Research article

Hybrid intelligence methods for modeling the diffusivity of light hydrocarbons in bitumen

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ABSTRACT

The solvent diffusivity is considered as a key factor in the design of solvent assisted processes in the bitumen field. In this study, a novel Adaptive neuro-fuzzy interference system (*ANFIS*) is employed to evaluate the diffusivity of the light hydrocarbons in the bitumen system. The particle swarm optimization (*PSO*) and genetic algorithm (*GA*) are adopted to promote *ANFIS* efficiency. The proposed models are established by a prepared dataset from multiple papers in the literature. Temperature (T), pressure (P) and molecular weight of alkanes (Mw) were considered as the input variables and on the other hand, Statistical parameters and graphical methods were used to appraise *ANFIS*, *ANFIS-PSO*, and *ANFIS-GA* performance. The results demonstrated that the highest correlation coefficient is related to *ANFIS-PSO* with $R^2 = 0.991$ and 0.987 for train and test data, respectively. In the end, the results indicated that the *ANFIS-PSO* model has a higher level of desirability based on statistical parameters.

1. Introduction

Bitumen is known with a specific gravity of less than 10 API [1, 2]. Due to the high viscosity of produced bitumen by conventional methods (i.e., commercial recovery procedures such as cyclic steam stimulation (*CSS*) and steam-assisted gravity drainage (*SAGD*) used to reduce the bitumen viscosity) [2, 3, 4, 5, 6], these processes require a great amount of steam per volume unit of the produced oil [3, 5, 7]. Environmental issues and greenhouse gas emissions are a product of burning natural gas so as to produce the steam required for viscosity reduction [3, 5, 8]. A superseded system based on solvent has been considered regarding its low energy-consuming less than 3% of SAGD, where water is not required in this procedure [9]. Solvent dissolution of bitumen in solvent-aided thermal recovery technique decreases the viscosity of bitumen by co-injecting a blend of saturated steam and solvent into bitumen [8]. The production rate of heavy oil recovery processes using hydrocarbon injection is dependent on the diffusivity of these solvents [2, 10]. Solvent diffusivity plays an essential role in the development of the solvent-assisted processes in the bitumen system [11, 12]. There are

some experimental studies on the light n-alkane diffusivity in heavy oils reported in the literature [2,13, 14, 15, 16, 17, 18, 19]. All of these measuring procedures are expensive and time-consuming for the computation of diffusivity coefficient, and it's because of the low rate of diffusion, composition analysis, and a few data sets available [19].

Recently, artificial intelligence technologies such as artificial neural network (*ANN*), adaptive neuro-fuzzy inference system (*ANFIS*), and support vector machine (*SVM*) have drawn researchers' attention because of their high capability, and flexibility in different applications including system classifications, predictive processes, and control systems [4, 20] that can be applied to a vast range of systems to predict the behavior of experimental systems [21, 22, 23, 24, 25]. To estimate diffusivity, different types of intelligent predictive tools have been reported [4,26, 27, 28, 29]. Based on the paper of Abbasi and et. Al., a multilayer perceptron and ANFIS approach were employed to predict the diffusivity of hydrocarbons combination. Eslamloueyan and et. Al studied a feed-forward neural network to estimate the binary diffusivity coefficient over a wide range of temperatures.

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In the current investigation, hybrid models are proposed equipped with an adaptive neuro-fuzzy inference system as a powerful, intelligent technique coupled with a Genetic algorithm (*GA*) and particle swarm optimization (*PSO*) to develop the ANFS model for the prediction of diffusivity of light n-alkane solvent in bitumen in operational conditions.

2. Methodology

2.1. ANFIS

The adaptive neuro-fuzzy inference system known as ANFIS was initially designed by Jang and Sun [30]. This intelligent system has been considered in detail due to incorporation of artificial neural network (*ANN*) with the Fuzzy Inference System (*FIS*) [31]. Regarding this ability, it is a powerful network structure, which is a popular and effective tool for function approximation application. To reach the optimized response, the ANFIS can be coupled with hybrid learning methods like GA, PSO, or Imperialist Competitive algorithm (*ICA*) [32, 33]. The ANFIS establishes a communication between input and output based on seers of Sugeno type of the If-Then rules. The model includes two fuzzy rules that can be explicated as follows:

Rule 1: If x is n_1 and y is m_1, then $z_1 = p_1x_1 + q_1y + v_1$ (1)

Rule 2: If x is n_2 and y is m_2, then $z_2 = p_2x + q_2y + v_2$ (2)

Where q_i, p_i, v_i are the consequent parameters, n_i and m_i are the linguistic labels.

    Layer 1:

$$d_{1,i} = \mu_{ni}(x)d_{1,i} = \mu_{mi}(y), \text{ for } i = 1, 2 \tag{3}$$

Where $d_{1,i}$ is the output of the *ith* node, and μ_{ni} and μ_{mi} represent membership function (*MF*).

    Layer 2:

$$d_{2,i} = \mu_{ni}(x) * \mu_{mi}(x) \text{ for } i = 1, 2 \tag{4}$$

Where d_{2i} is the output of layer 2.

    Layer 3:

$$d_{3,i} = \overline{w} = \frac{w_i}{w_1 + w_2} \text{ for } i = 1, 2 \tag{5}$$

Where $d_{3,i}$ is the normalized value, and w is the normalized firing strength.

    Layer 4:

$$d_{4,i} = \overline{w}_i z_i \quad \text{for } i = 1, 2 \tag{6}$$

Where $d_{4,i}$ denotes the defuzzification value.

    Layer 5:

$$d_{5,i} = \sum_i \overline{w}_i z_i \tag{7}$$

The ANFIS approach has five-layers including fuzzification layer, normalized layer, defuzzification layer, and an output layer, which are shown in Figure 1. In the first layer, a fuzzy set of input values are obtained by adaptive nodes with their functions. The weight of the rules (wi) in the second layer is obtained by multiplying the input values of each node by each other. In the third layer, the normalization of the weight of each rule is calculated. Defuzzification is fulfilled in the fourth layer, and finally the output is extracted [34].

