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Comparative Analysis of Computational Prediction Methods for Liquid-Liquid Equilibria in Ternary Water-Ethanol-Benzene Mixtures

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Abstract
Ethanol (EtOH) purification is a pivotal research pursuit, with liquid-liquid extraction emerging as a significant purification methodology. This study focuses on utilizing benzene solvent for EtOH purification and investigates the liquid-liquid equilibrium (LLE) within three-component systems comprising EtOH, water, and benzene. Thermodynamic modeling of EtOH-benzene-water systems at temperatures of 20 °C, 30 °C, 40 °C, and 55 °C was conducted. In this paper, the equations used for predicting mole fraction include Non-Random Two-Liquid (NRTL), Adaptive Neuro-Fuzzy Inference System (ANFIS), and Multilayer Perceptron Artificial Neural Network (MLP-ANN). First, the equation parameters were optimized using the particle swarm optimization (PSO) algorithm to employ the NRTL equation Experimental data was used to train the MLP-ANN and ANFIS methods, and the same experimental datasets were used for all models. These models estimated integral components across both phases, revealing effective system control across all methodologies. However, the comparative analysis indicated the superior performance of the MLP-ANN and ANFIS methods over the NRTL model. The Root Mean Square Deviation (RMSD) errors for the NRTL, MLP-ANN, and ANFIS models were 0.0253, 0.0035, and 0.0017, respectively. These results indicate that despite the low prediction error of all three methods, the NRTL equation has the highest error, and the ANFIS method has the lowest mole fraction prediction error.

Keywords
Liquid-liquid equilibria; Adaptive neuro-fuzzy inference system; Artificial neural network; NRTL model; Partial Swarm Optimization Algorithm

1.INTRODUCTION

There is a growing demand for purer products and improved efficiency in the chemical industry, leading to ongoing research into distillation techniques [1]. Distillation is a crucial separation process in the chemical and petrochemical industries, aiming to reduce energy consumption by utilizing the varying volatility of components [2]. However, current industrial practices for designing distillation processes can heavily rely on heuristic simulations, requiring numerous specific design specifications [3].

EtOH is a significant organic solvent used in thermometers and other applications, including fuel. Its production typically involves either the hydration of ethylene as an industrial feedstock or fermentation for fuel purposes. Unfortunately, most EtOH production processes results in an EtOH/water mixture, requiring distillation for purification. However, the presence of an EtOH/water azeotrope limits distillation, preventing the production of highly pure EtOH alone [4].

Nevertheless, azeotropic distillation is still the preferred method for obtaining highly pure EtOH in large-scale production. Furthermore, introducing a third component, benzene alters the vapor-liquid equilibrium and enables the formation of a new ternary azeotrope comprising EtOH, water, and benzene. The ternary azeotrope with the lower boiling point can be removed selectively, resulting in anhydrous EtOH [5].

Several methods have been used in the industry to separate azeotropic compositions. These methods include adding a third component that alters the vapor-liquid equilibrium (such as extractive distillation using a higher boiling solvent) and using heterogeneous azeotropic distillation to capture chemical components. However, vacuum distillation, which can be used to obtain absolute

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ethanol from an azeotropic feed, currently needs to be economically feasible [6, 7].

Therefore, this uses benzene as an entraining agent to break the azeotrope. The separation of water-EtOH mixtures has garnered significant research attention due to the potential utilization of EtOH as a sustainable fuel. Various technologies (pervaporation, zeolite adsorption, pressure-swing distillation, azeotropic distillation, extractive distillation, etc.) have been proposed for separating EtOH-water mixtures. Distillation is the primary method for separating ethanol and water, accounting for over 90% of all separation processes [8].

When multiple components are mixed, their behavior diverges from that of pure substances due to intermolecular interactions among their molecules. Consequently, determining the equilibrium behavior of phase systems becomes intricate. Practical measurements of thermophysical properties for systems such as water-EtOH-benzene involve significant costs, challenges, and time investment, particularly due to the impracticality of obtaining data across all necessary temperatures and pressures. The Non-Random Two-Liquid (NRTL) model, a significant tool in predicting phase equilibrium in non-ideal solutions, was pioneered by Renon and Prausnitz in 1968 [9]. This model, designed to address systems deviating from ideality, harnesses the concept of non-random intermolecular energies and their impact on solution behavior. By incorporating intermolecular interactions into its equations, the NRTL model can forecast solution phase behavior [10]. However, it does face challenges, particularly the requirement for experimental data to determine its parameters, which involves solving highly nonlinear equations. Furthermore, the model has limitations under specific conditions, such as at critical points [11].

