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Using Machine Learning Methods to Estimate the Molar Density of Benzene and Comparing the Methods with the Peng-Robinson EOS

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Abstract
In chemical industries, precision in calculations and process simulations is crucial. One of the most influential parameters is the molar density of a fluid under various pressure and temperature conditions. Equations of state (EOS) are common among the methods for determining molar density. Usually, the error resulting from predicting molar density using EOS is generally high at high temperatures and pressures due to the increased intermolecular effects. Additionally, due to the form of EOS concerning volume or molar density, calculating molar volume at specified temperature and pressure requires suitable numerical methods for root-finding. This article aims to present an effective method for estimating the molar density of benzene using two crucial machine learning methods, namely Multi-Layer Perceptron-Artificial Neural Network(MLP-ANN) and Adaptive Neuro-Fuzzy Inference System (ANFIS). This study used 302 sets of experimental data to train these two methods. Additionally, another set of 60 experimental data was used to compare the errors of the methods. The Peng-Robinson (PR) equation was also employed in this article to evaluate the performance of machine learning methods better and calculate molar density. The results showed that the mean relative errors (MRE) for the MLP-ANN, ANFIS, and PR methods for the 362 data points are 0.838%, 1.791%, and 4.834%, respectively. The results demonstrated that using machine learning methods can reduce computational errors, with the error from predicting using the PR equation being almost five times that of MLP-ANN. In this article, the MLP-ANN method outperformed ANFIS due to its computational efficiency and lower error in predicting molar density.

Keywords
Multi-Layer Perceptron-Artificial Neural Network; Adaptive Neuro-Fuzzy Inference System; MACHINE LEARNING; PVT; Peng-Robinson Equations of state.

1.INTRODUCTION

Benzene is an aromatic hydrocarbon with significant applications in the petrochemical, pharmaceutical, and petroleum industries. This material is used as an industrial solvent to produce plastic materials and various chemicals. Understanding the thermodynamic properties of fluids is crucial in designing equipment, modeling, and optimizing chemical processes. A fluid's most critical thermodynamic parameter is molar density, which depends on pressure and temperature. Typically, EOS is employed to obtain this property. EOS are categorized into three groups: empirical, semi-empirical, and theoretical [1-3]. However, these equations may only provide satisfactory performance in prediction. Predicting the thermodynamic properties of fluids at high temperatures and pressures often comes with relatively high errors due to deviations from ideal behavior [4]. Additionally, EOS for volume or molar density is usually of third order or higher, requiring numerical root-finding methods for volume or molar density calculations, which can pose a significant challenge.

In chemical engineering, modeling a system considering all phenomena is challenging and often costly. Over time, a vast amount of data has become available to researchers through modeling

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and laboratory experiments [5]. Researchers can use machine learning models to make accurate predictions in various fields, such as technical and engineering, basic sciences, medicine, and agriculture, resulting in cost-effective solutions. In implementing the machine learning model, with the help of experimental data, the best prediction algorithm should be presented by creating a relationship between the data and choosing the model [6].

Data is the first loop of the machine learning process obtained through simulations or laboratory experiments. These data can be accessed with minimal costs by examining various sources and articles. Additionally, the factors the studied parameters depend on regarding the data must be specified. Essentially, what data serves as input to the system and what constitutes its output need to be determined. Then, the type of machine learning model should be selected to achieve the best performance. Various machine learning models exist, including Principal Component Analysis (PCA), t-distributed Stochastic Neighbor Embedding (t-SNE), and Density-Based Spatial Clustering of Applications with Noise (DBSCAN) [7-10]. When using a machine learning model, there should be abundant data for learning to predict a system's different conditions. The learning model should also be appropriate to minimize errors. Adherence to these considerations may result in suboptimal outputs. Artificial Neural Network (ANN) and Adaptive Neuro-Fuzzy Inference System (ANFIS) are essential machine learning methods. With suitable experimental data, machine learning methods can be utilized with minimal error for predicting properties [11, 12].