2.2. PSO

PSO is known as one of the most potent hybrid techniques, which can lead to an excellent optimal output. This intelligent structure was represented by Kennedy and Eberhart in 1995 [35, 36]. Figure 2a shows the structure of PSO as a random optimization population-based method with accidental position and velocities, which are assigned to each particle. Initially, the algorithm is trying to reach the best optimal solution that leads to updating the position of the particles in a certain number of
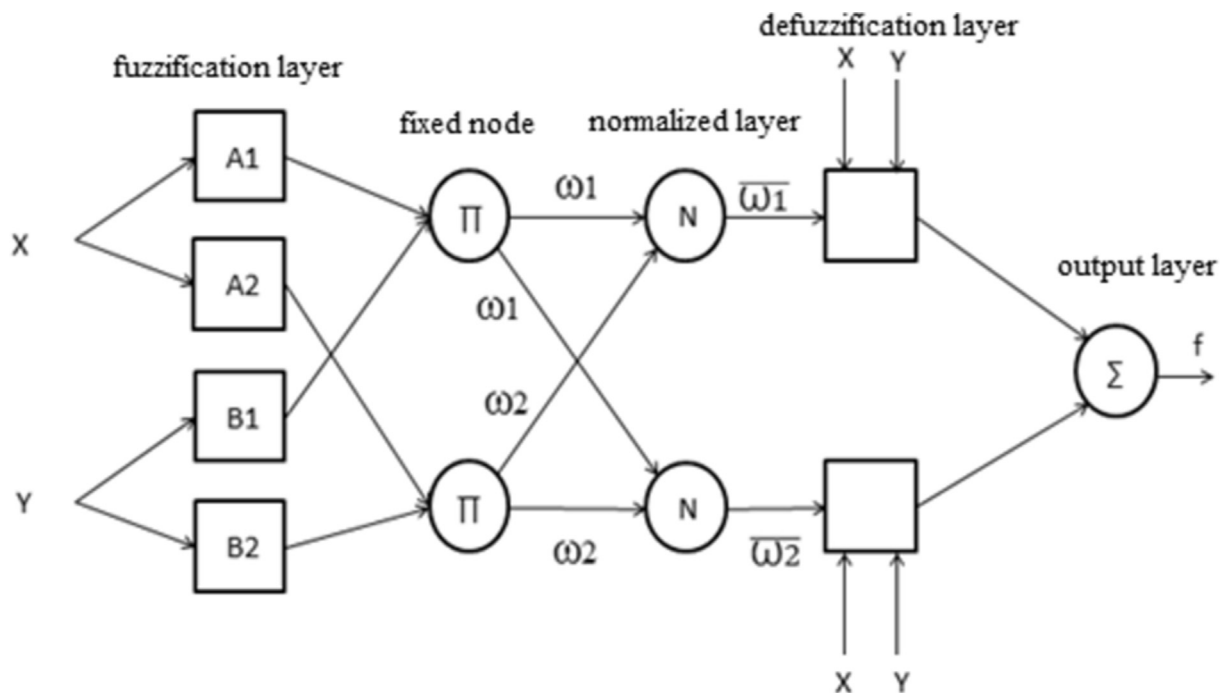

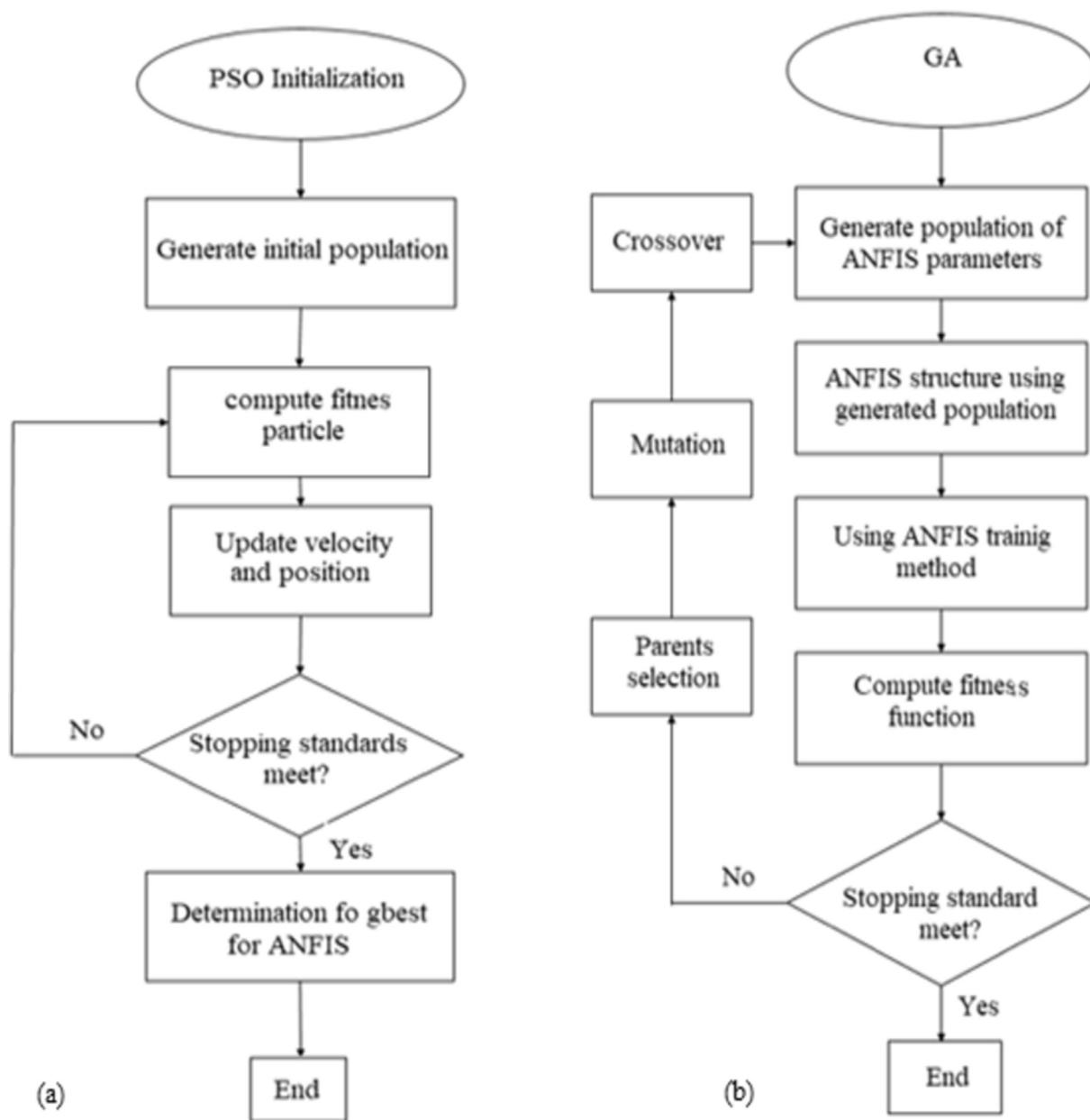**Figure 1.** The scheme of ANFIS structure.

