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RESEARCH PAPER

PSO-ANFIS and ANN Modeling of Propane/Propylene Separation using Cu-BTC Adsorbent

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Abstract

In this work, an artificial neural network (ANN) model along with a combination of adaptive neuro-fuzzy inference system (ANFIS) and particle swarm optimization (PSO) i.e. (PSO-ANFIS) are proposed for modeling and prediction of the propylene/propane adsorption under various conditions. Using these computational intelligence (CI) approaches, the input parameters such as adsorbent shape (S_A), temperature (T), and pressure (P) were related to the output parameter which is propylene or propane adsorption. A thorough comparison between the experimental, artificial neural network and particle swarm optimization-adaptive neuro-fuzzy inference system models was carried out to prove its efficiency in accurate prediction and computation time. The obtained results show that both investigated methods have good agreements in comparison with the experimental data, but the proposed artificial neural network structure is more precise than our proposed PSO-ANFIS structure. Mean absolute error (MAE) for ANN and ANFIS models were 0.111 and 0.421, respectively.

Keywords:
Adsorption,
ANN,
Cu-BTC,
Propylene/Propane,
PSO-ANFIS

Introduction

Olefins are one of the most important feeds in the petrochemical industries which are used for the production of various commodities. Light olefins such as ethylene and propylene are usually obtained by steam cracking or fluid catalytic cracking of heavy petroleum fractions and are mainly produced in mixtures with their paraffin homologs. The separation of these paraffin and olefin mixture is energy-intensive and also a costly process due to the very close relative volatility of components. Propylene as an important intermediate in the petrochemical industry is obtained by traditional separation process such as cryogenic distillation, which operates at low temperatures or high pressures, and needs a large number of distillation stages and very large reflux ratio due to the similarity of propylene and propane boiling points [1,2].

For example, the process for separation of propane/propylene was carried out at about 30 °C and 30 bar [3] and more than 150 theoretical stages are required to achieve high purity propylene (99.5%) [4]. So, the alternative propane/propylene separation processes to reduce the energy costs are required. For example, the separation techniques such as membrane, absorption, hydrogenation, and physical adsorption have been considered and adsorptive separation seems to be a more energy-efficient process for propane/propylene separation [5-10].

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Pressure swing adsorption (PSA), temperature swing adsorption (TSA) and also vacuum swing adsorption (VSA) techniques, based on solid molecular sieves, have been applied as an appropriate process. These processes have been considered for more than one decade [11-14] showing a satisfactory product recovery (87%) and very high purity (99%) [4]. In these processes, the separation is obtained in ambient temperature and no additional power was required to cool the gas mixture. Both commercial [4,11,13,15-17] and tailor-made adsorbents [18-21] have been used for separation of a propane-propylene mixture. Also, the use of activated carbon [22,23], carbon molecular sieves [24-26] and metal-doped adsorbents [27-30] for separation of olefin/paraffin mixture has been reported in the literature. The double bond of olefins can forms π-complexes with some transition metals which leads to making a difference in adsorption affinity between olefin and paraffin [18,31]. 13X and 4A zeolites were widely evaluated among the commercial adsorbents and have been demonstrated to be effective adsorbents for VSA process in order to produce high purity of propylene [13,14,32]. Da Silva and Rodrigues [33] studied adsorption isotherms of propylene and propane and investigated single component adsorption on commercial 13X and 4A zeolites at temperature between 273 and 473 K. It was shown that 13X zeolite shows a lower mass transfer resistance and higher adsorption capacity than 4A zeolite, while higher selectivity for propylene in mixture of propylene/propane has been reported for 4A zeolite relative to 13X. Also, in the other study, Grande and Rodrigues [34] reported that high purity propylene can be achieved using 4A zeolite. Commercial zeolite 4A presented excellent performance to be applied in vacuum pressure swing adsorption (VPSA) process; the propane diffusion within micro-pores is extremely slow which leads to reduce adsorbed propane. It was concluded that micro-pore diffusion strongly limits the adsorption rate of propane and thus, its adsorption can be controlled by the size of zeolite crystals [35,36]. Padin et al. [19] reported that the modification of commercial 4A zeolite with Li^+ cations (NaLiA zeolite) improve the uptake rate of propane. In a same study, the selective adsorption of propylene from the mixture with propane by Li-exchange zeolite 13X was studied. The results indicated that propylene is adsorbed preferentially over propane at low pressures and adsorption equilibrium can be described with Virial and multi-site Langmuir models [17]. Hanaa et al. [36] investigated the adsorption of propane/propylene onto the binary (introduction of Ni^{2+} or Cr^{3+} instead of Na^+) and ternary (introduction of Ni^{2+} and Cr^{3+} instead of Na^+) zeolites. They found that change in Henry's low slope indicates strong and weak interactions with propylene and propane, respectively. Iglesias et al. [37] verified 4A commercial zeolite for separation of C_3H_6/C_3H_8 mixture at a temperature below and above the critical temperature of propylene. They found that a certain amount of propylene was adsorbed irreversibly below the critical temperature. But at above the critical temperature, 4A zeolite could be excellent adsorbent for separation of propylene/propane mixtures in the temperature range of 150-180 °C.