The ANN method is a machine-learning approach inspired by the human brain. The human brain consists of many neurons, each responding to signals it receives. When interconnected in a network, these neurons can perform complex tasks such as image processing and language learning [13, 14]. Each neuron comprises weight coefficients, a transfer function, and a bias (threshold). The transfer function can be any function like tanh(x). Learning algorithms determine weight coefficients and bias [15]. Each data is multiplied by the weight coefficient of each neuron, then added to the bias and entered into the transfer function. The Feed-forward method is typically used to optimize weight coefficients and biases [16]. The available data are repeatedly entered into the neural network and reduced by adjusting the error coefficients in the output [17]. The simplest type of ANN is the Perceptron, and if it has multiple layers, it is called MLP (Multi-Layer Perceptron). Optimization methods such as Particle Swarm Optimization (PSO) can be used to optimize weight coefficients and biases. Shanhui Zhao [18] used the PSO algorithm to optimize the MLP-ANN modeling for enhanced performance. Asadollah Karimi et al. [19] utilized the PSO algorithm for optimizing biodiesel production, and Shiva Nazari et al. [20] used the same method for modeling cation exchange processes in gypsum walls.

Dr. Lotfi Ali Zadeh [21] first introduced fuzzy systems in 1965. These systems are more comprehensible due to their simple mathematical calculations, making it easier to model complex processes with the help of fuzzy systems. Fuzzy systems are comprised of membership functions and rules. Fuzzy systems eliminate classic if-then rules and implement a newer approach based on experts' knowledge of actual processes [22]. Each input can have multiple membership functions, and each function has specific data ranges between 0 and 1. Using fuzzy systems requires an expert to determine the number of membership functions, function ranges, and rules based on experience. The combination of MLP-ANN and FIS (Fuzzy interface system) has recently led to the creation of ANFIS. ANFIS determines its function ranges and rules using ANFIS learning algorithms to minimize output errors and eliminate the need for an expert. This optimization method is called a hybrid learning algorithm [23].

Considerable research has been conducted using machine learning methods to predict models or fluid properties. Dehaghani et al. [24] utilized ANFIS to predict the molar density of natural gas, yielding highly favorable results. Baghban et al. [25] compared the solubility of CO_2 in ionic solutions using both MLP-ANN and ANFIS methods alongside an EOS. They demonstrated that employing machine learning methods can significantly reduce prediction errors. Jhin et al. [26] predicted the radical scavenging activities of anthocyanins using the ANFIS method. Onu et al. [27] employed ANFIS to model the thermochemical purification process to produce energy from biogas, and Dolatabadi et al. [28] used MLP-ANN to model the adsorption of color and metal ions from aqueous solutions by sawdust. Additionally, Areerachakul [29] utilized MLP-ANN and ANFIS to estimate surface waters' biochemical oxygen demand (BOD) parameters.

This article aims to calculate and predict the molar density of benzene. Machine learning algorithms such as ANFIS and MLP-ANN were utilized to accurately predict benzene's molar density using experimental data. Furthermore, the PR EOS is also used to compare the performance of machine learning methods in predicting molar density. Ultimately, the methods are compared to predict molar density by comparing MRE.

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2.EXPERIMENTAL

Initially, 362 experimental data were compiled for the study by reviewing sources [30]. These data points have molar densities ranging from 0.00198 to mol/(cm^3) and 0.009302 mol/(cm^3). The temperature range is 428.14 K to 723.18 K, and the pressure range is 8.86 bar to 355.06 bar. Of these, 302 data were used to train ANFIS and MLP-ANN algorithms. Additionally, 60 data were randomly selected from the dataset for validation to ensure coverage across the molar density range. Machine learning methods rely on empirical data. In this article, temperature and pressure are considered input data to the system, while molar density serves as the output data from the system. Figure 1A illustrates a schematic of the ANFIS algorithm, showing its rules and membership function. Figure 1B depicts a schematic of MLP-ANN, specifying the number of neurons in the hidden layer, with its input and output similar to ANFIS.

