max} - \omega_{min}) \times k / k_{max} \quad (7)$$

Here, ω_{max} and ω_{min} denote the maximum and minimum inertial weight, respectively, $Pgbest(k)$ denotes the global best fitness at the k -th iteration, $Plbest_{ave}$ denotes the average local best fitness, k_{max} denotes the max iterations and k denotes the current iteration.

Furthermore, in CSPSO, the Lorenz chaotic operator is employed to generate acceleration coefficients (c_1, c_2). The Lorenz equations are defined as follows [51] :

$$\begin{cases} \frac{dx}{dt} = -a(x - y) \\ \frac{dy}{dt} = rx - y - xz \\ \frac{dz}{dt} = xy - bz \end{cases} \quad (8)$$

where a, b , and r are parameters that determine the system's behavior and are set as 10, 8/3 and 28, respectively. Given the dynamic properties of $x(t)$ and $y(t)$, which satisfy both ergodicity and randomness, the acceleration coefficients (c_1, c_2) are defined as follows:

$$\begin{cases} c_1 = x(t) \\ c_2 = y(t) \end{cases} \quad (9)$$

Table 1 shows the details of the CSPSO algorithm parameters.

Table 1. Details of the CSPSO algorithm parameters

Parameter	Description	Value
m	Number of particles	50
$itmax$	The iteration times	2000
$minerror$	Minimum error	1.00E-07

Parameter	Description	Value
w	Inertia weight	Self-adaptive
c_1	Cognitive component	Generated by Lorenz chaotic operator
c_2	Social component	Generated by Lorenz chaotic operator

2.3 CSPSO-KHM RBF ANN

RBF ANN is an efficient tool which can be trained with experimental information to map input and output data despite the complexity of their relation. It is a typical feed-forward ANN with three layers including input layer, hidden layer and output layer. In contrast to existing RBF ANN, we develop a specialized learning strategy that combines KHM clustering and CSPSO algorithm in this work, the fitness function is mean square error (MSE), the activation function is a Gaussian function as follow [52]:

$$g_i(x_k) = \exp\left(-\frac{\|x_k - c_i\|^2}{\sigma_i^2}\right) \quad (10)$$

where x_k ($1 \leq k \leq n$) is the k -th input vector, c_i ($1 \leq i \leq c$) are the centers of the basis functions, σ_i the respective spreads, n the number of samples, and c the number of hidden nodes. The estimated output of the network is given by equation (11):

$$O(x_k) = \sum_{i=1}^c w_i g_i(x_k) \quad (11)$$

where w_i is the connection weights of the i -th hidden node.

The training process of RBF ANN is accomplished through estimation of three kinds of parameters including the hidden centers, radial basis function spreads and the connection weights. The design process of a RBF ANN aims to determine optimal values for the three parameters:

c_i, σ_i, w_i . The selection of these parameters can be understood as a crucial and challenging problem. While the estimation of the connection weights and biases constitutes a standard regression problem, the determination of the spreads is carried out by specialized formulas that involve the distances between the centers. It turns out that the estimation of the basis function centers is the most important issue. Therefore, an optimization of the three parameters is necessary to improve the network's performance.

In this study, we employ KHM clustering algorithm to optimize the hidden centers and radial basis function spreads due to that the KHM clustering algorithm specialize in confirming the spreads based on the distance of the data centers. In the process of RBF ANN training, the hidden centers coincide with the cluster centers obtained by the KHM algorithm, and are updated as follow:

$$KHM(C_{basis-funtion}, C_{cluster}) \quad (12)$$

where $C_{cluster}$ is the cluster center according to KHM method, $C_{basis-funtion}$ is the basis function center. And each radial basis function spread is updated according to its hidden center.

The choice of connection weight and bias values for RBF ANN is a classical optimization problem, and the PSO algorithm has been verified that it has outstanding advantage to solve optimization problem. Therefore, we employ CSPSO algorithm to establish the connection weight and bias between the hidden layer and the output layer. The main objective of the proposed algorithm is to calculate optimal values for weight and bias. To accomplish this, we developed a specialized particle structure including the network weight and bias as follow:

$$particle(i) = [W_{h,o}, B_{h,o}] \quad (13)$$

where $W_{h,o}$ ($1 \leq h \leq c$), ($1 \leq o \leq p$) is the weight matrix between the h -th hidden note and the o -th output note, and $B_{h,o}$ the respective bias matrix, c is the number of hidden note, p is the number of output note. Every particle of CSPSO, called a single solution, represents a single RBF ANN and flies over the solution space in search for the optimal solution. The particles are evaluated using the standard MSE to seek the optimal solution. During the optimization process, the particles are updated accordingly using (5) and (6).

