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Determining the best constants of the eight-parameter non-Linear BWR equation using PSO and ACO algorithms to predict the PVT behavior of benzene

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ABSTRACT

Precision in computational analyses and simulations is paramount in the oil and gas sector. A critical aspect of these calculations involves ascertaining the molar density of gases and liquids under varying pressure and temperature conditions. For this purpose, the Benedict-Webb-Rubin (BWR) equation of state (EOS) stands out as a robust instrument for approximating the fluid's pressure-volume-temperature (PVT) properties. This article aims to introduce an effective technique for refining the BWR EOS by employing Particle Swarm Optimization (PSO) and Ant Colony Optimization (ACO) algorithms. The Super-Halley method was used to determine the molar volume or molar density. This article details how, using a dataset of 360 experimental observations, the most effective constants (comprising eight parameters) were ascertained utilizing the PSO and ACO algorithms. Furthermore, an additional set of 50 experimental data points was analyzed to assess the accuracy of the BWR EOS. The results indicated an error margin of 2.164% for PSO and 2.768% for ACO, respectively. Subsequently, the predictive error associated with the 11-parameter Benedict-Webb-Rubin-Starling (BWRS) equation was found to be 3.75%. In contrast, the simpler, three-parameter Soave-Redlich-Kwong (SRK) equation exhibited a notably higher error rate of 9.866%. These findings underscore a general trend: as the number of parameters in an EOS increase, the prediction error tends to decrease. Interestingly, its error rate is approximately double even though the BWRS equation features three additional parameters compared to the empirical BWR equation. This observation suggests that experimental approaches significantly enhance predictive accuracy despite the increased computational demands in determining optimal constants.

1. Introduction

Equations of state are fundamental tools defining the interrelations among essential thermodynamic variables pressure, volume, and temperature for specific substances or mixtures [1]. The SRK, BWR, and BWRS equations are prominent examples of such equations in the field. A common and intricate task within these equations involves the determination of volume or molar density, presenting an attractive challenge for numerical experts. Broadly, equations of state are categorized into three distinct groups: experimental, semi-empirical, and theoretical [2-4]. Empirical EOS, renowned for their high reliability, are primarily developed based on experimental data. Notable among these equations are the Beattie-Bridgeman and the BWR EOS [5-8]. A distinctive characteristic of these equations is their reliance on many parameters, which must be meticulously calculated or determined before application. These parameters are typically derived from rigorous experimental procedures.

Consequently, empirical equations are predominantly utilized for specific materials and within certain operational ranges where high accuracy is paramount. However, their extensive reliance on experimental data increases costs [9]. Moreover, determining optimal coefficients in these equations necessitates a profound understanding of optimization techniques. Semi-empirical equations of state represent an optimal fusion of

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experimental data with theoretical calculations. Examples of such equations include Van der Waals EOS, Redlich-Kwong, SRK, and BWRS [10]. A key advantage of semi-empirical equations lies in their computational efficiency and reduced reliance on experimental parameters. This combination of simplicity and practicality contributes to their widespread popularity in various applications [11]. Theoretical equations of state are fundamentally rooted in molecular models, finding extensive applications across molecular sciences and quantum physics. Notable among these are Michelson's and Morse's EOS, although their use in PVT calculations is somewhat limited due to various challenges [12]. The relevance of EOS extends to numerous practical applications, including separation processes, distillation columns, enhancing oil recovery in hydrocarbon reservoirs, and calculating water density and viscosity [13]. Aromatic compounds are indispensable in modern chemistry, pharmaceuticals, petrochemicals, and materials science. Their versatile chemical properties make them valuable in various industrial and scientific fields [14]. Benzene is an aromatic hydrocarbon with essential applications in the petrochemical, pharmaceutical, and petroleum industries. It serves as an industrial solvent in producing plastics and various chemicals. Understanding benzene's thermodynamic properties, such as PVT, is crucial for designing and optimizing industrial processes. In this context, EOSs are invaluable, as they provide precise predictions and descriptions of these properties, enabling engineers to develop more effective and efficient processes [15]. Various methods and specialized algorithms are employed to optimize processes and equations. Notably, PSO and ACO are extensively used in determining the constants of EOS, especially for those with multiple parameters like the BWR EOS. For instance, Koch et al. utilized the PSO algorithm to optimize the parameters of multiphase EOSs, demonstrating that optimization can significantly enhance EOS performance [16]. In their research, Lazos et al. applied both PSO and ACO algorithms to fine-tune the activity coefficient of the Non-Random Two-Liquid (NRTL) EOS for a 20-component mixture, revealing that these algorithms effectively predict the equilibrium behavior of liquid-vapor systems [17]. In a separate study, Lazos et al. employed the PSO algorithm to optimize the activity coefficients for mixtures of 14 different alcohols with water, finding that the predictive capability of the PSO algorithm surpassed that of traditional equations of state [18]. Furthermore, the BWR equation can be seen as an evolution of the Beattie-Bridgeman empirical equation [19]. Addressing the shortcomings of the Beattie-Bridgeman EOS in critical regions, Benedict et al. introduced a modified version known as equation 1, which enhances the original by incorporating additional parameters.