Consequently, computational prediction methods such as artificial neural networks (ANN) and ; Adaptive neuro-fuzzy inference system (ANFIS) have recently gained considerable attention due to their proven reliability.

Computer-based methods have made significant contributions to the accurate prediction of material properties and characteristics. Techniques like ANN and ANFIS are particularly effective in determining the complex nonlinear relationships between input and output characteristics. These models are especially useful for systems whose equations cannot be accurately predicted [12, 13]. The applications of ANN are diverse, ranging from enhanced oil recovery, drilling, and well completion to predicting parameters like activity coefficients and kinetic coefficients [14-18]. Similarly, ANFIS has found use in predicting properties in various domains such as rubber, carbon dioxide solubility, CO_2 capture in amines, density of ionic mixtures, and thermal conductivity [19-23].

The investigation utilizes benzene-water-EtOH phase equilibrium data at various temperatures to determine the molar composition of constituents using the NRTL equation. Initially, the NRTL equation parameters are optimized using experimental data and the PSO algorithm. Additionally, ANN and ANFIS methodologies are employed to further explore and optimize the system's modeling. These methodologies, which rely on experimental data, provide robust modeling capabilities. Consequently, this study leveraged ANFIS and ANN techniques to effectively determine the molar composition of components in LLE, contributing to comprehensive system analysis and modeling.

2.EXPERIMENTAL

2.1.Parameter optimization using the Partial Swarm Optimization method

The PSO algorithm, developed by R.C. Eberhart in 1995 [24], takes inspiration from the collective behaviors observed in animal swarms. In this computational method, individual particles are endowed with initial randomized attributes, including positions and velocities [25]. These particles iteratively explore the solution space, aiming to locate optimal solutions by moving towards promising regions, mirroring the behaviors of natural swarms. Nevertheless, a significant downside of PSO is its tendency for slow convergence, where the algorithm may need numerous iterations to reach an optimal solution. Researchers have significantly addressed this challenge through various strategies and enhancements [26].

In determining the LLE within ternary systems, equations that govern the activity of individual components across two coexisting phases are utilized. These equations provide valuable insights into the dynamics and interplay among constituents in the liquid phases, enabling the precise computation of equilibrium compositions. By considering activity coefficients and their correlation with mole fractions of the components, the prediction of phase equilibrium is become more precise, fostering a deeper comprehension of the studied system's behavior (Equation 1):

$$x_i'\gamma_i' = x_i''\gamma_i'' \quad i=1,2,3 \qquad (1)$$

Where x_i and γ_i represent the mole fraction and activity coefficient of component i, respectively, for the two phases denoted $'$ and $''$.

The NRTL equation is a powerful tool for assessing the activity coefficients of individual components within a system. This equation , with its ability to accommodates the non-random nature and inherent asymmetry in molecule distribution

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across liquid phases. By integrating parameters representing molecular size, shape, and polarity, the NRTL equation offers a robust framework for estimating activity coefficients. Through the analysis of these coefficients, the intricate dynamics and intermolecular interactions within ternary systems can be precisely delineated, thereby enabling reliable predictions of LLE. This precision and depth of understanding instill confidence in the NRTL equation's application.

The NRTL equation and its constants are according to equations 2-7 [9]:

$$\ln\gamma_i = \frac{\sum_{j=1}^{N}\tau_{ji}G_{ji}x_j}{\sum_{k=1}^{N}G_{ki}x_k} + \sum_{j=1}^{N}\frac{x_jG_{ij}}{\sum_{k=1}^{N}G_{kj}x_k}\left(\tau_{ij} - \frac{\sum_{l=1}^{N}\tau_{lj}G_{lj}x_l}{\sum_{k=1}^{N}G_{kj}x_k}\right) \quad (2)$$

$$G_{ji} = \exp\left(-\alpha_{ji}\tau_{ji}\right) \quad (3)$$

$$\tau_{ji} = A_{ji} + \frac{B_{ji}}{T} \quad (4)$$

$$\alpha_{ji} = \alpha_{ij} \quad (5)$$

$$\tau_{ji} \neq \tau_{ij} \quad (6)$$

$$\tau_{ii} = \tau_{jj} = 0 \quad (7)$$

Where G_{ji} and τ_{ji} are binary NRTL parameters, A_{ij} and B_{ij} are the fitting parameters, α_{ji} is a non-randomness parameter, and T is the temperature (K).