Artificial neural network (ANN) and adaptive neuro-fuzzy inference system (ANFIS) have been used in many studies to determine and also anticipate the physical and chemical properties in various industrial processes [38-54]. Reviewing the related studies showed that, propylene/propane adsorption has not been investigated using ANN and PSO-ANFIS methods.

In this study, the effects of temperature, pressure and Cu-BTC adsorbent structures on the adsorption of propylene/propane were investigated and modeling of PSO-ANFIS and ANN for this process were performed and the model with the best matching of the experimental data was determined.

Experimental Methods

Various factors have an effect on the adsorption of propylene and propane. Among them, the materials used as adsorbent and its shape have a great impact on the adsorption. In addition, the

operating pressure and temperature have important roles in adsorption efficiency. In this study, with emphasis on the metal-organic framework (MOF) adsorbent and the Cu-BTC molecular structure, the adsorption rates of propylene and propane were studied. A set of 271 experimental data points of propylene and propane adsorption on Cu-BTC adsorbent were collected from previous studies [55-57]. The difference in the data was in the shape of Cu-BTC adsorbent which was in extrudate [55], sphere [56], tablet [56], and powder [57] shapes. Temperature and pressure were applied in the range of 423-323 K and 0-520 kPa, respectively. Statistical analysis of the input and output data are shown in Table 1.

Table 1. Statistical analysis of the input and output variables of the proposed models

Factors	Symbol	Unit	Minimum	Maximum	Median	Average	SD
Input							
Adsorbent shape*	S_A	-	1.00	4.00	2.50	2.50	1.29
Pressure	P	kPa	0.00	520.00	45.57	89.23	118.28
Temperature	T	K	323.00	423.00	348.00	358.52	29.19
Output (Adsorption)							
Adsorbed propylene	$n_{C3=}$	mol/kg	0.00	8.02	3.07	3.76	2.43
Adsorbed propane	n_{C3}	mol/kg	0.00	7.14	2.37	2.86	2.13

* For adsorbent shape: (1)=extrudate, (2)=sphere, (3)=tablet, and (4)=powder

Description of Proposed Models

In this paper, precise PSO-ANFIS and ANN models are introduced for the modeling and prediction of propylene/propane adsorption under several conditions. In these computational intelligence (CI) structures, the inputs are an adsorbent shape (S_A), temperature (T), and pressure (P).

Artificial Neural Network

ANN structures [58,59] basically consist of interconnected neurons. A neuron is the basic processing part of ANN. The weights in ANNs are equivalent to the synapses of biological neurons. the weights are adjusted Using an error-minimization technique i.e. back-propagation method. Between the ANN models, the multi-layer perceptron (MLP) network is the most commonly used ANN which consists of a number of neurons [58,59].