$$P = RT\rho + \left(B_0RT - A_0 - \frac{C_0}{T^2}\right)\rho^2 + (BRT - A)\rho^3 + A\alpha\rho^6 + \frac{C\rho^3}{T^2}(1 + \gamma\rho^2)\exp(-\gamma\rho^2) \qquad (1)$$

The equation previously discussed is widely recognized as the BWR EOS [20]. Furthermore, an alternative representation of the BWR EOS is formulated in terms of the compressibility coefficient, which is referred to as equation 2:

$$Z = 1 + \frac{B_0}{V} - \frac{A_0}{VRT} - \frac{C_0}{VRT^3} + \frac{B}{V^2} - \frac{A}{V^2RT} + \frac{A\alpha}{V^3RT} + \frac{C}{V^3T^3}\left(1 + \frac{\gamma}{V^2}\right)\exp\left(-\frac{\gamma}{V^2}\right) \qquad (2)$$

Where A_0, B_0, C_0, A, B, C, α, and γ are the eight constants of this EOS. Initially, the BWR EOS was primarily utilized to predict the thermodynamic properties of light hydrocarbons, pure substances, and their mixtures [21, 22]. Further investigations have revealed that equation 2 can also be used for non-hydrocarbon materials [23, 24]. The BWR EOS is particularly lauded for its precise predictions of the thermodynamic properties of light hydrocarbons and their mixtures, making it one of the most reliable EOS for assessing the PVT properties of hydrocarbons [22]. Additionally, it has been noted for its adeptness in covering critical areas because thermodynamic studies of fluids in critical areas are crucial [25, 26]. Further studies revealed the versatility of BWR EOS, extending its predictive capabilities to liquids and gases. This led to modifications enhancing its accuracy in predicting liquid behavior [27]. Determining its constants is one of the main problems when using the BWR EOS. For this reason, many efforts were made to provide a suitable method to find the constants of the BWR equation. One of the most common techniques is using the least square error technique. Ramolo and Frizzell notably developed a method employing this technique to determine the BWR EOS's constants accurately. Then, with the help of this method, they determined constants for ammonia in both liquid and vapor phases [28]. Similarly, Crane and Sontak developed another approach for data fitting using the least square error technique, applying it to calculate the BWR equation constants for nitrogen [29]. However, the least square error technique, typically more suited for linear equations, faces limitations when applied to the non-linear BWR EOS, often leading to less satisfactory results [30, 31]. To address this issue, Mateo Gomez and Tados introduced a non-linear regression method based on Markratt's optimization technique [32]. This method, while effective, requires accurate initial guesses for all eight parameters. Bragg et al. [33] proposed an alternative approach that necessitates only an initial guess for the γ parameter. They derived the value of γ graphically; however, this graphical approach tends to diminish the method's validity and the accuracy of the resulting constants [33]. The efforts of the researchers show that when the optimization of a non-linear equation such as BWR is considered, it is necessary to provide suitable optimization methods. These researches efforts underscore the critical need for appropriate optimization techniques, especially when dealing with non-linear equations like the BWR EOS. The primary objective of this article is to determine the optimal coefficients for the BWR EOS, specifically for benzene. Benzene PVT data originates from various studies. Consequently, the optimal constants for the BWR EOS are determined using the PSO and ACO algorithms. A comparative analysis of the BWR EOS and other EOS, such as BWRS and SRK EOS, focuses on their predictive accuracy with experimental data. It is important to note that the Super-Halley method calculates volume or molar density. This method significantly enhances the convergence speed of the BWR equation in these calculations, thereby accelerating the program's overall runtime.

2. Materials and Methods

Initially, 410 sets of benzene PVT data were prepared after reviewing various sources [1]. Optimization was performed using 360 of these data sets. The best constants for the BWR equation were determined by employing the PSO and ACO algorithms. Each repetition required 360 volume or molar density calculations in this phase. This necessity led to the choice of the super-Halley method, which is notable for its high convergence speed. This process was repeated until the optimal constants for the BWR equation were identified. An additional 50 data sets were then used to evaluate the error rate and, in essence, the predictive capability of the EOS. To further demonstrate the predictive efficiency of the BWR equation with optimal coefficients, it was compared with the 3-parameter SRK equation and the 11-parameter BWRS equation. Subsequently, the PSO, ACO, and Super-Halley methods are briefly discussed.