The following objective function is used for parameter regression (Equation 8):

$$F_a = \sum_{i=1}^{3}\sum_{k=1}^{M}(x'_{ik}\gamma'_{ik} - x''_{ik}\gamma''_{ik})^2 \quad (8)$$

Equation 9 is derived from equation 8 to facilitate correlation quality assessment.

$$F_a = \sum_{i=1}^{3}\sum_{k=1}^{N}\sigma_{ik} \quad (9)$$

$$\sigma_{ik} = \begin{cases} \frac{(x'_{ik}\times\gamma'_{ik})}{(x''_{ik}\times\gamma''_{ik})} - 1, & \text{if } \frac{(x'_{ik}\times\gamma'_{ik})}{(x''_{ik}\times\gamma''_{ik})} \geq 1 \\ \frac{(x''_{ik}\times\gamma''_{ik})}{(x'_{ik}\times\gamma'_{ik})} - 1, & \text{if } \frac{(x''_{ik}\times\gamma''_{ik})}{(x'_{ik}\times\gamma'_{ik})} < 1 \end{cases}$$

Equation 9, which encapsulates the objective function pertinent to parameter estimation, is minimized, elucidating the values of parameters within the NRTL equation. This optimization endeavor reduces the disparity between calculated and empirically observed equilibrium data. The efficacy of regression, denoting the model's fidelity to experimental findings, is commonly assessed through metrics such as the mean relative error (MRE), R-squared, and RMSD.

$$MRE = \frac{1}{N}\sum_{i=1}^{N}\frac{\left|x_i^{exp} - x_i^{calc}\right|}{x_i^{exp}} \quad (10)$$

$$R_{square} = 1 - \frac{\sum_{i=1}^{N}\left(x_i^{exp} - x_i^{calc}\right)^2}{\sum_{i=1}^{N}\left(x_i^{exp} - \bar{x}\right)^2} \quad (11)$$

$$, \bar{x} = \frac{1}{N}\sum_{i=1}^{N}x_i^{exp}$$

$$RMSD = \sqrt{\left(\frac{\sum_{i=1}^{N}\left(x_i^{exp} - x_i^{calc}\right)^2}{6N}\right)} \quad (12)$$

To accurately determine the values of x_1, x_2, and x_3, it is necessary to solve the machine of nonlinear equations accurately. Numerical methods such as Newton's or similar techniques are needed for the machine. The arc-length continuation method is another exact method for solving the machine of nonlinear equations [27]. It is linear according to equation 2, and the device for the nonlinear equations has 3 equations corresponding to the three components of the two-phase system.

$$\begin{cases} f_1 = x'_1\gamma'_1 - x''_1\gamma''_1 = 0 \\ f_2 = x'_2\gamma'_2 - x''_2\gamma''_2 = 0 \\ f_3 = 1 - x''_1 - x''_2 - x''_3 = 0 \end{cases} \quad (13)$$

Equation 13 involves molar components in the phase " that are currently unknown. To determine their exact value, we use Newton's method, which requires the determination of the Jacobian matrix. The activity coefficient depends on the number of molar components. Additionally, f_3 in equation can be the same as f_1 and considered f_2. However, since the problem's condition states that the sum of the molar components in the second phase equals 1, this condition is used to solve the equation.

$$\begin{bmatrix} \frac{\partial f_1}{\partial x''_1} & \frac{\partial f_1}{\partial x''_2} & \frac{\partial f_1}{\partial x''_3} \\ \frac{\partial f_2}{\partial x''_1} & \frac{\partial f_2}{\partial x''_2} & \frac{\partial f_2}{\partial x''_2} \\ \frac{\partial f_3}{\partial x''_1} & \frac{\partial f_3}{\partial x''_2} & \frac{\partial f_3}{\partial x''_3} \end{bmatrix} \times \begin{bmatrix} \Delta x''_1 \\ \Delta x''_2 \\ \Delta x''_3 \end{bmatrix} = -\begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix} ; \Delta x = x_{n+1} - x_n \quad (14)$$

(2-6)

To solve equation 14, it is important to start with an initial guess for all three components. Once the initial guess is determined, the Jacobian matrix and the values of f are specified. Using these, we can determine the value of Δx and then obtain the next value. For a better understanding, refer to Figure 1 for calculating the molar components in the phase '; this method can also be used.