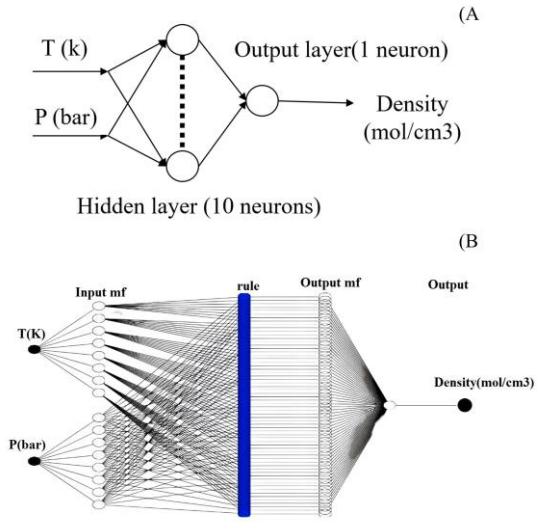

Fig. 1. Schematic of algorithms (A: MLP-ANN, B: ANFIS)

In Figure 1(a), it can be observed that the data is first multiplied by the weight coefficients of each neuron. It is then summed with bias and input into the transfer function.

The MRE, as indicated in Equation 1, was employed to assess errors.

$$MRE = \frac{1}{N}\sum_{i=1}^{N} \frac{|Density_{calc} - Density_{exp}|}{Density_{exp}} \quad (1)$$

This paper also employed the PR EOS to compare with machine learning methods. According to Equation 2 (The constants of the equation are given in equations 2-1 to 2-5.), the constants of the PR equation can be calculated by having T_c, P_c, ω, and k. The PR EOS is among the best equations for estimating hydrocarbon materials' molar density [31].

$$P = \frac{RT}{(V-b)} - \frac{a\alpha}{V(V+b)+b(V-b)} \quad (2)$$

$$a = \frac{0.45724R^2T_c}{P_c} \quad (2\text{-}1)$$

$$b = 0.07780\frac{RT_c}{P_c} \quad (2\text{-}2)$$

$$\alpha = \left[1 + k\left(1 - \sqrt{T_r}\right)\right]^2 \quad (2\text{-}3)$$

$$k = 0.037464 + 1.54226\omega - 0.26992\omega^2 \quad (2\text{-}4)$$

$$T_r = \frac{T}{T_c} \quad (2\text{-}5)$$

As it turns out, the PR EOS is a third-degree polynomial in molar volume with temperature, pressure, and constants. Molar density is the inverse of molar volume. Therefore, the PR function is also a third-degree function concerning molar density. Numerical root-finding methods must be employed to determine molar density. This paper utilized the super-Halley method, a powerful root-finding technique [32], to calculate molar density. The iteration function of the super-halley method is given by Equation 3.

$$x_{n+1} = x_n - \left[1 + \frac{1}{2}\frac{f'(x_n)^{-1}f''(x_n)f(x_n)f'(x_n)^{-1}}{1-f'(x_n)^{-1}f''(x_n)f(x_n)f'(x_n)^{-1}}\right]\frac{f(x_n)}{f'(x_n)} \quad (3)$$

The algorithm for the super-Halley method to calculate the molar volume of benzene is presented in Figure 2. It is worth noting that, to solve the super-Halley equation, an initial guess is required to start the trial-and-error process. Investigations indicate that the super-Halley method heavily depends on the initial condition; therefore, choosing a suitable initial condition is necessary to prevent the super-Halley method from diverging. Studies show that the best initial condition for the trial-and-error process is the molar volume calculated assuming an ideal gas. Hence, for a given temperature and pressure, the initial guess is determined first based on Equation 4, the ideal gas law:

$$V = \frac{RT}{P} \quad (4)$$

Then, following the algorithm presented in Figure 2, the super-Halley method determines the molar volume. It is important to note that, according to the algorithm, if $|V_{n+1} - V_n| < \varepsilon$ or $|f(V)| < \varepsilon$, the desired solution is obtained. Otherwise, by substituting V_{n+1} into V_n, the process of finding the root of the equation is repeated until the absolute result becomes less than ε. In this paper, the value of ε is considered 10^{-15} to enhance calculation accuracy.