2.1. PSO and ACO algorithms

The PSO algorithm is a population-based algorithm for solving optimization problems. This algorithm draws inspiration from the collective behavior of birds and fish in nature. In PSO, a group of particles is initialized with random positions and velocities within the search space. Each particle represents a potential solution to the optimization problem and retains the best positions discovered so far [34]. The ACO algorithm, similar to PSO, is an optimization algorithm. In this approach, a population of ants is placed within the search space, and each ant independently explores paths while being influenced by the others. Upon traversing a path, each ant deposits a certain amount of pheromone (a chemical signal) along its trail. These pheromones play a crucial role in the ants' decision-making process. Paths with a higher concentration of pheromones indicate locations identified as effective by other ants. As a result, subsequent ants are more inclined to follow these more pheromone-rich routes [35]. In this article, the PSO and ACO algorithms have been utilized to optimize the molar density of benzene using the BWR EOS. The Super-Halley method, employing temperature and pressure data, initially determines the molar density from the BWR EOS (Equation 1). Subsequently, the calculated molar density is compared and evaluated against experimental data. The Mean Relative Error (MRE) function, defined based on these discrepancies, is selected as the objective function for the algorithm.

Each particle is initially assigned a random position and velocity in the PSO algorithm. Notably, each particle represents the coefficients of the BWR EOS. The performance of each particle is then evaluated using the MRE function. It is updated if a particle discovers a new position that is more optimal than its previous best. The best place among all particles is identified and recorded during each iteration. The ACO algorithm functions similarly to the PSO, with the distinction that positions leading to error reduction are marked with a higher pheromone concentration. This serves to guide other ants towards these more successful positions. Ultimately, the best place identified by the ants is the optimal solution to the problem. In these algorithms, a certain threshold is a fixed value that the objective function must reach for the algorithm to end. In other words, the algorithm stops if the MRE becomes less than or equal to this threshold. Suppose the number of iterations reaches the maximum. In that case, the algorithm continues up to a certain number of iterations. After getting this number, the algorithm stops even if the objective function has not reached the desired threshold.

$$\mathrm{MRE} = \frac{1}{N}\sum_{i=1}^{N} \frac{|\mathrm{Density_{calc}} - \mathrm{Density_{exp}}|}{\mathrm{Density_{exp}}} \quad (3)$$

The implementation of this algorithm demonstrates the potential to attain the optimal molar density for benzene. This method is capable of predicting molar density with high precision and exceptional efficiency. It holds promise as a powerful tool in oil and gas engineering and various other industrial processes. As illustrated in Figure 1, the optimization steps are delineated using the PSO and ACO algorithms.

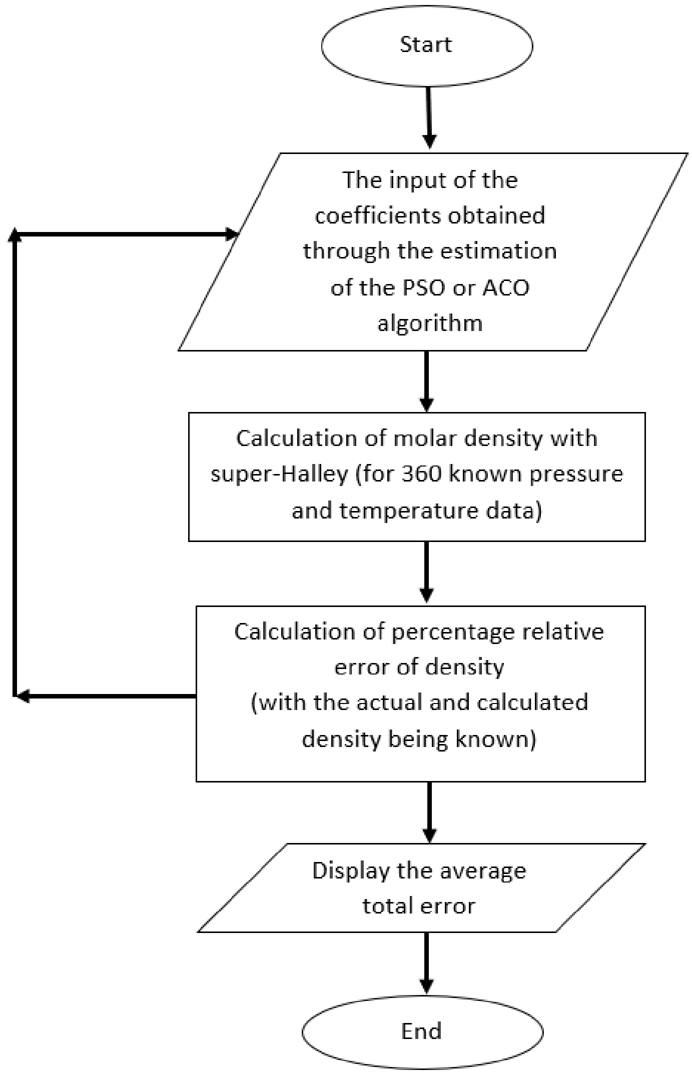

Fig. 1. Flowchart illustrates the method for calculating the constants of the BWR EOS using the PSO and ACO algorithms.