The procedure for CSPSO-KHM RBF ANN can be summarized as follows:

Step 1: Model initialization. Randomly initialize basis function centers, connection weight, bias, the positions and velocities of a group of PSO particles.

Step 2: Input training samples. Set basis function centers accordingly using equation (12); set the connection weight and bias based on equation (13).

Step 3: Model training. Apply the KHM to update the basis function centers based on equations (1) - (4); apply the CSPSO to update the connection weight and bias based on equations (5) and (6).

Step 4: Calculate the network outputs and errors. If network converges or the maximum number of iterations occurred then stop, else go to step 3.

3. EXPERIMENTAL MODEL

3.1 Experimental data and pre-processing

CSPSO-KHM RBF ANN is designed for solubility prediction of $SCCO_2$ in 10 polymers including PS, CPE55, CPE60, CPE67, PLLA, PLGA, PBSA, PBS, PP and HDPE. All experimental data are collected from literature. After comprehensive evaluation of the experimental data, a database containing 327 data points is established. Table 2 shows the sources of statistical experimental solubility data used in this work. For each $SCCO_2$ /polymer system, the database is randomly divided into three subsets including training, validation and testing sets. The training set, contained about 70% data points, is used to train the ANN model. The validation and testing set, contained about 15% each, are used to verify and test the prediction capability.

Table 2. Experimental data in this work

Polymer	T (K)	P (Mpa)	S (g/g)	Data points	Reference
PS ^[a]	338.22-473.15	7.540-44.410	0.02641-0.16056	70	[53-56]
CPE55 ^[b]	306.00-343.00	10.370-31.020	0.09840-0.63660	20	[57]
CPE60	306.00-344.00	10.150-29.910	0.14210-0.56840	18	[57]
CPE67	309.00-343.00	10.380-31.000	0.12810-0.58950	18	[57]
PLLA ^[c]	308.00-323.00	9.620-31.460	0.16520-0.43010	27	[58]
PLGA ^[d]	308.00-323.00	10.140-31.470	0.09030-0.29630	27	[58]
PBSA ^[e]	323.15-453.15	7.870-20.127	0.04763-0.17410	29	[53, 59]
PBS ^[f]	323.15-453.15	8.008-20.144	0.04534-0.17610	31	[53, 59]
PP ^[g]	313.20-483.70	7.400-24.910	0.03950-0.26170	67	[53, 60-62]
HDPE ^[h]	433.15-473.20	10.731-18.123	0.00551-0.12296	20	[53, 60]
total	306.00-483.70	7.400-44.410	0.00551-0.63660	327	

^[a]Polystyrene. ^[b]Carboxylated polyesters. ^[c]Poly(L-lactide). ^[d]Poly(D,L-lactide-co-glycolide). ^[e]Poly(butylene succinate-co-adipate). ^[f]Poly(butylene succinate). ^[g]Polypropylene. ^[h]High-density polyethylene.

3.2 Assessment

The prediction capabilities of different models are evaluated in terms of average relative deviation (ARD), root mean square error of prediction ($RMSEP$), and squared correlation coefficient (R^2). ARD and $RMSEP$ are defined as follows:

$$ARD = \frac{1}{N} \sum_{i=1}^N \frac{|y_i - \hat{y}_i|}{y_i}$$

$$RMSEP = \sqrt{\frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2}$$

where N is the number of data samples; the y_i and \hat{y}_i are the reference and predicted value for the i -th test sample, respectively.

3.3 Architecture

In this work, two process variables, temperature T and pressure P , have been selected as input parameters, the output layer has one neuron that predicts solubility by the model. The number of neurons in the hidden layer is unknown and needs to be optimized. Therefore, the number of neurons in the hidden layer is optimized heuristically. Then, 13 CSPSO-KHM RBF ANN models are generated assuming the number of neurons in the hidden layer from 3 to 15. The optimum number is selected based on the minimum ARD value. In Figure 1, ARD against different number of neurons in the hidden layer is plotted for the training set. It can be seen that the ARD has its minimum value when the number of the neurons is 8.