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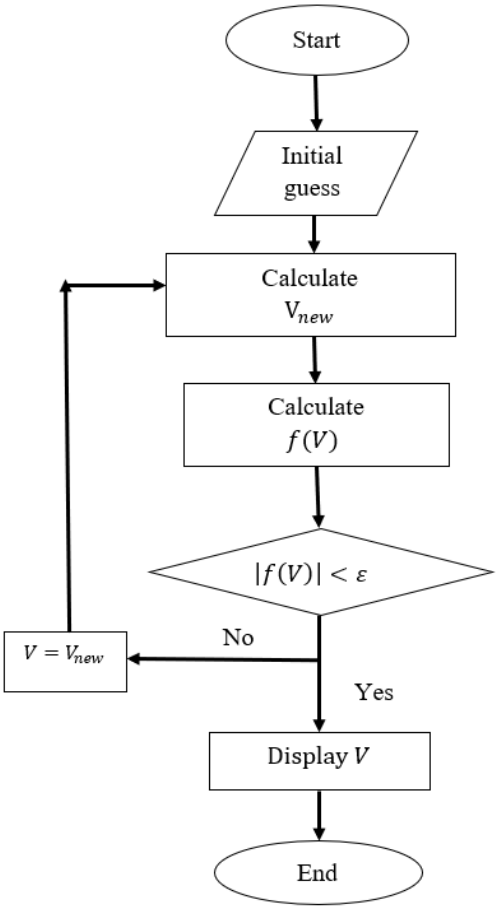

Fig. 2. Molar volume rooting algorithm

The weaknesses of the ANFIS and MLP-ANN algorithms include their extensive computational requirements and time-consuming program execution. Notably, the challenges associated with the ANFIS algorithm are significantly more severe. If the input parameters for ANFIS are numerous, the computational workload of ANFIS becomes excessively high. Additionally, when experimental data are scarce for both algorithms, the training process becomes challenging, increasing the prediction error for these two algorithms.

3.RESULTS AND DISCUSSION

As mentioned in sections 1 and 2, a relatively large amount of experimental data is required to train MLP-ANN and ANFIS to ensure a successful learning process. For this purpose, 302 benzene data were used to train both methods. In the MLP-ANN method, the inputs consist of temperature and pressure, while the output is the molar density. The type of neural network used is MLP, with 10 neurons in its hidden layer. In general, the neural network used has a hidden layer, which, as mentioned, has 10 neurons, and an output layer, which has one neuron. The way these neurons are connected can also be seen in Figure 1a. The neuron is connected to all the neurons in the next layer. The Bayesian Regularization learning algorithm was employed for MLP-ANN training, and an epoch of 1000 was considered .Also, the log-sigmoid transfer function (logs) was used for the hidden layer, and the linear transfer function (purely) was used for the output layer. The obtained error for 302 benzene data is 0.84%, and for 60 data, it is 0.83%, indicating excellent estimation of benzene data.

In ANFIS, the training data are precisely the same as those for MLP-ANN, encompassing 302 benzene data. This algorithm has 8 membership functions of the trimf (triangular membership function) type for each input. The reason for using trimf can be understood by considering Figure 3 because different membership functions such as gaussmf(Gaussian membership function), dsigmf (difference between two sigmoidal membership functions), and trapmf (trapezoidal membership function) were examined. It was shown that the trimf membership function had the best performance for this system, and as there are two inputs, the number of rules is 64. Also, a trimf membership function is considered for each rule. The Hybrid learning algorithm was utilized for training, with an epoch of 3 and zero tolerance. The errors obtained for 302 data are 1.82%, and for 60 data, it is 1.59%.

Furthermore, to compare the capabilities of machine learning methods, the results of predicting MLP-ANN and ANFIS methods were compared with the PR EOS. The prediction error for the PR EOS is 4.63% for 362 data. According to Table 1, the prediction errors of the methods are presented.