2.2. Determining the Volume or Molar Density of PVT Equations Using the Super-Halley Method

The Super-Halley method is a numerical technique used for root-finding, particularly effective with complex functions. This article used the Super-Halley method to calculate molar density. It is important to note that an initial estimate of the molar density is required when determining it under any given pressure and temperature conditions. This initial guess is determined using the ideal gas for each operating condition. The formulation and algorithm of the Super-Halley method are as follows:

$$x_{n+1} = x_n - \frac{f(x)}{f'(x)}\left(1 + \frac{1-\frac{f(x_n)f''(x_n)}{2\,|f'(x_n)|^2}}{1+\frac{f(x_n)f''(x_n)}{2\,|f'(x_n)|^2}}\right) \tag{4}$$

One of the advantages of the Super-Halley method is its high accuracy and rapid convergence rate. Additionally, this method proves highly effective in scenarios where the function exhibits rapid changes or discontinuities. However, a notable drawback of the Super-Halley method is its requirement for the first and second derivatives of the function, which can pose a challenge with certain functions [36]. According to Figure 2, the algorithm of the Super-Halley method for determining the molar density is presented.

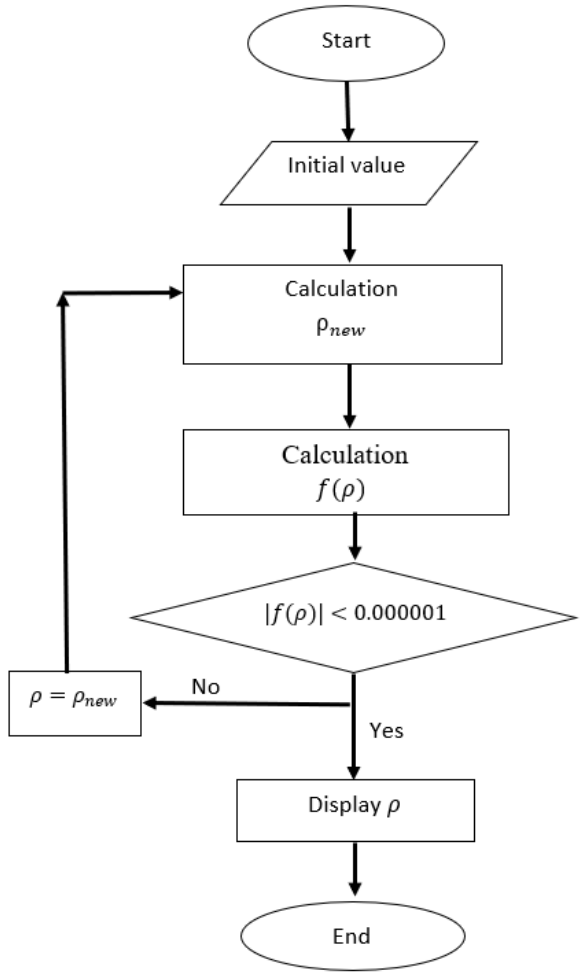

Fig. 2. Flowchart of the molar density root-finding algorithm using the Super-Halley method.

3. Results and Discussion

The Super-Halley method was employed to calculate the molar density. Initially, the function f(ρ) was established based on Equation 1, aiming to determine the molar density by setting this function to zero. The molar density is first estimated using the ideal gas for the given pressure and temperature to initiate the trial-and-error process. Subsequently, as illustrated in Figure 2, and following the algorithm of the Super-Halley method, the molar density is determined using Equation 5.

$$f(\rho) = RT\rho + \left(B_0RT - A_0 - \frac{C_0}{T^2}\right)\rho^2 + (BRT - A)\rho^3 + A\alpha\rho^6 + \frac{C\rho^3}{T^2}(1 + \gamma\rho^2) \times \exp(-\gamma\rho^2) - P = 0 \quad (5)$$