Figure 2. Optimized ANFIS with PSO (a),and GA(b).

iterations [37, 38]. Eqs. (3) and (4) update the velocity, and position of each swarm in each iteration.

$$g_i^{k+1} = w g_i^k + c_1 r_i^k \left(p_i^k - x_i^k \right) + c_2 r_2^k \left(p_{gbest}^k - x_i^k \right) \qquad (8)$$

$$x_i^{k+1} = x_i^k + g_i^{k+1} \qquad (9)$$

Where $g_i^{(k+1)}$, x_i, and w denote the velocity of the ith swarm in the kth iteration, position of the swarm, and the premier weight, respectively. r_1 and r_2 are random numbers between [0,1]. C_1 and C_2 are cognitive acceleration and social acceleration, respectively. P_{gbest} is the optimum solution obtained from swarms, and p_i indicates the global best position [39].

At first, an initial population is generated, and the random velocities and positions are distributed. In the next level using regression analysis, every swarm is examined. As the best swarm's compatibility rate met the stopping criterion, the algorithm should be stopped. On the other side, if the compatibility rate doesn't meet the stopping criterion, the positions and velocities of swarms must be updated.

Table 1. The range of experimental data.

n-alklane	Temperature (K)	Pressure (MP)	Diffusivity*10^{-10} (m^2/s)	Ref
CH$_4$	297–449	3.33–8	0.6–168	[15, 16]
C$_2$H$_6$	297–373	0.77–8	1.3–9.5	[13, 14]
C$_3$H$_8$	288–360	0.33–2.3	0.3–11.5	[2, 17, 18]
C$_4$H$_{10}$	299–365	0.22–0.99	2.7–22	[2]

Table 2. Specification of ANFIS structure.

ANFIS structure	Description values
Fuzzy structure	Sugeno-type
Initial FIS for training	Genfis 3
Membership function type	Gaussian
Number of input	12
Number of output	1
Optimal method	Hybrid
Training maximum epoch number	2000
Step size decrease rate	0.059
Step size increase rate	0.95

2.3. GA

GA is a type of random optimization procedures based on genetics theories. GA is divided into three principal steps, known as elementary population generation, GA operators (selection, crossover, and mutation), and assessment through the adjustment function, which are described more precisely in [40, 41].

- In GA, the solution is considered as a chromosome. The initial population is a set of solutions in optimization problem conditions.
- In the selection operator, each solution with high compatibility values has a higher chance of continuing the process.
- In the crossover operator, a new chromosome is created by the scattered random method.
- The mutation operation avoids trapping to local optima.
- In the assessment section, the fitness function is computed for any individual solution.

The scheme of the GA optimization method is shown in Figure 2 b.

2.4. Data processing

For the development of the proposed models, a set of reliable experimental data is gathered from the literature, which is shown in Table 1. To enhance the model accuracy, the collected data are normalized using the following formula [42].

$$n_i = \frac{n - n_{\min}}{n_{\max} - n_{\min}} \tag{10}$$

Where n_i is the normalized value, n is the initial value, nmin minimum variable value, and nmax denotes maximum variable value.

Generally, the error values are used as a credible evaluation for the model's prediction. The results offer that the reliable model is considered as the main model with the lowest error values. To evaluate the accuracy of models, the statistical values such as mean absolute relative deviation (MARD), mean squared error (MSE), maximum absolute error (MAE) and, R^2 were considered.

$$MSE = \frac{\sum_{i=1}^{k} (a - P)^2}{k} \tag{11}$$

$$MAE = \frac{1}{k} \sum_{i=1}^{k} \frac{|P - a|}{a} * 100 \tag{12}$$

$$MARD = \frac{\max|P - a|}{a} * 100 \tag{13}$$
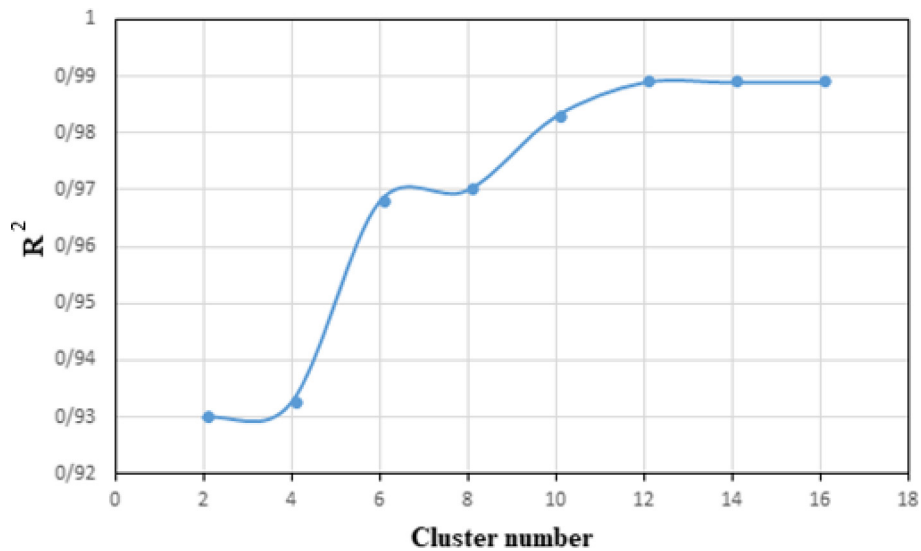
Where a is the actual value, and p is the predicated value.