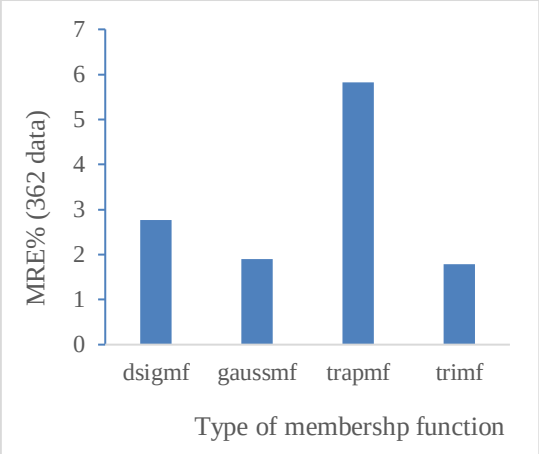

Fig. 3. Error types of membership functions

Table 1. MRE obtained for the studied methods

	MLP-ANN	ANFIS
Train data (302)	0.84%	1.82%
Test data (60)	0.83%	1.59%

MLP-ANN and ANFIS exhibit acceptable errors.

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Examining the error between MLP-ANN and ANFIS suggests that, due to the presence of adjustable parameters in the MLP-ANN method, such as weight coefficients and biases, the performance of MLP-ANN is superior to ANFIS. As shown in Figure 1B, the neural network consists of two layers. The hidden layer comprises 10 neurons, and the output layer has one neuron. To further investigate the number of neurons in the hidden layer and how many neurons to select in the hidden layer, an investigation was conducted, which can be seen in figure 4; according to figure 4, it is clear that the higher the number of neurons in the hidden layer The error also decreases, but the error increases again after 10 neurons in the hidden layer. It can be concluded that 10 neurons are very suitable for the hidden layer

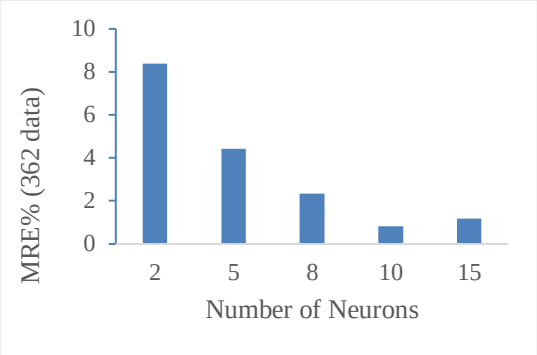

Fig. 4. The error of the number of neurons in the hidden layer

The system has two inputs. Since each must connected to all neurons in the next layer, each neuron in the hidden layer has two inputs. Therefore, each neuron has two weight coefficients and ten biases. In the next layer, with one neuron and ten inputs, there are ten weight coefficients and one bias. Thus, the number of parameters in the MLP-ANN method is 41. In contrast, in the ANFIS method, considering eight membership functions for each input, each with three unknown parameters and 112 variables in the output according to 64 rules, the number of parameters is very high, resulting in a longer learning and optimization time than MLP-ANN.

The choice of the learning algorithm is crucial. In this article, the Levenberg-Marquardt learning algorithm was used for MLP-ANN training in addition to the Bayesian Regularization learning algorithm. The results showed that the MRE for the Levenberg-Marquardt learning algorithm for 302 data was 3.84%. In other words, in the MLP-ANN method, incorrectly selecting the Levenberg-Marquardt learning algorithm, compared to Bayesian Regularization, led to a 457% increase in the MRE for predicting the molar density of benzene. One of the most significant reasons for this error may be the data not falling within the range. If the data are not in the range due to reasons such as errors in the experimental method or different fluid behavior at that point compared to the surrounding data, the algorithm's learning will have errors, especially in ANFIS, as it changes the membership function ranges based on the data value, disrupting the function's performance in that range.