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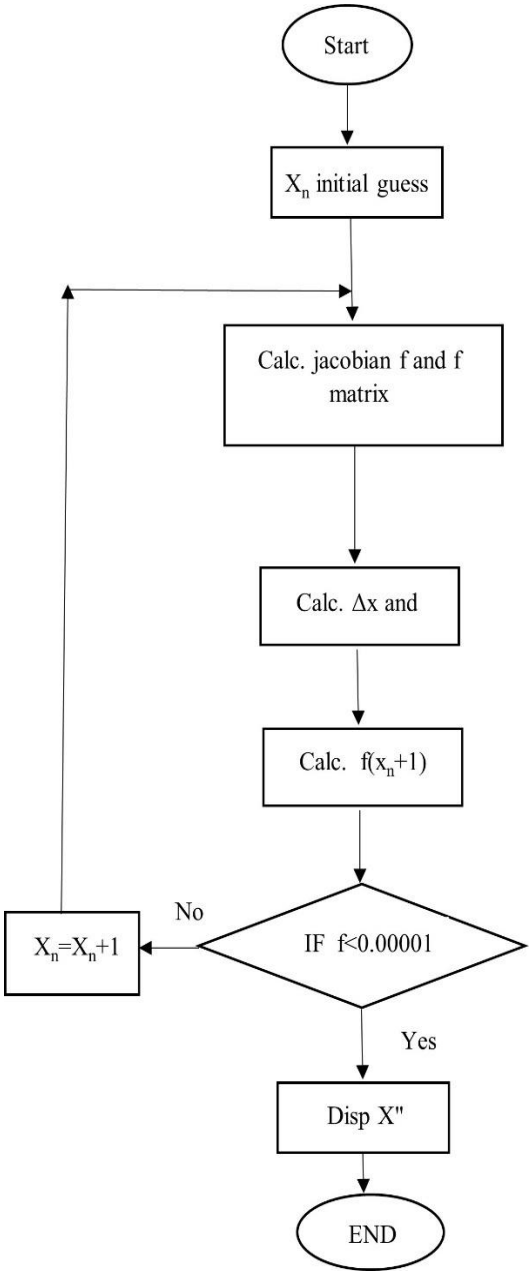

Fig. 1. Flowchart for solving sets of nonlinear equations using Newton's method

2.2.Artificial Neural Network

Neural networks imitate the structure and functionality of biological neural networks present in the human brain [28]. Computational models known as ANNs have been developed based on this paradigm. Information processing in ANNs occurs through interconnected units called neurons. [29]. Each neuron processes input data by applying weighted coefficients, activating a specified function, and integrating outcomes with bias or threshold values to generate an output [30]. Determining weight and bias coefficients in neural networks typically involves the feed-forward approach. This method involves iteratively providing input data to neurons and adjusting weights and biases to minimize output errors. This iterative refinement process is essential to neural networks' learning mechanism. [31].

Neural networks are valuable tools for analyzing complex systems characterized by intricate interrelations among components. One of the foundational architectures is the perceptron, which represents the simplest neural network structure comprising input, neuron, and output layers. However, real-world applications typically leverage multiple layers of neurons, giving rise to the Multi-Layer perceptron ANN (MLP-ANN). These MLP-ANNs offer enhanced capabilities to discern and model convoluted relationships within datasets, rendering them adept pattern recognition, classification, and regression tasks [32].

2.3.Adaptive Neuro-Fuzzy Inference System

The inception of fuzzy systems dates back to 1965 when Dr. Lotf Alizadeh [33] introduced the concept, witnessing a surge in applications over subsequent decades. Fuzzy logic has an advantage over conventional mathematical frameworks with its continuum-based approach, spanning from 0 to 1 [34]. This characteristic makes it easier to understand and model complex nonlinear systems, where precise mathematical descriptions are often challenging to obtain.

Fuzzy logic systems comprise membership functions and rules. Membership functions establish mappings between input variables and linguistic terms, while rules govern their interactions. Typically, domain experts formulate these rules based on their insights into the system under scrutiny, which can be seen as a limitation of fuzzy logic.

In response to this limitation, researchers have combined ANNs with fuzzy logic, leading to the development of ANFIS [12]. These systems combine various types of ANNs, with the Tagaki-Sugeno logic system as their foundation [35]. By incorporating fuzzy logic to handle uncertain and imprecise data, along with the neural network's ability to learn and adjust parameters using available system data, ANFIS provides a strong framework for addressing complex modeling challenges.

In the ANFIS, membership function parameters undergo determination and optimization utilizing existing system data. Typically, a hybrid learning algorithm is employed to ascertain the parameters of the Sugeno-type fuzzy logic system. This algorithm combines gradient descent with the least square error method to calculate membership function parameters. This reduces experts' need for manual intervention to establish interval values for membership functions [36].

Nevertheless, a potential drawback of this approach arises when the system's input

parameters increase, resulting in a significant rise in learning time. This scalability limitation requires careful consideration when deploying neuro-fuzzy systems to handle extensive and complex datasets [37].