The MLP is a feed-forward network, which has three or more layers: one input layer, one or more hidden layers and one output layer [58,59]. In Fig. 1a, x_1, x_2,…, x_N are the inputs, y_1, y_2, …, y_M are the outputs and k is the number of hidden layer neurons. Also, N and M are the number of inputs and outputs, respectively. The output of tth neuron in the hidden layer is described as below:

$$z_j = f\left(\sum_{p=1}^{N}\left(x_p w_{pt}\right) + b_j\right), \qquad t = 1, 2, \ldots, k \tag{1}$$

where f is the hidden layer activation function, x is the input, w is the weighting factor and b is the bias term. The output of the jth neuron in the output layer is given by:

$$y_m = \sum_{p=1}^{k}\left(\theta_p W_{pm}\right) + b_m, \qquad m = 1, 2, \ldots, M \tag{2}$$

Adaptive Neuro-fuzzy Inference System/PSO Algorithm

ANFIS is a combination of ANN and fuzzy inference system (FIS), which has both ANN and FIS advantages [60,61]. An ANFIS structure has five layers. Each ANFIS layer contains some

nodes, which have their node functions. If a FIS has one output (f) and two inputs (x, y), the following equation describes a single fuzzy if-then rule:
Rule1: *if* x *is* A_1 *and* y *is* B_1, *then* $f_1 = p_1x + q_1y + r_1$
Rule2: *if* x *is* A_2 *and* y *is* B_2, *then* $f_2 = p_2x + q_2y + r_2$
where, p_i, q_i, and r_i are called consequent parameters (linear output parameters) and i=1,2. A sample of an ANFIS structure is shown in Fig. 1b. Each node in layer 1 has the following node function:

$$O_{1,i} = \mu_{A_i}(x), \qquad i = 1,2 \tag{3}$$
$$O_{1,i} = \mu_{B_{i-2}}(y), \qquad i = 3,4 \tag{4}$$

i is the membership grade of A_1, A_2, B_1, and B_2 and $O_{1,i}$ is the node i output. As an example, the Gaussian function is given by:

$$\mu_A(x) = \exp(-\frac{(x-c)^2}{2\sigma^2}) \tag{5}$$

where c and σ are called premise parameters. Each node in layer 2 denotes the firing strength of a rule and multiplies all incoming signals with the following output:

$$O_{2,i} = w_i = \mu_{A_i}(x)\mu_{B_i}(y) \ , \quad i = 1,2 \tag{6}$$

The nodes in layer 3 are called normalized firing strengths with the following node functions:

$$O_{3,i} = \overline{w_i} = \frac{w_i}{w_1 + w_2} \ , \quad i = 1,2 \tag{7}$$

Each node in layer 4 has the node functions given by:

$$O_{4,i} = \overline{w_i} f_i = \overline{w_i}(p_i x + q_i y + r_i), \quad i = 1,2 \tag{8}$$

where, $\overline{w_i}$ is a normalized firing strength from layer 3 and $\{p_i, q_i, r_i\}$ are named consequent parameters. Finally, layer 5 computes the only output with the following equation:

$$O_{5,i} = \sum_i \overline{w_i} f_i \ , \quad i = 1,2 \tag{9}$$

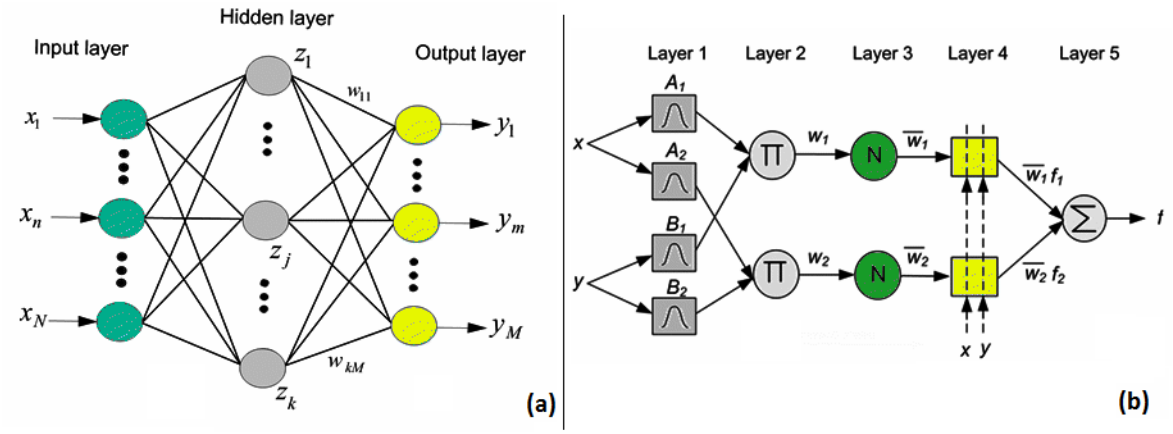

Fig. 1. (a) MLP structure (b) ANFIS structure

Modeling Approach

In this work, ANN and PSO-ANFIS approaches were used to predict the effect of several parameters influencing on propylene/propane adsorption. In Table 1, the input and output variables of the presented PSO-ANFIS and ANN models are shown. An ANFIS model has two sets of parameters (premise and consequent parameters). During the training process, these parameters are adjusted. Some existing training approaches for ANFIS structure may cause the local minimum problem. To solve this problem and for updating the premise and consequent parameters of ANFIS, PSO technique can be applied. PSO, first proposed by Kennedy et al. [62], is an evolutionary computational method which is widely used in many optimization applications [63]. PSO is a population-based search technique. In PSO, each possible solution is represented as the swarm, which is a particle in a population. In the presented PSO-ANFIS technique, we used PSO method for adjusting the parameters of membership functions. This method is more flexible and less expensive in hardware implementation in comparison with the conventional ANFIS methods. In this method, at first, the ANFIS structure is trained by the hybrid learning algorithm, which is based on the least-squares and gradient descent techniques. After that, the number of ANFIS membership functions (MFs) and their parameters are adjusted by the PSO method. For this step, mean absolute error (MAE) as the fitness function is used. The training and testing data sets required for the presented PSO-ANFIS and ANN models are obtained from the previous studies [55-57]. For this study, 271 experimental data were used, about 70% of them are applied for training the presented models. MATLAB 7.1 software was used to develop PSO-ANFIS and ANN structures. For obtaining the best ANN model, different configurations were tested with a different number of hidden layers. Also, epochs and the hidden layer neurons were changed from 50 to 500 and 1 to 10, respectively. To obtain the best PSO-ANFIS structures, epochs, the number and the types of input MFs were changed. Then, the PSO parameters such as the number of epochs and the number of particles for each population were determined. Tables 2 and 3 show the best ANN and PSO-ANFIS models obtained.

To compare the developed models with the experimental data, we used the MAE, correlation factor (R), and root mean square error (RMSE) whose equations are given as follow:

$$\mathrm{MAE} = \frac{1}{N}\sum_{i=1}^{N}\left|x_{i_{exp}} - x_{i_{pred}}\right| \tag{10}$$

$$\mathrm{RMSE} = \left[\frac{\sum_{i=1}^{N}\left(x_{i_{exp}} - x_{i_{pred}}\right)^2}{N}\right]^{0.5} \tag{11}$$

$$\mathrm{R} = 1 - \left[\frac{\sum_{i=1}^{N}\left(x_{i_{exp}} - x_{i_{pred}}\right)^2}{\sum_{i=1}^{N}\left(x_{i_{exp}}\right)^2}\right] \tag{12}$$

where, '$x_{i_{exp}}$' and '$x_{i_{pred}}$' are the experimental and predicted values (ANN and PSO-ANFIS), respectively, and *N* is the total number of data.