Therefore, according to equation 4, first and second-order derivatives are needed to use the Super-Holley method. Once these derivatives are determined, an initial guess of the molar density is required. As previously discussed, this initial estimate is obtained using the ideal gas. Subsequently, this estimated molar density of the ideal gas is placed on the right side of Equation 4 for computation, resulting in a new molar density value. If a discrepancy exists between the initially estimated density and this new value, the new density is adopted as the initial guess for the next iteration. This procedure is repeated until the value of the function, $f(\rho_{new})$, is reduced to less than 0.00001. The rooting program algorithm will be stopped, and the desired molar density will be obtained. Depending on the PSO and ACO algorithms, molar density calculations are determined according to the number of particles or ants and the number of repetitions to reach the optimal coefficients. After calculating the molar density, the focus shifts to the PSO method. As previously explained, this algorithm computes the coefficients of the BWR equation. Upon specifying the particles, each having 360 molar density points, the PSO algorithm calculates the sum of the relative error at all these points. This sum is then used as the objective function. A configuration of 100,000 particles and 50 iteration steps was selected for optimal performance of the PSO algorithm. The critical role of the Super-Halley method becomes apparent considering the high volume of molar density calculations, a result of the substantial number of particles and repetition steps in the PSO method. Due to this volume, a robust root-finding method is essential to enhance convergence speed and minimize rooting errors. Thus, the Super-Halley method was selected for its ability to accelerate convergence. In the PSO algorithm, numerous estimations are made for the coefficients to ascertain the most optimal set, aiming to minimize the error percentage of the method. As indicated in Table 1, the optimal coefficients determined by the PSO algorithm are presented. An evaluation of 50 data points for validation revealed that the prediction error of molar density based on the PSO algorithm was 2.164%. The ACO algorithm requires selecting a specific number of ants and repeating steps to ensure optimal performance. The article applies the ACO algorithm using 1000 ants and 100 steps. After the optimization process and the determination of the optimal coefficients, as indicated in Table 2, an evaluation using 50 data points for validation revealed that the prediction error for molar density based on the ACO algorithm was 2.768%. As discussed in the sections detailing the PSO and ACO algorithms, it is essential to note that the fundamental principles of optimization in these algorithms are similar. However, despite the algorithms being equal, the optimal coefficients for the BWR equations, as shown in Tables 1 and 2, are different. Nonetheless, the average prediction error for both algorithms is nearly the same. Also, the unit used in this study is for pressure (bar), temperature (k), molar density ($\frac{mol}{cm^3}$), and the universal constant of gases (R=83.1447 $\frac{cm^3 bar}{molK}$). according to the units used and equation 1, the units of the values in Tables 1 and 2 are determined.

Table 1. Coefficients derived from optimizing the BWR equation using the PSO algorithm

coefficient	value
A_0	18633947.541384
A	499998125.44673
α	1089205.3519701
B_0	122.47979955401
B	32090.087672453
C_0	−20000
C	18448652.139781
γ	7000000000

Table 2. Coefficients derived from optimizing the BWR+ equation using the ACO algorithm

coefficient	value
A_0	19421803.9350
A	28887672.93
α	17417106.45331
B_0	148.5008
B	23519.574752
C_0	253936208455.2842
C	1560614370908.894
γ	59997935482.18781

Next, to compare the performance of PSO and ACO algorithms with semi-empirical state equations, the predictive ability of the BWR equation was compared with SRK and BWRS equations. A critical factor in the more accurate prediction of molar density may be the number of parameters in the EOS. An increase in the number of parameters leads to a reduction in prediction error. The SRK equation is a three-parameter model, whereas the BWRS equation encompasses eleven parameters. An analysis of 50 experimental data points for validation indicates that the BWRS equation significantly outperforms the SRK equation. Figures 3A-C corroborate these findings. As demonstrated in Figure 4, the prediction errors for molar density using the SRK and BWRS methods are 9.866% and 3.75%, respectively. In other words, increasing the number of EOS parameters from three to eleven significantly reduces the prediction error. This article compares these two semi-empirical state equations with the empirical BWR equation, which has eight parameters. As previously mentioned, the eight parameters of the BWR equation were optimized using the PSO and ACO algorithms. Based on the parameters of the BWR and BWR^+ equations presented in Tables 1 and 2, the relative error of both the BWR and BWR^+ equations in predicting the molar density of benzene are much lower compared to the BWRS equation. According to Figure 4, the error rate of the BWR equation in predicting molar density is 2.164%, while for the BWRS equation, it is 3.75%. In other words, despite having three more parameters, the semi-empirical BWRS EOS has an average error of more than 73% higher than that of the BWR EOS in predicting the molar density of benzene. The results demonstrate that with proper optimization of the coefficients in empirical state equations, these empirical models can outperform their semi-empirical counterparts. Therefore, the primary purpose of this article is the role of PSO and ACO optimization algorithms in determining optimal coefficients and then accurately predicting molar density.

Figure 3 illustrates the impact of pressure and temperature on the molar density of benzene. This figure shows that the predictive abilities of the SRK, BWRS, BWR, and BWR^+ equations were evaluated against experimental data. Specifically, the temperatures investigated in Figure 3A-C were 603.15 K, 653.15 K, and 703.16 K, respectively. The results indicate that the SRK EOS, a three-parameter model, shows limited agreement with the experimental data. In contrast, the BWRS equation, which incorporates eleven parameters, demonstrates significantly better predictive accuracy than the SRK equation. Furthermore, Figure 3 suggests that by employing the meta-heuristic optimization algorithms of PSO and ACO, the prediction errors for both BWR and BWR^+ are substantially reduced, resulting in a closer alignment with the experimental findings.