Figure 3. Performance of ANFIS for different cluster.

Table 3. Specification of PSO structure.

PSO structure parameters	Description values
Maximum iteration	2000
Particle number	50
Initial inertia weight	0.9
Inertia weight damping ratio	0.99
Cognitive acceleration (C1)	1.05
Social acceleration (C2)	2.05

Table 4. Specification of GA structure.

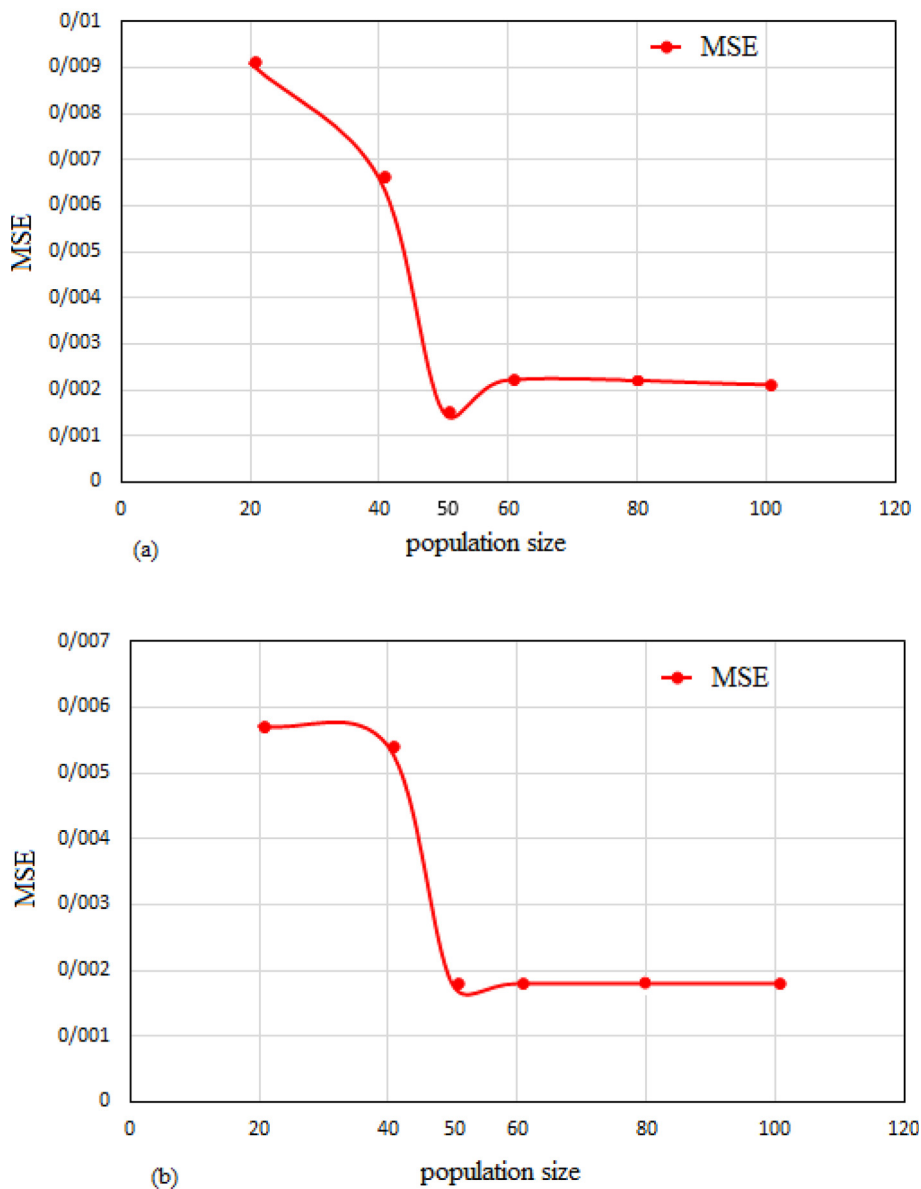| GA structure parameters	Description values
Population size	50
Maximum number of generation in GA	2000
Crossover %	0.8
Selectin pressure	8
Mutation rate	0.15

Figure 4. Performance of ANFIS PSO (a), and ANFIS GA (b) based on MSE for various population size.

Table 5. Comparison of performance of developed model for test and train data.

Models	Training				Testing			
	R^2	MSE	MAEA%	MAAE%	R^2	MSE	MAEA%	MAAE%
ANFIS	0.97	0.0025	2.46	26.4	0.98	0.0038	3.41	24.32
ANFIS-GA	0.989	0.0012	1.59	23.02	0.984	0.0032	2.72	26.06
ANFIS-PSO	0.991	0.0010	1.30	23.01	0.987	0.0027	1.98	23.48

3. Result and discussion

Since the purpose of this study is diffusivity modeling of light hydrocarbons in various operational conditions in bitumen, the temperature, pressure, and molecular weight of alkanes were set as input parameters. Choosing the input parameters for the preparation of the