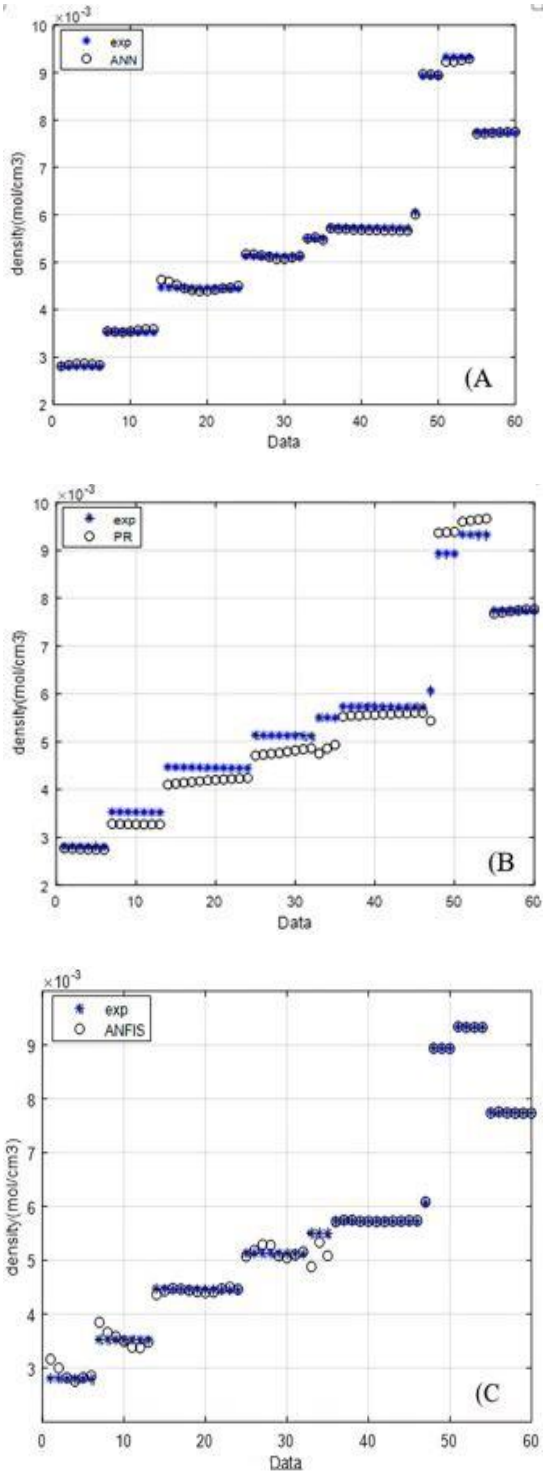

Fig. 5. Comparison diagram between A) MLP-ANN methods, B) ANFIS, and c) PR EOS with experimental data

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According to Figure 5, the validation of machine learning methods, MLP-ANN and ANFIS, along with the PR EOS, is demonstrated with 60 experimental data points. Based on Figure 5A, the ANN has effectively estimated the molar density. The PR EOS (Figure 5B) exhibits a high MRE. Only very high and low molar densities can be predicted well, and the prediction of intermediate molar densities has a significant error. In Figure 5C, corresponding to the ANFIS method, it is observed that it performs better in predicting high densities than all methods; however, it has a significant prediction error for low densities. By comparing the predictive capabilities of the studied methods, the MLP-ANN method is the most suitable for predicting the molar density of benzene. Despite its very low prediction error, it requires fewer training computations than the ANFIS machine learning method. Moreover, unlike the PR EOS, it does not require the calculation of molar density through numerical root-finding methods. Therefore, in this study, the ANN machine learning method is the most suitable among MLP-ANN, ANFIS, and the PR EOS. In this research, an appropriate solution for predicting material properties has been presented. Usually, experimental equations require laboratory data to determine their parameters using optimization tools. With this solution, these equations usually cannot cover all the data well. It may cause problems at some points, but machine learning methods with proper training can easily cover all data and have fewer prediction errors. Most importantly, the steps of machine learning training are much easier than empirical equations.