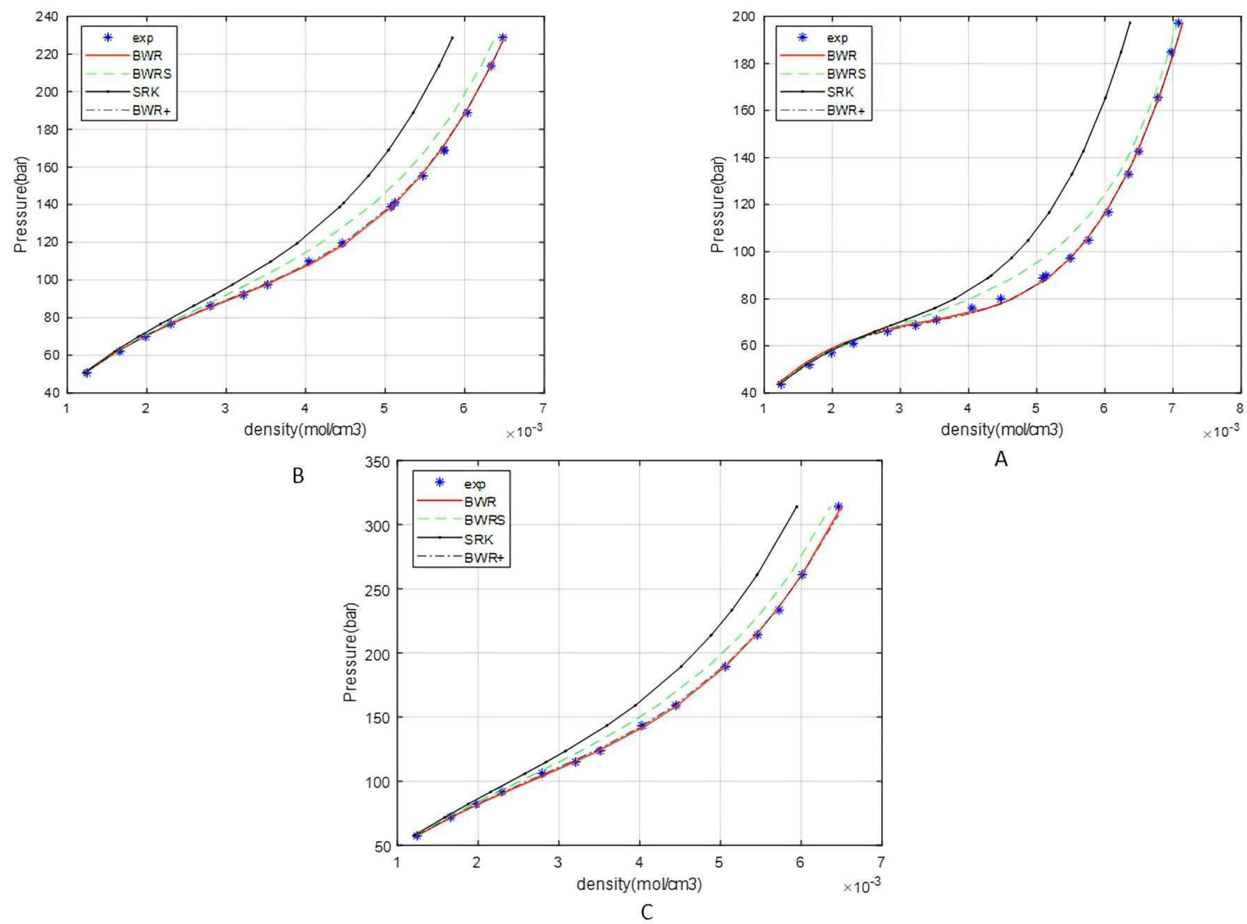

Fig. 3. The diagram of changes in molar density relative to pressure at various temperatures (A: 603.15 K, B: 653.15 K, C: 703.16 K)