Results and Discussions

The proposed models will be outstanding if MAE=0, RMSE=0, and R=1. The obtained errors for our proposed models are presented in Table 4. From this table, it can be observed that the ANN model is capable of predicting the adsorption of propylene/propane values better than PSO-ANFIS model. Also, Figs. 2 and 3 show the comparison between the experimental results

and the predicted values for testing and training data. As can be seen in these figures, PSO-ANFIS structure is less precise than our ANN structure. A membership function in a fuzzy system is more complicated than a neuron in an ANN structure, thus if we assume that a neuron in ANN model is equivalent to a membership function in ANFIS model, an ANN model will have a simpler structure than PSO-ANFIS model. Therefore, in the hardware implementation, the presented ANN model is faster, cheaper, and more flexible.

Table 2. Properties of the best ANN structure

Type of ANN	MLP
No. of the hidden layers	2
The input layer neurons	3
The first hidden layer neurons	4
The second hidden layer neurons	4
The output layer neurons	1
Learning rate	0.5
Epochs	250
Adaption learning function	Trainlm
Activation function	Tansig

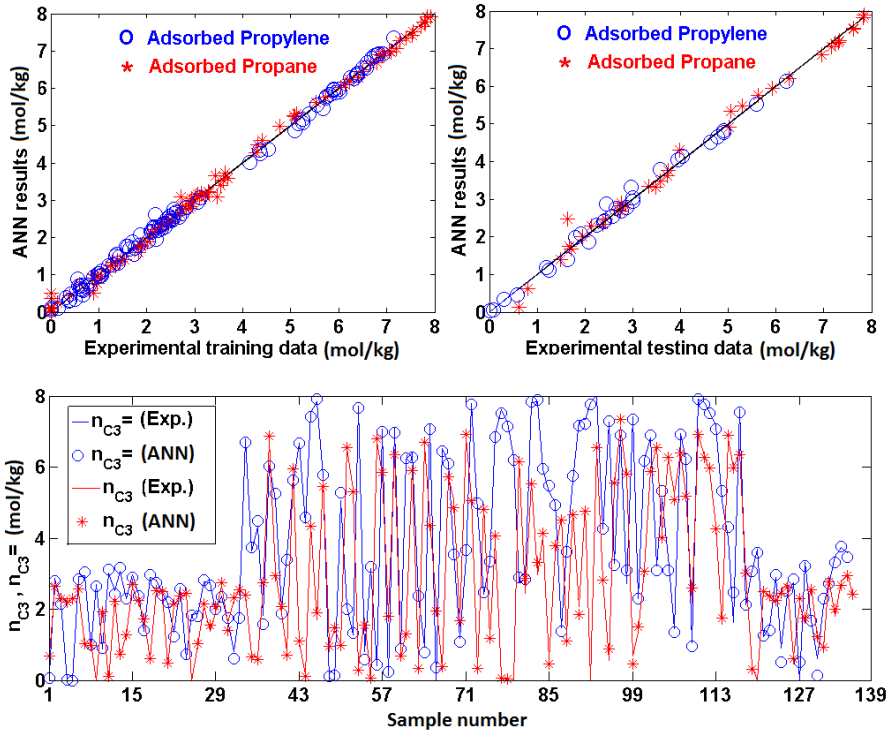

Fig. 2. The results of ANN model

In Fig. 4, a better evaluation between the presented ANN model and the experimental data for the testing and training propylene/propane adsorption is demonstrated. It can be obviously observed from Fig. 4 that in all of the adsorbent shapes, the amount of propylene/propane adsorption increases by increasing the pressure and also, decreasing the temperature. Fig. 4 also indicates that a greater amount of propylene is adsorbed on Cu-BTC surface in comparison with propane. This difference in the amount of adsorption is the basis for the separation of these two components which this pattern is repeated in the various temperatures and pressures and for all shapes of the adsorbents. Accoring to Fig. 4, it is clear that the results obtained using the ANN model is more compatible with the experimental data in all adsorbent shapes and operating conditions.