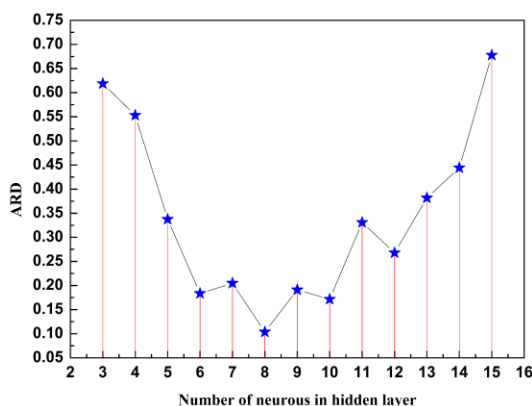


Figure 1. Results of topology studies for optimal ANN configuration

4. RESULTS AND DISCUSSION

In this work, a three-layer RBF ANN trained by the CSPSO and KHM (CSPSO-KHM RBF ANN) was developed; the optimum architecture is 2-8-1. Then, the CSPSO-KHM RBF ANN is employed to investigate solubility of SCCO_2 in 10 polymers.

4.1 Results of the proposed model

Table 3 indicates the statistical values of CSPSO-KHM RBF ANN for predicting SCCO_2 solubility in various polymers. The results in Table 3 clearly demonstrate the capability of the proposed model in predicting the values of SCCO_2 solubility in polymers accurately. The output of the CSPSO-KHM RBF ANN model show well agree with the target, regardless of the training set, or validation set, or testing set. Particularly, for CPE55, CPE60, and PBS, show better correlation between the prediction and the experimental, the R^2 is more than 0.9980.

Table 3. Values of ARD , R^2 and $RMSEP$ for the proposed model

Compounds	Training set			Validation set			Testing set		
	ARD	R^2	$RMSEP$	ARD	R^2	$RMSEP$	ARD	R^2	$RMSEP$
PS	0.1080	0.9978	0.0112	0.1066	0.9977	0.0114	0.1058	0.9972	0.0116
CPE55	0.1068	0.9968	0.0113	0.0981	0.9986	0.0120	0.1066	0.9989	0.0104
CPE60	0.1020	0.9979	0.0097	0.1050	0.9988	0.0094	0.1040	0.9983	0.0102
CPE67	0.0968	0.9975	0.0096	0.1041	0.9978	0.0113	0.1047	0.9971	0.0109
PLLA	0.1037	0.9989	0.0103	0.1051	0.9968	0.0112	0.1034	0.9965	0.0109
PLGA	0.0978	0.9975	0.0112	0.1102	0.9967	0.0104	0.0972	0.9975	0.0096
PBSA	0.0984	0.9976	0.0111	0.1049	0.9987	0.0110	0.1104	0.9962	0.0106
PBS	0.1070	0.9969	0.0104	0.1014	0.9965	0.0098	0.1045	0.9980	0.0104
PP	0.1054	0.9976	0.0103	0.1039	0.9979	0.0103	0.1064	0.9976	0.0107
HDPE	0.1105	0.9982	0.0106	0.1031	0.9966	0.0105	0.1081	0.9979	0.0113
Average	0.1036	0.9977	0.0106	0.1042	0.9976	0.0107	0.1051	0.9975	0.0107

In the CSPSO-KHM RBF ANN model, the training set is used to fit the parameters, the validation set is used to estimate the error rate in order to tune the model parameters, and the testing set is used to investigate the prediction capability of the proposed model. For the testing set, Figure 2 and Figure 3 plot the correlations between experimental data and prediction value. We can note that the superiority of the solubility prediction by CSPSO-KHM RBF ANN. It is obvious that the proposed model has excellent prediction accuracy and good correlation between experimental data and prediction value.

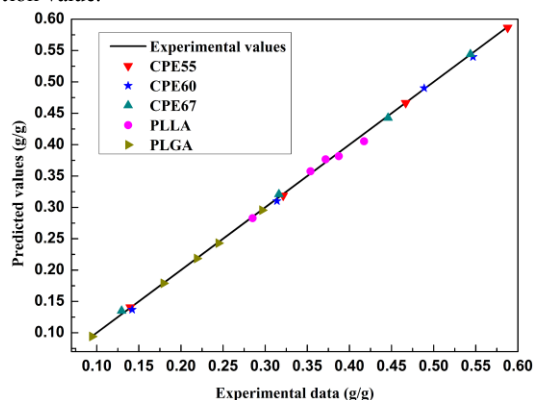


Figure 2. Predicted data by CSPSO-KHM RBF ANN in the testing set (a)