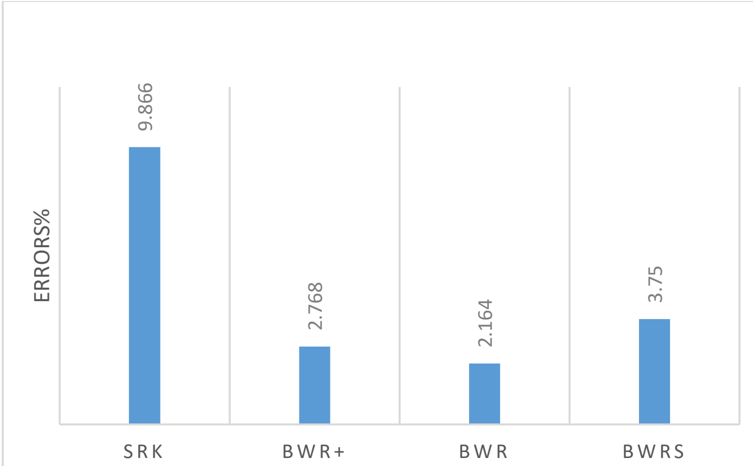

Fig. 4. Comparative Analysis of Error across Different Equations

Additionally, an examination of Figure 3 reveals that most equations exhibit diminished performance at high pressures. The results indicate that the system's behavior more closely approximates the ideal state as pressure decreases, enabling state equations to perform PVT calculations with reduced error. Moreover, Figure 3 demonstrates that the prediction error of the SRK and BWRS state equations increases with higher temperatures. Notably, under varying pressures and temperatures, the optimally tuned BWR equation consistently demonstrates accurate predictions of experimental data for benzene, maintaining good agreement with the experimental results throughout. Also, this optimization has a significant limitation: the coefficients of the equation of state. It can be used for one substance, which in this research is benzene. It does not include all substances, but on the other hand, since the coefficients are specific for each substance, the previous nose error is significantly reduced.

4. Conclusion

This article evaluates and compares the performance of various state equations in calculating benzene's PVT properties. Given the complexity and non-linearity of the BWR equation, this study explored the use of meta-heuristic algorithms such as the PSO and ACO to optimize the equation's coefficients. The optimization of the BWR state equation coefficients using the PSO and ACO algorithms yielded highly accurate results. Our investigations revealed that the average prediction error percentage for 50 PVT data points was 2.164% with the PSO algorithm and 2.768% with the ACO algorithm. In other words, the prediction errors of both the PSO and ACO algorithms were nearly identical, and these error rates were lower than those of all other state equations examined in this study. Figure 4 indicates that the prediction error for molar density using the SRK and BWRS state equations is 9.866% and 3.75%, respectively. This outcome highlights the significant impact of precise optimization of coefficients on the predictive accuracy of the BWR EOS. A critical insight from this article is that with highly accurate optimization, there is less necessity for equations with more coefficients. Notably, the 8-parameter BWR equation, when optimized using the PSO and ACO algorithms, demonstrates markedly higher efficiency than the 11-parameter BWRS equation.

Meta-heuristic algorithms like PSO and ACO are supported by limitations when optimizing the coefficients of equations. The differences in outcomes can be attributed to the nature of these meta-heuristic algorithms; this is because, by each algorithm's framework, the particles in PSO and the ants in the ACO algorithm endeavor to find the most effective route for optimizing the problem. While the optimization paths may differ based on the algorithm used, the ultimate objective remains to optimize the problem efficiently. Consequently, both algorithms, despite their different approaches, eventually converge towards the best possible solution. Given that both algorithms have achieved nearly identical error rates and the results from both methods are satisfactory, the ACO algorithm emerges as the more efficient choice regarding computational speed. This is especially true considering that the ACO algorithm utilizes 1000 ants, whereas the PSO algorithm uses 100,000 particles. Therefore, in terms of computational speed, the ACO algorithm is preferable. An essential outcome of optimizing the BWR state equation coefficients is that meta-heuristic algorithms like PSO and ACO can effectively optimize complex equations. A critical factor in successfully applying these methods is the availability of extensive experimental data, essential for obtaining optimal coefficients and validating the equation.