ANFIS is vital as a challenge in the nonlinear system modeling [40]. As mentioned earlier, the data set are normalized between (0,1) and then divided randomly into 70% for training and 30% for the test. An ANFIS approach was proposed to determine the diffusivity of light n-alkane. To this end, a Gaussian type membership function)MF(was used to develop the ANFIS model in which contains 12 rules based on
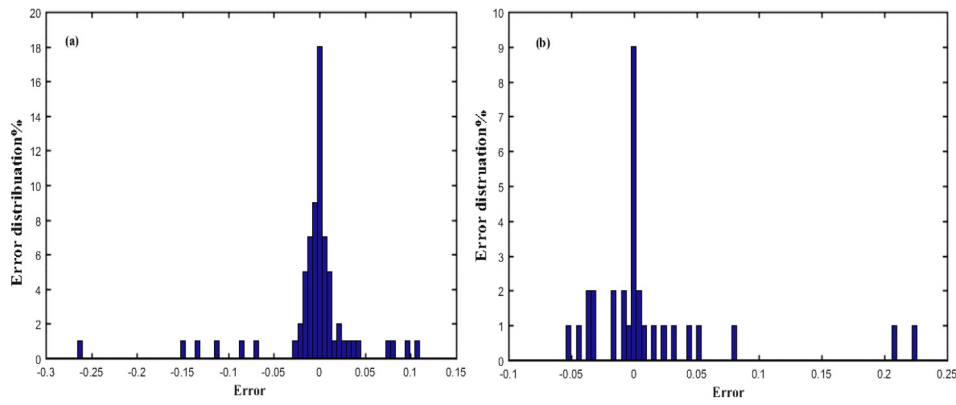
Figure 5. Error histogram of ANFIS for train (a) and test (b).
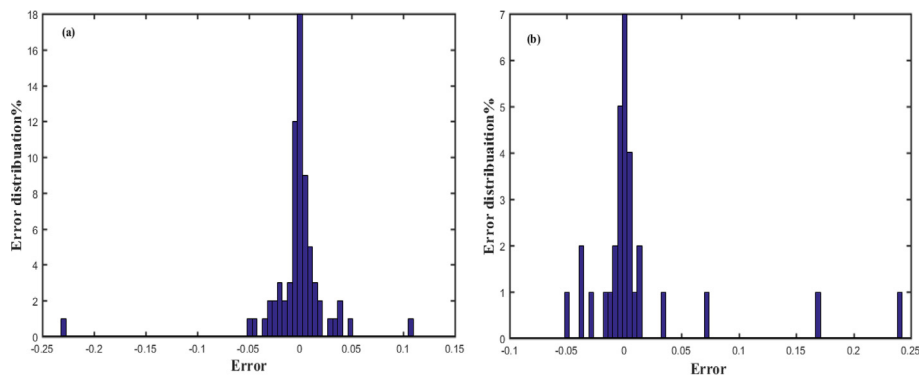

Figure 6. Error histogram of ANFIS-GA for train (a) and test (b).

the FCM model. The structure of the prepared model is shown in Table 2. The ANFIS training was performed with 2000 epochs. The number of clusters of the ANFIS structures plays an important role in the efficiency of this model [43]. Therefore, the coefficient determination of this network was evaluated based on different number of clusters and is shown in Figure 3. As can be seen, the model with 12 clusters has a suitable performance.

To reach high accuracy, the developed model is coupled with the PSO and GA optimization methods. PSO and GA were used to train the ANFIS and specify the optimal values of ANFIS results. In the case of ANFIS-PSO, the best solution of PSO parameters can be obtained from the parameter investigation (i.e., maximum iterations count, maximum particle numbers, initial inertia weight (Wmin), inertia weight damping ratio (Winamp), cognitive acceleration (C1) and social acceleration (C2)). The optimum values of these parameters were obtained based on a trial and error technique. The Gaussian function was considered as MF. Table 3 shows the best parameter structure of PSO (i.e, particles number = 50, maximum iterations number = 2000, C1 = 1.05, C2 = 2.05, Win = 0.9 and Wdamp = 0.99).

Also, the Gaussian MF was used to develop the ANFIS-GA model. Trial and error techniques were employed to reach the best optimal parameters for the GA structure. The GA parameters are shown in Table 4.
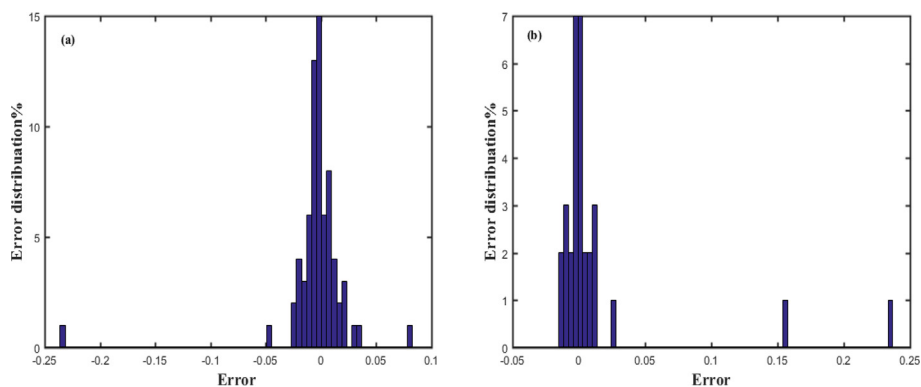

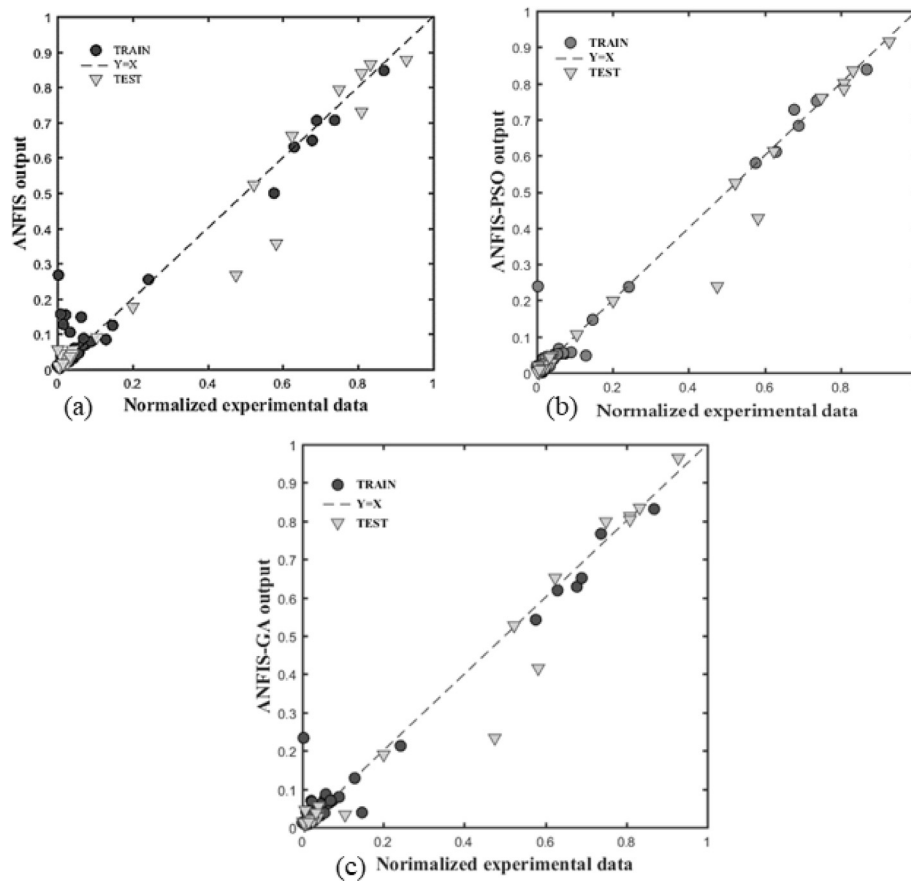**Figure 7.** Error histogram of ANFIS-PSO for train (a) and test (b).