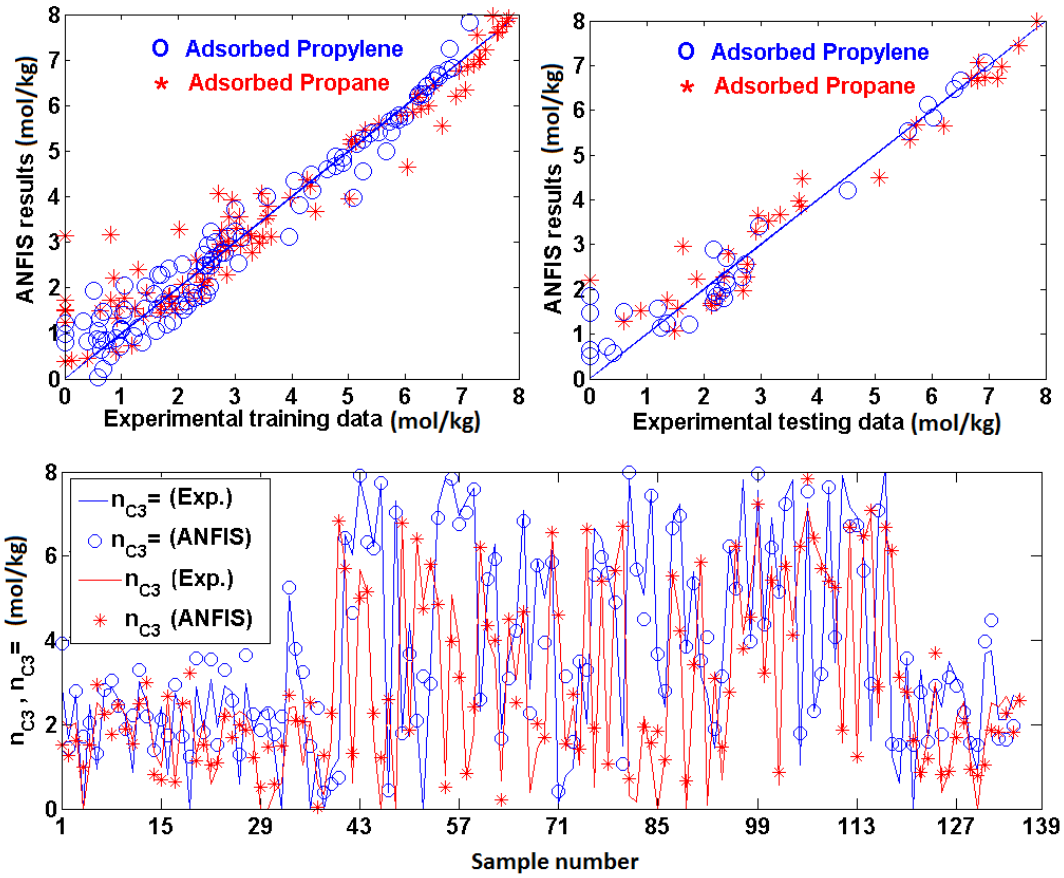

Fig. 3. The results of PSO-ANFIS model

Table 3. Properties of the best PSO-ANFIS structure

Type	Sugeno
Number of the inputs	3
Number of the outputs	1
Number of membership functions for each input	3
Number of membership functions for the output	3
Type of the input membership function	Gaussian
Type of the output membership function	Linear
Total number of fuzzy rules	3
Total number of nonlinear parameters	36
Total number of linear parameters	15
Epochs (for each population)	420
Number of particles (for each population)	84
w1 (inertia weight)	1
w2 (inertia weight damping ratio)	0.99
C1 (personal learning coefficient)	1
C2 (global learning coefficient)	2