4.CONCLUSION

This article focused on evaluating and comparing two machine learning methods and an EOS for calculating the molar density of benzene. For this assessment, 302 experimental data were used to train ANFIS and MLP-ANN algorithms for predicting the molar density of benzene. These data points have molar densities ranging from 0.00198 to mol/(cm^3) and 0.009302 mol/(cm^3). The temperature range is 428.14 K to 723.18 K, and the pressure range is 8.86 bar to 355.06 bar. Additionally, 60 randomly selected data out of 362 benzene experimental data were chosen for validation. Both machine learning methods, ANFIS and MLP-ANN, could effectively predict benzene's molar density. However, the PR EOS predicted benzene molar density with a higher relative error. Using the MRE for the 302 experimental data, MLP-ANN and ANFIS demonstrated good predictions with errors of 0.84% and 1.82%, respectively. The PR EOS, with a relative error of 4.81%, predicted benzene molar density but with higher error rates. The obtained errors for 362 data for PR, MLP-ANN, and ANFIS were 4.634%, 0.838%, and 1.791%, respectively. Therefore, it can be concluded that the predictive performance order is MLP-ANN > ANFIS > PR EOS for determining benzene molar density. Additionally, the MRE for the validation of benzene molar density was 0.83% for MLP-ANN and 1.59% for ANFIS. Again, it can be concluded that the predictive performance order is MLP-ANN > ANFIS > PR for determining benzene molar density. From comparing the prediction power of the studied methods, the MLP-ANN method is the most suitable method for predicting the molecular density of benzene. Despite the very low prediction error, compared to the ANFIS machine learning method for training, it does not have many calculations for training. Therefore, the training time of the MLP-ANN method is much lower than the ANFIS method. Also, unlike the PR EOS, there is no need to calculate the molar density through numerical rooting methods. Therefore, in this study, the ANN machine learning method is the most appropriate method among the ANFIS machine learning method and PR EOS. In this study, two learning algorithms, Levenberg-Marquardt and Bayesian Regularization, were studied using the MLP-ANN method to emphasize the importance of the learning algorithm. The results showed that selecting the Levenberg-Marquardt learning algorithm instead of Bayesian Regularization led to a 457% increase in the MRE for predicting benzene molar density. It was also revealed that for the MLP-ANN hidden layer, the number of neurons is 10, and for the ANFIS for membership function type, trimf has the lowest error. It can be said that machine learning methods are an essential tool for optimizing experiments and simulations because they have fewer prediction errors and can model complex systems well. Machine learning is an essential and widely used tool because it can be used in all fields, such as the environment, pure chemistry, Medicine, etc.

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استفاده از روش‌های یادگیری ماشین برای تخمین چگالی مولی بنزن و مقایسه روش‌ها با معادله حالت پنگ-رابینسون

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چکیده

در صنایع شیمیایی، دقت در محاسبات و شبیه سازی فرآیند بسیار مهم است. یکی از پارامترهای تاثیرگذار، چگالی مولی سیال در شرایط مختلف فشار و دما است. معادلات حالت (EOS) برای تعیین چگالی مولی رایج است. معمولاً خطای ناشی از پیش‌بینی چگالی مولی با استفاده از EOS در دماها و فشارهای بالا به دلیل افزایش اثرات بین مولکولی زیاد است. علاوه بر این، با توجه به شکل EOS در مورد حجم یا دانسیته مولی، محاسبه حجم مولی در دما و فشار مشخص نیاز به روش‌های عددی مناسب برای ریشه‌یابی دارد. هدف این مقاله ارائه روشی موثر برای تخمین چگالی مولی بنزن با استفاده از دو روش یادگیری ماشینی مهم، یعنی MLP-ANN و ANFIS است. این مطالعه از ۳۰۲ مجموعه داده های تجربی برای آموزش این دو روش استفاده کرد. علاوه بر این، مجموعه دیگری از ۶۰ داده تجربی برای مقایسه خطاهای روش ها استفاده شد. معادله پنگ رابینسون (PR) نیز در این مقاله برای ارزیابی عملکرد روش‌های یادگیری ماشین و محاسبه چگالی مولی مورد استفاده قرار گرفت. نتایج نشان داد که میانگین خطاهای نسبی (MRE) برای روش هایMLP-ANN ، ANFIS و PR برای ۳۶۲ نقطه داده به ترتیب ۰.۸۳۸، ۱.۷۹۱، و ۴.۸۳۴ درصد است. نتایج نشان داد که استفاده از روش‌های یادگیری ماشینی می‌تواند خطاهای محاسباتی را کاهش دهد، خطای پیش‌بینی با استفاده از معادله PR تقریباً پنج برابر MLP-ANN است. در این مقاله، روش MLP-ANN به دلیل کارایی محاسباتی و خطای کمتر در پیش‌بینی چگالی مولی، عملکرد بهتری از ANFIS داشت.

کلید واژه ها

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