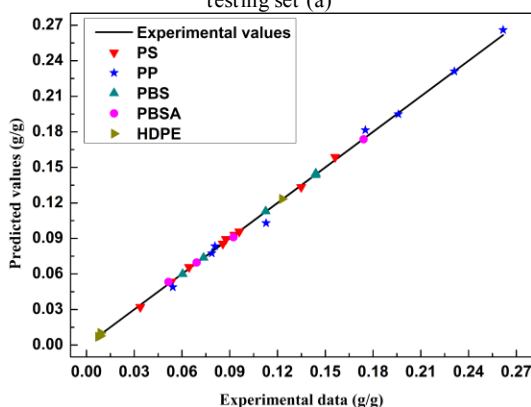


Figure 3. Predicted data by CSPSO-KHM RBF ANN in the testing set (b)

4.2 Comparison of the proposed model against the others

To verify the efficiency and validity of the proposed computational model, two well-known models, RBF ANN and PSO ANN, are employed as comparative models. Figure 4 plots the curves of mean square error (MSE) versus epoch of the different models. According to the figure, it is noticeable that the CSPSO-KHM RBF ANN is superior in terms of converging speed and accuracy and shows the best prediction performances.

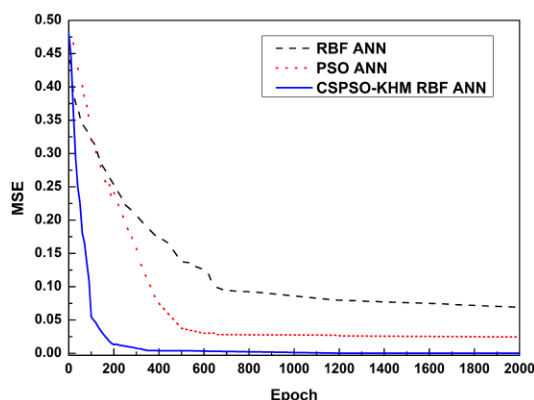


Figure 4. Curve of MSE VS. Epoch

Furthermore, to substantiate the proposed model outperforms RBF ANN and PSO ANN, another testing database containing 60 data points (picked 6 data points each polymer at random) is additionally established for comparison among the different models. Figure 5 describes the correlation between prediction and experimental values. From Figure 5, it is evident that the output of the CSPSO-KHM RBF ANN model shows better agreement with the target by comparing RBF ANN and PSO ANN, the results report the superiority of CSPSO-KHM RBF ANN, and indicate that the proposed model has better prediction capability.

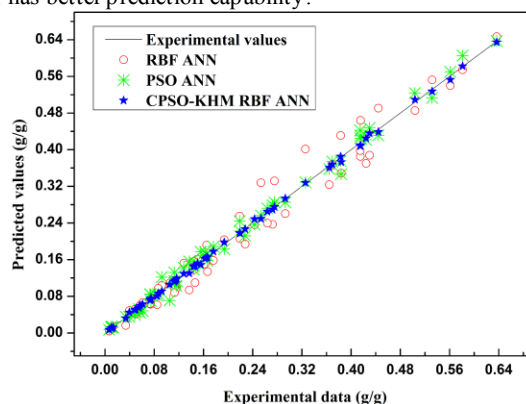


Figure 5. Predicted data VS. experimental data in the testing database

In particular, a comparative performance is further evaluated in terms of ARD , R^2 , $RMSEP$, $best\ fitness$, MSE , and computation time, respectively. Running every model successively five times and then taking the average result is performed, Table 4 displays the performance comparison among the comparison models based on the testing database.

Table 4. Statistical parameters of the comparison models

Model	ARD	R^2	$RMSEP$	$Best\ Fitness$	MSE	Time (S)
RBF ANN	0.3812	0.9541	0.0644	6.47E-06	9.76 E-04	10.82
PSO ANN	0.2629	0.9754	0.0418	8.63 E-07	8.63 E-04	18.67
CSPSO-KHM RBF ANN	0.1051	0.9975	0.0107	4.52 E-07	1.91 E-04	21.76

What is more, the ARD for Adaptive Neuro-Fuzzy Inference System (ANFIS) and RBF ANN proposed by Khajeh and Modarress [32] are 0.2543 and 0.6498, respectively, whereas the ARD is 0.1051 in this work. The ANN trained by unified PSO proposed by Ahmadi, M. A. [63] has a R^2 of 0.99493, whereas R^2 is 0.9975 in this work.

4.3 Result analysis

Obviously, from Table 3 and Figures 2-3, it is apparent that the proposed model presents the best performances for solubility prediction, regardless of the correlation or accuracy. In the uniform data set, as shown in Table 4 and Figures 4-5, we can note the

superiority of the CSPSO-KHM RBF ANN to RBF ANN, PSO ANN. Especially, the *ARD* and *RMSEP* values, shown in Table 4, record the proposed model could predict SCCO₂ solubility in polymers with high accuracy, and the good correlations shown by *R*² describe that the predicted data are observed to mutually agree with experimental values.