3.RESULTS AND DISCUSSION

Acquiring empirical data is crucial to enhancing the development of ANN and ANFIS frameworks. These datasets, sourced from scholarly references, comprise molar component profiles observed across four discrete thermal conditions, specifically at 20 °C, 30 °C, 40 °C, and 55 °C [38-41]. A total of 45 data points were used, with ten randomly selected for model testing and the rest for model training. To refine the model, predicting the molar composition in phase 2 (water-rich phase) requires temperature readings and molar component data from phase 1 (hydrocarbon-rich phase). The models have three input parameters: water and benzene molar compositions in phase 1 (x_3' and x_2', respectively) and system temperature. The resulting output provides the predicted molar compositions of water and benzene in phase 2 (x_3'' and x_2'', respectively).

Triangular membership functions (TRIMF) were deployed to construct the ANFIS, wherein each input encompasses four distinct membership functions, each governed by three variable parameters. A hybrid optimization approach was used to fine-tune the membership function parameters. Notably, ANFIS yields a single output; hence, two separate systems were instantiated—one for benzene molar output and the other for water molar output, although they share identical inputs.

Transitioning to the MLP-ANN model, akin input data utilized in ANFIS was adopted, with the output directly representing the mole fraction of benzene and water within phase 2. It's crucial to note that the number of neurons within the hidden layer significantly impacts output error is crucial. After iterative refinement and experiential insights, a neural network configuration comprising ten neurons was chosen for hidden layer MLP-ANN and considered. Also, the log-sigmoid transfer function (logsig) was used for the hidden layer and the linear transfer function (purelin) was used for the output layer. The Levenberg-Marquardt algorithm facilitated training, with iterative learning cycles persisting until the error approached its minimum threshold, ensuring a precise estimation of molar component compositions across both methodologies.

As mentioned before, using the NRTL equation involves obtaining the necessary parameters to estimate activity coefficients and molar component compositions in phase 2. The initial step is to determine parameters by using experimental data at specific temperatures and optimizing them through an optimization method. In this case, the PSO algorithm minimizes the objective function defined in Equation 4. The algorithm utilized 50,000 particles over 100 iterations to ensure the error reached its optimal value, especially considering the challenge of working with a limited dataset and numerous parameters. Each particle in the algorithm represents NRTL equation parameters, and optimal constants were chosen to minimize risk within the search space. The search ranges were intentionally selected to allow unconstrained optimization while keeping the α_{ij} coefficients within 0 to 1 to maintain physical validity [42].

Figures 2, 3, 4, and 5 illustrate the output outcomes of an ANN and an ANFIS across various temperature settings. To compare these outcomes with those produced by the NRTL method, data obtained from the NRTL's adjustable coefficients through the PSO optimization method, as outlined in Table 1, are presented alongside the ANN and ANFIS results for comparative analysis.

The NRTL method faces several challenges, particularly in solving sets of nonlinear equations to determine molar components across different phases after adjusting adjustable parameters. The NRTL equation system in this problem was solved using the fsolve function in MATLAB. Additionally, Newton's method was employed for further investigation. Interestingly, the results obtained from both methods were identical with no differences. It's worth noting that initial guess values for both methods were chosen to be close to the experimental values to ensure convergence to the desired values. This method also requires a large amount of data to fine-tune the adjustable parameters and adjust parameters to accommodate varying activities at different temperatures. In contrast, the ANN and ANFIS methodologies avoid these complexities by effectively modeling systems through data assimilation independently of system complexity. Unlike the NRTL equation, which may fail to cover certain system conditions, machine learning methods are explicitly used for scenarios where equations are insufficient to model systems comprehensively.

The NRTL method requires solving nonlinear equations, unlike the ANN and ANFIS methodologies. The ANN and ANFIS methods use algebraic equations and straightforward operations to present results directly, making it easier to compare with laboratory data. Table 2 contains R-squared, RME, and RMSD values for all three methods. Despite these evaluations, NRTL is not as effective as alternative methods in predicting the behavior of complex systems, such as the water-EtOH-benzene three-component system