Figure 8. Estimated data versus real data for ANFIS(a)ANFIS-PSO(b), and ANFIS-GA(c).
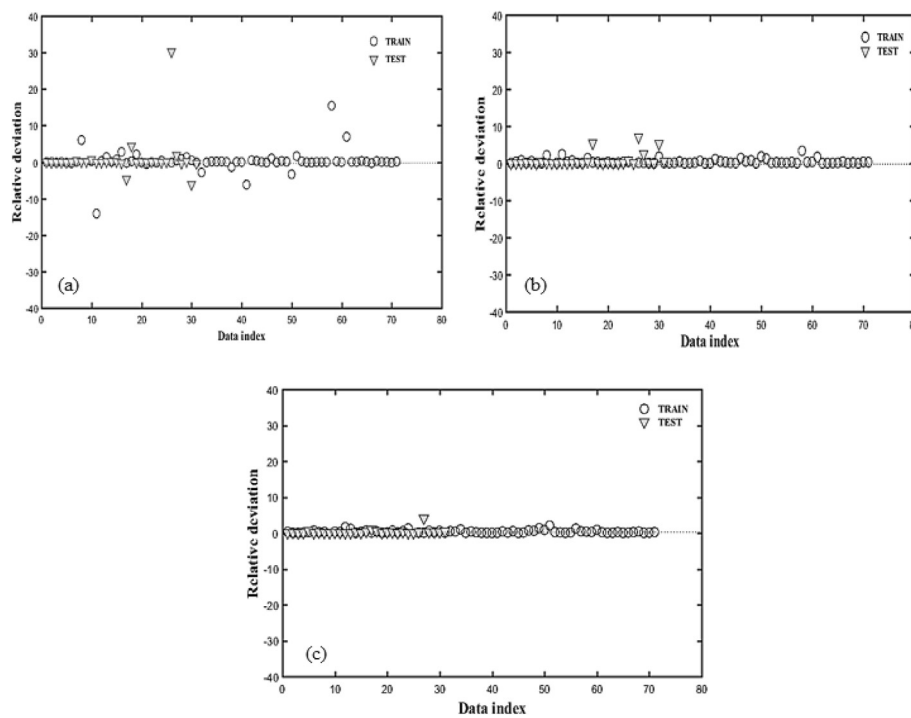

Figure 9. Relative deviation plot for ANFIS(a), ANFIS-GA(b), and ANFIS-PSO(c).

Table 6. Effect of outlier on performance of ANFIS-PSO model.

Run numb	R^2	MSE	MAAE%	MEAE%	Out numb
1(a)	0.989	0.0015	23.6	1.52	3
2(b)	0.993	0.0011	18.99	1.46	2
3(c)	0.973	0.0035	49.8	2.04	3

Table 7. Comparison of developed model with previous work.

Solvent	ANFIS-PSO		ANFIS-GA		ANFIS		Richardson et al., (2019)	
	MAE%	MARD%	MAE%	MARD%	MAE%	MARD%	MAE%	MARD%
Methane	3	10.23	3.87	24.2	6.01	26.04	5	11
Ethane	2.5	14.41	8.3	19.42	24.83	54.5	15	45
Propane	5.62	35.78	5.87	74.3	6.52	40.45	18	45
Butane	14.35	27.83	9.75	16.62	9.68	16.63	28	33

Figure 4 presents the performance of ANFIS-GA and ANFIS-PSO through the population size. As can be seen for both models, the best efficiency was attained by 50 particles, with MSE = 0.0018, and MSE = 0.0013 respectively.

Table 5 demonstrates the capability of the proposed models based on statistical parameters. A predictive model is reliable with high performance when error values are close to 0 and R^2 to 1 [40]. Due to this fact, statistical parameters in Table 5 for ANFIS-PSO are in high accordance to real data in comparison with the ANFIS and ANFIS-GA models. Figures 5, 6, and 7 illustrate the error histograms of three models for test and train data. Error histogram plots show that the obtained results have a normal curve based on the error distribution. As can be seen, most of the error values of the ANFIS-PSO model are near to zero compared with the values of the two other models. It indicates the high reliability of the developed model [44].

Figure 8 represents the forecasted values versus the normalized actual amounts for test and train values. The agglomeration of the estimated amount close to the Y = X line exhibits the appropriate capability of the models [45]. The R^2 value for ANFIS, ANFIS-GA, and ANFIS-PSO models were 0.979, 0.987, and 0.989, respectively; This expresses that the forecasting of diffusivity by three established models are in good agreement with experimental values but the ANFIS-PSO technique is more suitable than the ANFIS and ANFIS-GA structures.