The comparison among the different models shows that CSPSO-KHM RBF ANN has higher accuracy and better agreement than ANFIS, RBF ANN and PSO ANN but consumes more computation time. By contrast, RBF ANN consumes less computation time with lower accuracy. Generally, if the computation time is acceptable, the accuracy is of great practical significance. Table 4 shows that the computation time is acceptable.

In terms of efficiency, accuracy and correlation, the results show that the performance of the proposed model is better. There are two major factors that lead to the superiority of the proposed model, one is that the training algorithm based on self-adaptive strategy and chaos theory is employed to concentrate on premature convergence; and the other is that the KHM clustering method is used to tune the hidden centers and radial basis function spreads.

It is important to note that there are some notable characters for the CSPSO-KHM RBF ANN model.

(1) Compared with the traditional computation methods, such as perturbed-hard chain theory, lattice-fluid theories and cubic equation of states, the CSPSO-KHM RBF ANN could avoid the PVT corrections due to the influence of high pressure and temperature, and gives high accuracy. At the same time, it presents excellent prediction capability and high accuracy compared with the others algorithms, such as ANFIS.

(2) The solubility prediction trend is concordant with the experimental. Take PP for instance, Figure 6 depicts the corrections between predicted values and experimental data at different pressure from 7.44 (Mpa) to 17.376 (Mpa) and under the different temperatures of 453.20 (K), 423.20 (K), 370.20 (K) respectively.

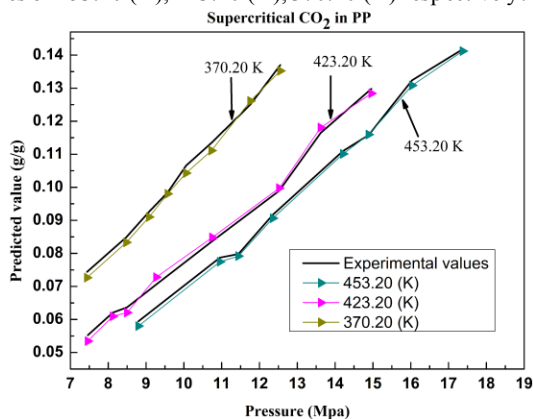


Figure 6. Corrections between predicted values and experimental data. From our predictive experiments, we can determine that the solubility of SCCO₂ in PP increased almost linearly with pressure, and decreased with increasing temperature. The solubility prediction trend is concordant with the experimental trend. Generally, many SCCO₂/polymer systems have the solubility trend similar to that of SCCO₂/PP.

5. CONCLUSION

Solubility of supercritical carbon dioxide (SCCO₂) in many polymers is substantial in polymer processing. The present study is conducted to seek a novel prediction model so as to replace the costly and time-consuming measurement in laboratory. For this purpose, we have developed a hybrid prediction model based on ANN, self-adaptive PSO, chaos theory, and KHM clustering method to predict the solubility of SCCO₂ solubility in polymers. The conclusion is that the proposed CSPSO-KHM RBF ANN model is a reliable and accurate

method for predicting SCCO₂ solubility in polymers, and is a practicable method for analyzing and designing polymer processing technology. It has a good application prospects, such as system of experimental data processing, prediction of material performance and properties, optimization, and simulation of material processing technology. Meanwhile, in the future, we will use some heuristic techniques for the data uncertainty pretreatment to reduce the computation cost for higher efficiency, such as ordering, pruning, etc. At the same time, we will follow up on this subject all the time and focus on applying the proposed model to solve more realistic problems.

ABBREVIATIONS

PVT	Pressure, Volume, Temperature
ANN	Artificial Neural Network
RBF	Radial Basis Function
SCCO ₂	Supercritical carbon dioxide
PSO	Particle Swarm Optimization
CSPSO	Chaotic Self-adaptive Particle Swarm Optimization
KHM	K-harmonic means
PBS	Poly(butylene succinate).
PBSA	Poly(butylene succinate-co-adipate).
PP	Polypropylene.
PS	Polystyrene.
CPEs	Carboxylated polyesters
PLLA	Poly(L-lactide)
PLGA	Poly(D,L-lactide-co-glycolide)
HDPE	High-density polyethylene
ARD	Average Relative Deviation
R ²	Squared Correlation Coefficient
MSE	Mean Square Error
RMSEP	Root Mean Square Error of Prediction
ANFIS	Adaptive Neuro-Fuzzy Inference System

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