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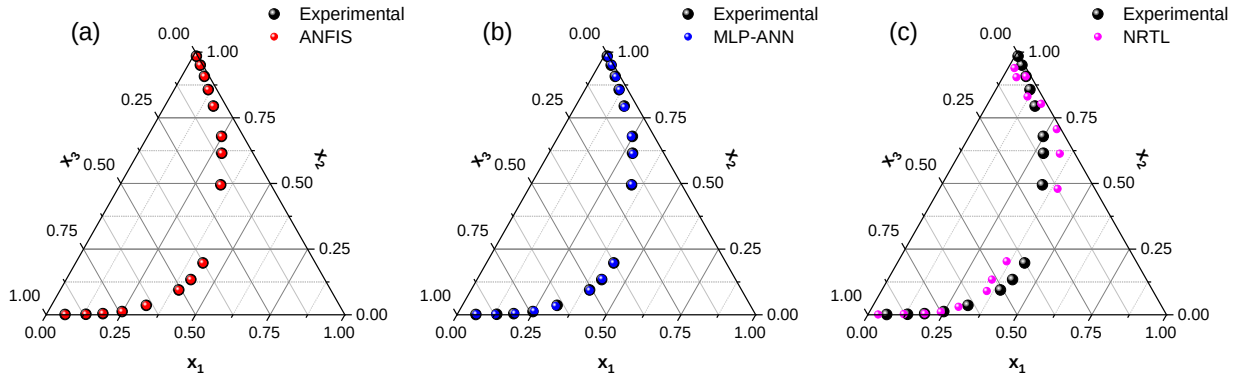

Fig. 2. Phase diagrams for the ternary system EtOH-benzene-water at 20 °C using a) ANFIS, b) MLP-ANN, c) NRTL

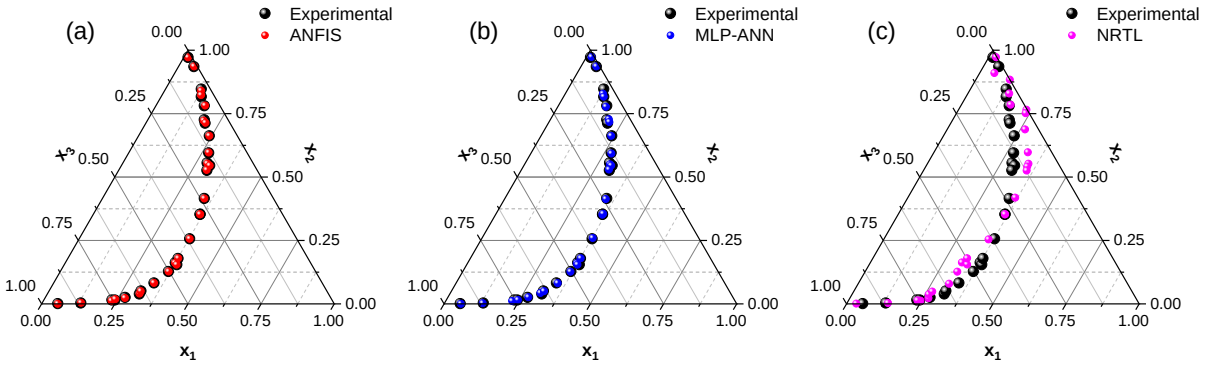

Fig. 3. Phase diagrams for the ternary system EtOH-benzene-water at 30 °C using a) ANFIS, b) MLP-ANN, c) NRTL

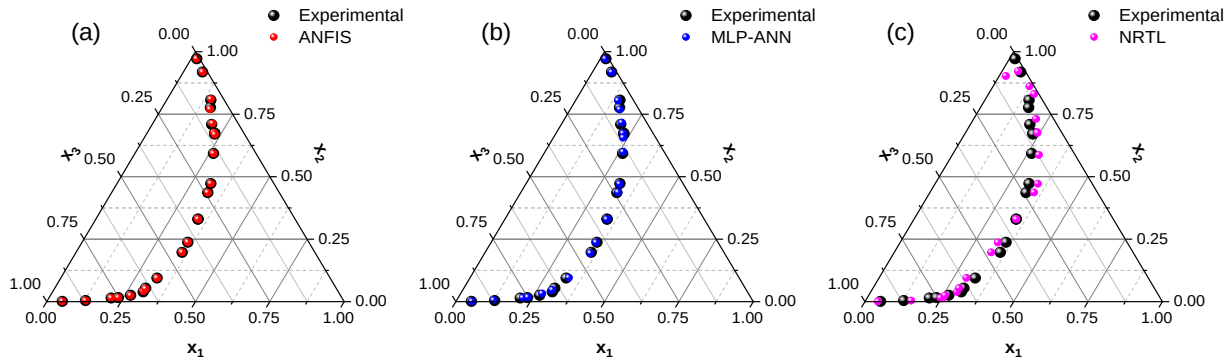

Fig. 4. Phase diagrams for the ternary system EtOH-benzene-water at 40 °C using a) ANFIS, b) MLP-ANN, c) NRTL