As a matter of fact, the determined coefficient can't be the only way to show the reliability of the developed model, thus, a relative deviation plot has been used to investigate the capability of developed models to make the best decision. Therefore, the relative deviation for train, and test has been calculated by Eq. (9):

$$IE = \frac{P_i - R_i}{R_i} \qquad (14)$$

The IE shows the relative deviation, Pi is output amount, and Ri is the real one. The agglomeration of IE values beside zero of horizontal line axes demonstrates the high ability of the models [38, 46]. Figure 9 shows the relative deviation of ANFIS, ANFIS-GA, and ANFIS-PSO. As can be seen, ANFIS-PSO has a suitable performance in comparison to the ANFIS and ANFIS-GA models.

The assessment of the developed model by statistical and relative deviation values shows the high accuracy of the ANFIS-PSO model to predict the diffusivity of light hydrocarbon in the bitumen. Therefore, ANFIS-PSO model was selected as the best model for predicting the diffusivity value.

Additionally, to get over any hesitancy on experimental data that can affect the validation of the proposed model, the sensitivity analysis should be considered. This hesitancy on experimental values may occur because of human error or device error [47]. In data processing, some of these samples reduce the performance of the proposed model called outlier [24]. In this study, William's plot is applied to the detection of Outliers for the ANFIS-PSO model as the selected model based on the Leverage approach method (Figure 10). In this case, standardized residual and Hat values are plotted in horizontal and vertical axes, respectively. HAT values are obtained as follow:

$$H = X(X^T X)^{-1} X^T \qquad (15)$$

$$H^* = 3(N+1)/P \qquad (16)$$

H presents an (m*m) matrix, and X shows an (n*m) matrix where m and n are parameter number and data point number, respectively. H* is the critical leverage value, where N is the count of parameters, and P is related to the count of data points [24, 48]. Based on William's plot, the detected outlier is eliminated from the data set for each Run. The proficiency of ANFIS-PSO model was investigated by statistical parameters. Table 6 indicates that the performance of the proposed model was improved based on $R^2 = 0.993$, MSE = 0.0011, MAAE = 18.99, and MEAE = 1.46.

Another advantage of ANFIS is that it can estimate a specific parameter for different inputs in the training data [40]. As mentioned earlier, the ANFIS-PSO algorithm has the best performance for the prediction of diffusivity of light hydrocarbons in the bitumen system. Figure 11 shows the distribution of diffusivity of light n-alkanes based on operational conditions. Figure 11 a,b and c show the diffusivity of CH_4, C_2H_6, and C_3H_{10} versus temperature and pressure. As can be seen, the diffusivity of hydrocarbons are increased by increasing the pressure, and it's because of the mass transfer controlled by the molecular diffusion mechanism [15, 49], while the temperature does not have a significant effect on the diffusivity of C1–C3 in bitumen. Figure 11-d demonstrates the C_4H_{10} diffusivity versus temperature and pressure. The C_4H_{10} diffusivity is increased by rising temperature and pressure.