Table 4. The obtained standard errors for the introduced models

Network	Data	MAE	RMSE	R
ANN	Training	0.09	0.12	0.9986
	Testing	0.12	0.17	0.9966
PSO-ANFIS	Training	0.40	0.58	0.9679
	Testing	0.43	0.57	0.9699

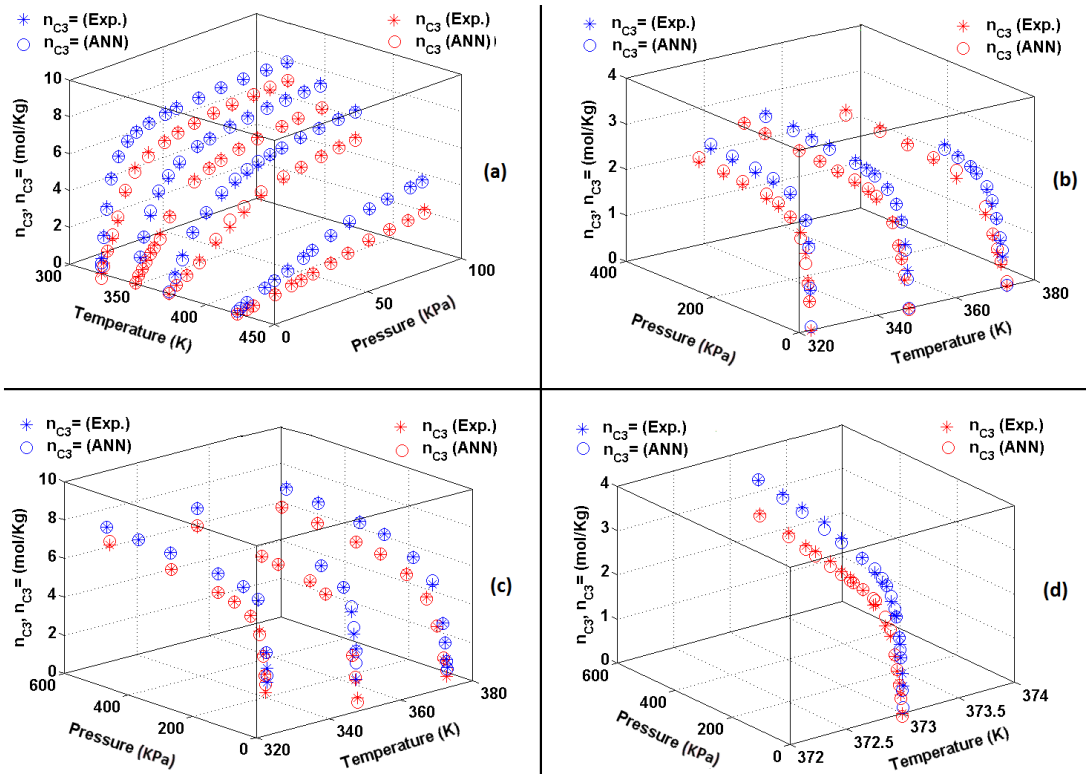

Fig. 4. Comparison results of the presented ANN structure, and adsorbent shapes (a) sphere, (b) extrudate, (c) tablet, and (d) powder

Conclusions

In this work, ANN structure along with a novel and effective hybrid approach are proposed for prediction of propylene/propane separation by Cu-BTC adsorbent. The proposed hybrid method is based on the combination of PSO and ANFIS structures. We compared the predictions of the proposed ANN and PSO-ANFIS models with the experimental data. The results showed that the PSO-ANFIS and ANN approaches have high accuracies. Also, the ANN model with less complicated structure was found to be more accurate than the PSO-ANFIS model. The MAE for ANN model had an average value of 0.111, outperforming PSO-ANFIS approach. Therefore, the proposed models could be used to solve more complex scientific problems.

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