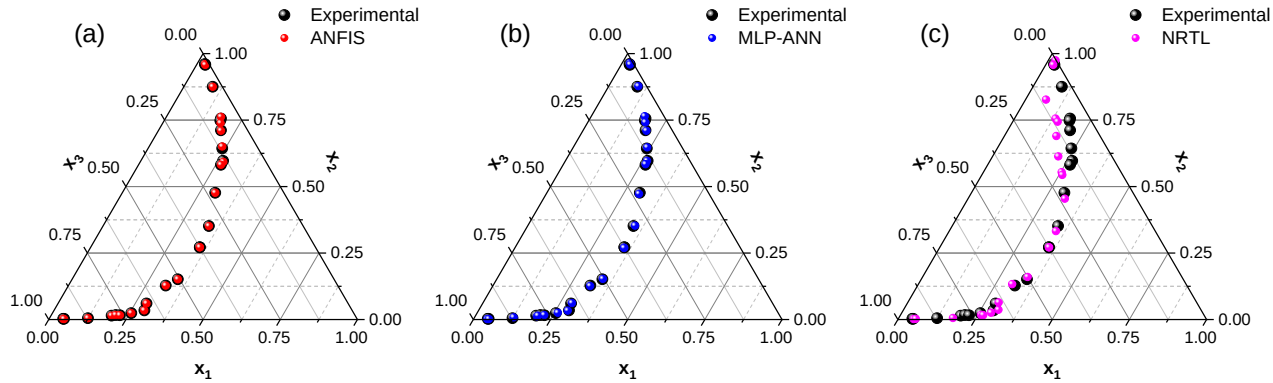

Fig. 5. Phase diagrams for the ternary system EtOH-benzene-water at 55 °C using a) ANFIS, b) MLP-ANN, c) NRTL

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Table 1. Optimized parameters of the NRTL model for ternary LLE EtOH-benzene-water systems

System	i-j	α_{ij}	A_{ij}	A_{ji}	B_{ij}	B_{ji}
EtOH (1)	1-2	0.200001	0.367489	0.62030	-2.560444	-0.379293
Benzene (2)	1-3	0.200003	0.178274	-37.50	-26.893267	400.00
Water (3)	2-3	0.200000	0.766352	1.696453	332.196148	155.550857

Table 2. R-squared, RME, and RMSD for NRTL, MLP-ANN, and ANFIS Models.

Method	Error	Test Data (10)	Train Data (35)	All Data (45)
NRTL	Rsquare	0.98848	0.99119	0.99076
	MRE	0.05386	0.09277	0.08413
	RMSD	0.02428	0.02568	0.02537
MLP-ANN	Rsquare	0.99953	0.99987	0.99982
	MRE	0.02391	0.05784	0.0503
	RMSD	0.00489	0.00303	0.00353
ANFIS	Rsquare	0.99992	0.99996	0.99995
	MRE	0.01802	0.01499	0.01566
	RMSD	0.00203	0.00162	0.00173

Table 3. Experimental and calculated plait points data for the ternary system EtOH-benzene-water at various mperatures.

Method	Temperature	Plait Point (x_1)	Plait Point (x_2)	Plait Point (x_3)
Experimental	20 °C	0.3912	0.3600	0.2488
	30 °C	0.3650	0.3530	0.2820
	40 °C	0.3440	0.3300	0.3260
	55 °C	0.3540	0.2710	0.3750
NRTL	20 °C	0.3912	0.3600	0.2488
	30 °C	0.3650	0.3530	0.2820
	40 °C	0.3440	0.3300	0.3260
	55 °C	0.3540	0.2710	0.3750
MLP-ANN	20 °C	0.3880	0.3601	0.2519
	30 °C	0.3660	0.3553	0.2787
	40 °C	0.3429	0.3291	0.3280
	55 °C	0.3543	0.2690	0.3767
ANFIS	20 °C	0.3913	0.3601	0.2486
	30 °C	0.3650	0.3530	0.2820
	40 °C	0.3440	0.3300	0.3260
	55 °C	0.3540	0.2709	0.3751

Based on Figures 2-5, the NRTL equation shows minimal error for one of the components, likely due to the mixture behaving similarly to a pure fluid, which the equation can predict accurately. However, most of its deviations are noticeable, as shown in Figure 2C. On the other hand, the ANFIS and MLP-ANN methods show predictive solid capabilities for the system, regardless of the specific temperatures or types of molar components. According to Table 2, the error metrics for ANFIS across test, training, and combined datasets are consistent, indicating its stable performance across various error measurement methods. There are discrepancies in performance between learning and test errors with other methods, indicating less robust performance. The MRE values for NRTL, MLP-ANN, and ANFIS methods, computed over 35 data points, are 0.09277, 0.05784, and 0.01499, respectively. The corresponding MRE values for 10 test data points

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are 0.05386, 0.02391, and 0.00203. This stark contrast highlights the effectiveness of ANFIS as an estimator. Using various error metrics allow for better identification of differences; for instance, the R-squared error provides insights not easily captured by other measures.