The comparison between the proposed models and previous correlation is shown in Table 7. Table 7 clearly indicates that the hybrid intelligent models have improved the MAE and MARD values. Results show the high capability of the hybrid model of ANFIS–PSO model to estimate the diffusivity with high accuracy and reliability. Therefore the
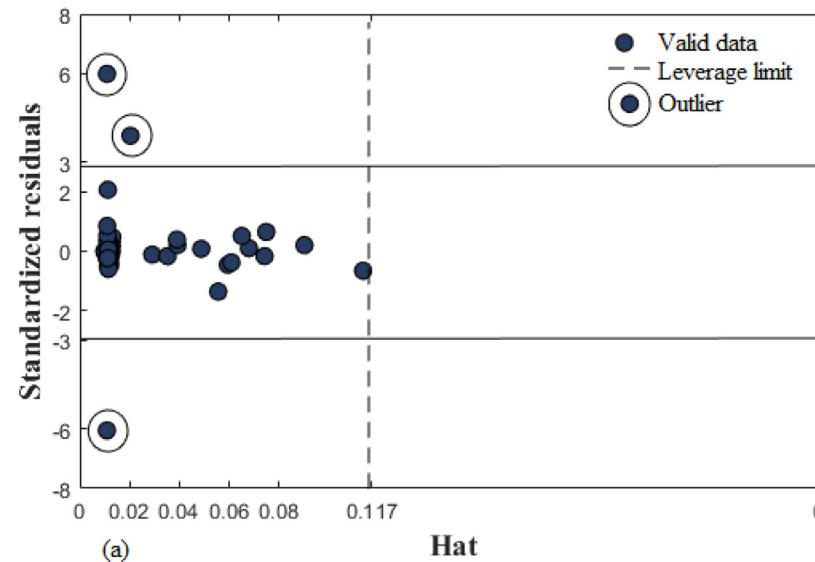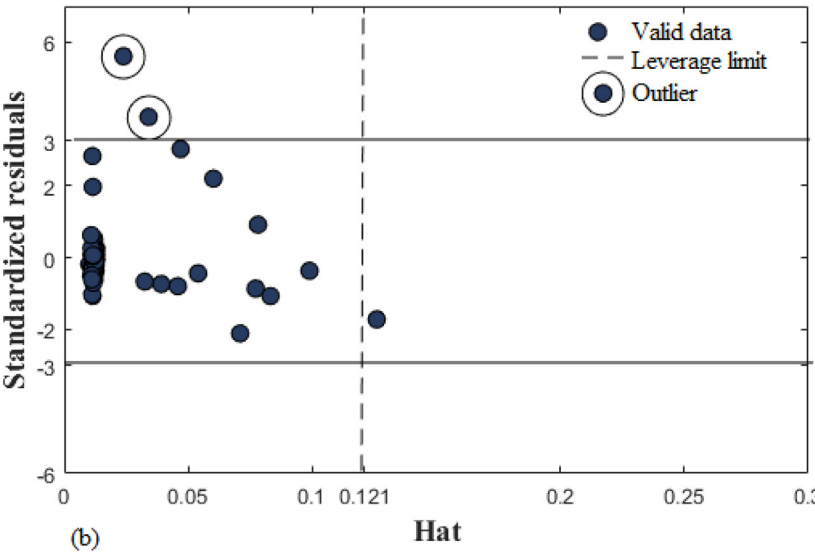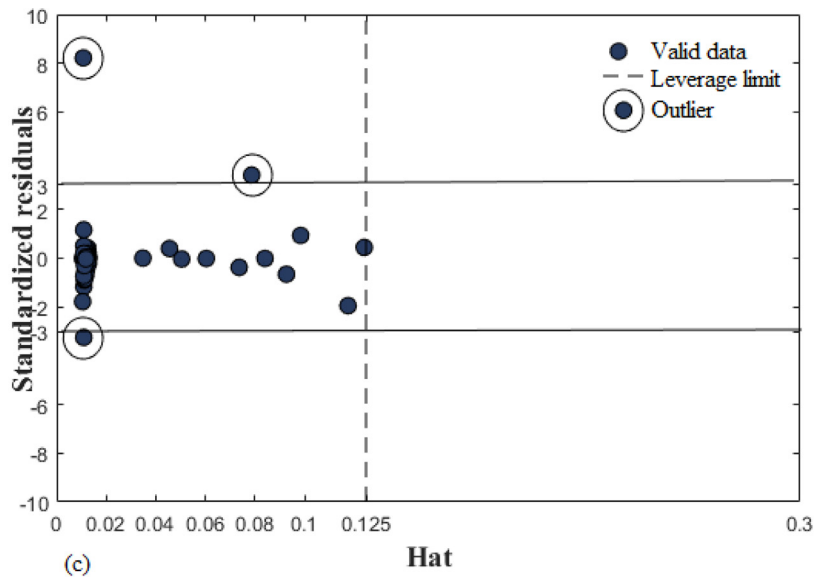
Figure 10. Detection of outliers for: (a) first run, (b) second run, (c) third run, (d).
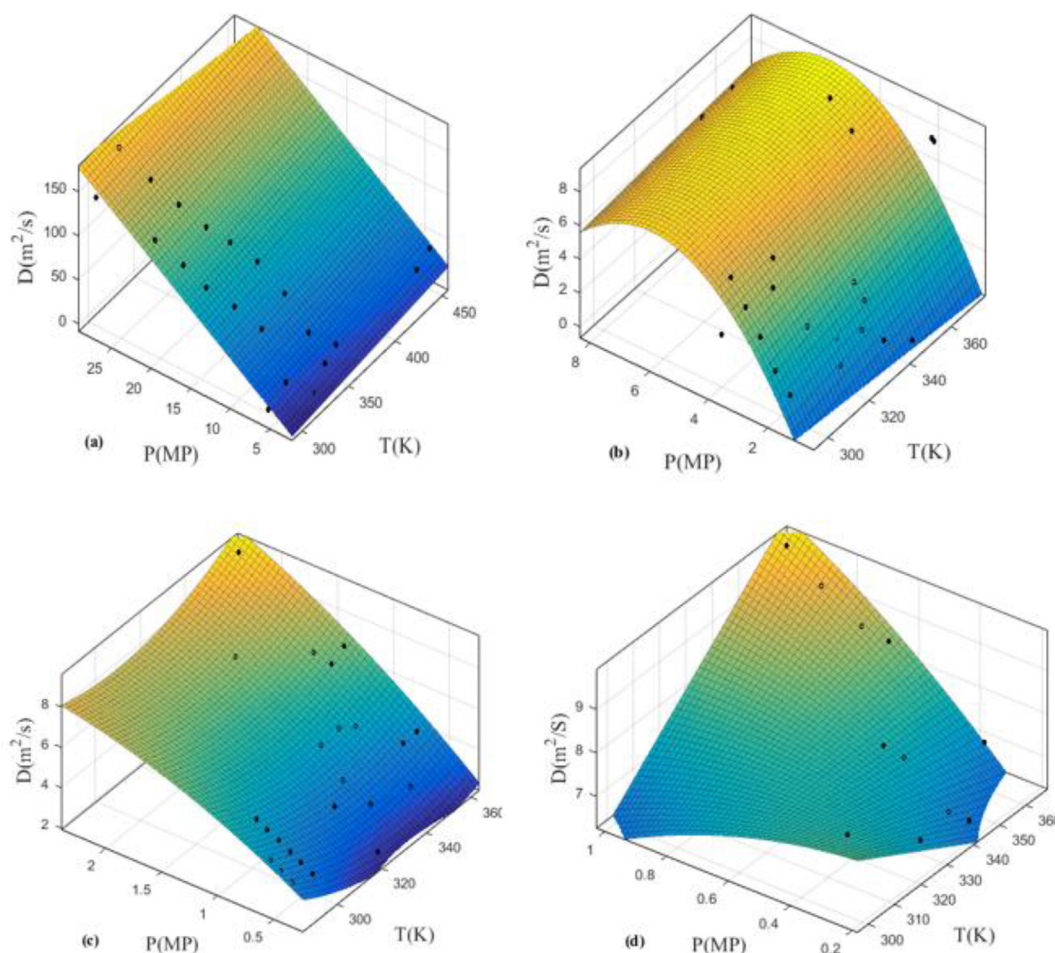
Figure 11. Effect of diffiusivity of CH_4 (a),C_2H_6 (b),C_3H_8 (c),andC_4H_{10} (d)for different conditions.

ANFIS-PSO model establishes a relation between inputs and outputs without any consideration of difficult thermodynamic concepts [50].

4. Conclusion

In this work, the diffusivity of light hydrocarbons in the bitumen system was evaluated in operational conditions. The results show the capability of ANFIS model to predict diffusivity. Also, the application of hybrid intelligent methods such as PSO and GA for the optimization of ANFIS performance was evaluated. The comparison of three proposed models (based on statistical parameters and graphical method) shows that the ANFIS-PSO model with $R^2 = 0.993$ was more suitable than ANFIS-GA and ANFIS models with $R^2 = 0.987$ and $R^2 = 0.979$, respectively.

Declarations

Author contribution statement

Hossein Rajabi Kuyakhi: Conceived and designed the experiments; Analyzed and interpreted the data.

Omid Zarenia: Contributed reagents, materials, analysis tools or data; Wrote the paper.

Ramin Tahmasebi Boldaji: Performed the experiments; Analyzed and interpreted the data.

Competing interest statement

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

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