According to Table 2, the MRE for the NRTL equation is about five times higher than that for ANFIS, indicating a significant difference. The MLP-ANN and ANFIS methods are considered more user-friendly, although they are not without challenges. For example, unlike the NRTL equation, MLP-ANN or ANFIS require training to estimate the mole fraction of components for each phase, making them less adaptable as standalone comprehensive systems.

4.CONCLUSION

The distillation of EtOH is challenging due to azeotropes. Benzene is often used as a third component to resolve this issue. This paper utilized a conventional thermodynamic system modeling approach using the NRTL equation. The parameters of this equation are experimentally obtained at different temperatures, resulting in 15 adjustable parameters. The PSO algorithm minimizes an objective function derived from the NRTL equation and experimental data. To enhance the performance of the PSO, the number of particles has been increased to 50,000, with 100 iterations. Additionally, MLP-ANN methods are employed, which require experimental data similar to the NRTL equation for learning. The input parameters for MLP-ANN and ANFIS models include temperature and molar components in one phase, with the output indicating the molar components in the other phase. The NRTL parameters was determined using 35 data point, and 10 data points are selected for testing. Also, to solve the non-linear equations of the NRTL equation, Newton's method and the fsolve ready command of MATLAB were used, which yielded the same results, although the initial guess was very effective, and for convergence, we tried to consider the same points close to the experimental data. ANFIS and MLP-ANN learning are also performed following the same procedure. The MRE error of 45 data for NRTL, ANFIS, and MLP-ANN is 0.08413, 0.01566, and 0.0503, respectively, demonstrating that the ANFIS method has outperformed both previous methods. Unlike the NRTL equation, MLP-ANN, ANFIS, and related methods bypass limitations associated with media polarity and nonlinear rate device calculations, providing efficient determination of molar components through simple algebraic operations. These results highlight the effectiveness of machine learning methods in modeling multicomponent thermodynamic systems, which is superior to traditional approaches such as the NRTL equation.

Conflicts of interest

There are no conflicts of interest to declare.

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تحلیل مقایسه‌ای روش‌های پیش‌بینی محاسباتی برای تعادل مایع-مایع در مخلوط‌های سه‌جزئی آب- اتانول- بنزن

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چکیده

خالص‌سازی اتانول یک تحقیق محوری است که استخراج مایع-مایع به‌عنوان یک روش خالص‌سازی قابل توجه در حال ظهور است. این مطالعه بر روی استفاده از حلال بنزن برای خالص‌سازی اتانول تمرکز دارد و تعادل مایع-مایع (LLE) را در سیستم‌های سه‌جزئی شامل اتانول، آب و بنزن بررسی می‌کند. مدل‌سازی ترمودینامیکی سیستم‌های اتانول-بنزن-آب در دماهای ۲۰، ۳۰، ۴۰ و ۵۵ درجه سانتی‌گراد انجام شد. در این مقاله، معادلات مورد استفاده برای پیش‌بینی کسر مولی عبارتند از: دو مایع غیر تصادفی (NRTL)، سیستم استنتاج تطبیقی عصبی-فازی (ANFIS) و شبکه عصبی مصنوعی پرسپترون چند لایه (MLP-ANN). البته ابتدا پارامترهای معادله NRTL با استفاده از الگوریتم بهینه‌سازی ازدحام ذرات (PSO) بهینه شدند. داده‌های تجربی برای آموزش روش‌های MLP-ANN و ANFIS، با مجموعه داده‌های تجربی یکسان برای همه مدل‌ها مورد استفاده قرار گرفت. این مدل‌ها اجزای مولی را در هر دو فاز تخمین زدند. با این حال، تجزیه و تحلیل مقایسه‌ای نشان داد که روش‌های MLP-ANN و ANFIS نسبت به مدل NRTL عملکرد بهتری دارند. خطاهای ریشه میانگین مربعات انحراف (RMSD) به دست‌آمده برای مدل‌های NRTL، MLP-ANN و ANFIS به‌ترتیب ۰/۰۲۵۳، ۰/۰۰۳۵ و ۰/۰۰۱۷ بود. نتایج نشان می‌دهد که با وجود خطای کم پیش‌بینی هر سه روش، معادله NRTL بیشترین خطا و روش ANFIS کمترین خطای پیش‌بینی کسر مولی را دارد.

کلید واژه ها

تعادل مایع-مایع، مدل دو مایع غیر تصادفی، سیستم استنتاج تطبیقی عصبی-فازی، شبکه عصبی مصنوعی پرسپترون چند لایه، الگوریتم بهینه‌سازی ازدحام ذرات

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