References

[1] G.C. Straty, M.J. Ball, and T.J. Bruno, PVT measurements on benzene at temperatures to 723 K. J CHEM ENG DATA, 32 (1987) 163-166.
[2] J.B. West and J. B West, The Original Presentation of Boyle's Law. Essays on the History of Respiratory Physiology, (2015) 55-60.
[3] S. Saeki, M. Tsubokawa, J. Yamanaka, and T. Yamaguchi, Semiempirical equation of state and the Grüneisen parameter for polymers and rare gas solids. Polymer, 32 (1991) 3170-3176.
[4] S. Saeki, Empirical equation of state for supercritical fluids. J. Supercrit. Fluids, 8 (1995) 30-45.
[5] M. Vestfálová. Thermodynamic properties of real gases and BWR equation of state. in EPJ Web of Conferences. 2015. EDP Sciences.
[6] Equation of State. In Developments in Petroleum Science, (1998) 129-166.
[7] P.L. Hagelstein, Equation of State and Fugacity Models for H2 and for D2. J. Condens. Matter Nucl. Sci., 16 (2015) 23-45.
[8] J.A. Beattie and O.C. Bridgeman, A new equation of state for fluids. I. Application to gaseous ethyl ether and carbon dioxide1. J. Am. Chem. Soc., 49 (1927) 1665-1667.
[9] P.E. Savage, Spreadsheets for thermodynamics instruction. Chem. Eng. Educ., 29 (1995) 262-269.
[10] S. ZHANG, H. IWASHITA, and K. SANADA, Soave-Redlich-Kwong adiabatic equation for gas-loaded accumulator. Journal of the Japan Fluid Power System Society, 49 (2018) 65-71.
[11] R.N. Lichtenthaler, E.G.d. Azevedo, and J.M. Prausnitz, Molecular thermodynamics of fluid-phase equilibria. (No Title), (1998).
[12] B. Poling, J. Prausnitz, and J. O'connell, The properties of gases and liquids2001McGraw-Hill. New York, 21 (2001).
[13] (a) R. Smith, Chemical process: design and integration. John Wiley & Sons (2005). (b) F. Zarei, R. Razavi, A. Baghban, and A.H. Mohammadi, Evolving generalized correlations based on Peng-Robinson equation of state for estimating dynamic viscosities of alkanes in supercritical region. J. Mol. Liq., 284 (2019) 755-764.
[14] (a) B. Hashemzadeh, L. Edjlali, P. Delir Kheirollahi Nezhad, E. Vessally, A DFT studies on a potential anode compound for Li-ion batteries: Hexa-cata-hexabenzocoronene nanographen, Chem. Rev. Lett., 4(4) (2021) 232-238. (b) S. Soleimani-Amiri, Identification of Structural, Spectroscopic, and Electronic Analysis of Synthesized….,. Polycyclic Aromat. Compd., 41 (2021) 635-652. (c) S. Soleimani-Amiri, A systematic investigation on the structure, energy, aromaticity, and stability of substituted $X_5Y_5C_{10}$ nanocages (X=B, Al, Ga, and Y=N, P, As). Heteroat. Chem, 28 (2017) e21380. (d) S. Soleimani-Amiri, Z. Hossaini, Z. Azizi, Synthesis and Investigation of Biological Activity of New Oxazinoazepines: Application of Fe3O4/CuO/ZnO@MWCNT Magnetic Nanocomposite in Reduction of 4-Nitrophenol in Water, Polycycl. Aromat. Compd., 43 (2022) 2938-2959. (e) A. K. O. Aldulaimi, A. H. Adhab, H. R. Saud, M. Ubaid, M. H. Sami, Chemical Fixation of CO2 with 2-Aminobenzenethiols into Benzothiazol(on)es: A Review of Recent Updates, Chem. Rev. Lett., 7 (2024) 241-252.
[15] K. Isinkaralar, Experimental evaluation of benzene adsorption in the gas phase using activated carbon from waste biomass. Biomass Conversion and Biorefinery, (2023) 1-10.
[16] G. Cox and M.A. Christie, Fitting of a multiphase equation of state with swarm intelligence. J. Condens. Matter Phys., 27 (2015) 405201.
[17] J. Lazzus, M. Rivera, I. Salfate, G. Pulgar-Villarroel, and P. Rojas, Application of particle swarm+ ant colony optimization to calculate the interaction parameters on phase equilibria. J. Eng. Thermophys., 25 (2016) 216-226.
[18] J.A. Lazzús, Optimization of activity coefficient models to describe vapor–liquid equilibrium of (alcohol+ water) mixtures using a particle swarm algorithm. Comput. Math. Appl., 60 (2010) 2260-2269.
[19] G.A. Neece and D.R. Squire, Tait and related empirical equations of state. The Journal of physical chemistry, 72 (1968) 128-136.
[20] E. Mansour, A. Farag, F. El-Dars, S. Desouky, M. Batanoni, and M. Mahmoud, Predicting PVT properties of Egyptian crude oils by a modified Soave–Redlich–Kowng equation of state. Egypt. J. Pet., 22 (2013) 137-148.
[21] M. Thol and I.H. Bell, Empirical fundamental equations of state for pure fluids and mixtures, (2020).
[22] R.S. Markadeh, A. Arabkhalaj, and M. Birouk, On the density prediction of multicomponent hydrocarbon mixtures at near-and supercritical conditions. Fluid Ph. Equilibria, 562 (2022) 113560.
[23] J. Tkaczuk, Equations of state for the thermodynamic properties of cryogenic mixtures. 2021, Université Grenoble Alpes [2020-....].
[24] Z. Zhang, M. Gao, X. Chen, X. Wei, J. Liang, C. Wu, and L. Wang, The Joule–Thomson effect of (CO2+ H2) binary system relevant to gas switching reforming with carbon capture and storage (CCS). Chin. J. Chem. Eng., 54 (2023) 215-231.
[25] R. Shahsavan Markadeh, A. Arabkhalaj, and M. Birouk, On the Density Prediction of Multicomponent Hydrocarbon Mixtures at Near-and Supercritical Conditions. Available at SSRN 4076714.
[26] J. Ban, C. Li, W. Yang, W. Zhang, X. Yuan, and Y. Xu, Prediction of physical properties and phase characteristics of ethane and ethane mixture in the ethane pipeline. Processes, 11 (2023) 2283.
[27] T. Tsuji and T.-a. Hoshina, Measurement of Vapor-liquid Equilibria (VLE) for the Ternary, Propane+ Dimethyl Ether+ Butane, and the Three Constituent Binaries, and Predicted Values by the Benedict-Webb-Rubin (BWR) Equation of State: Measurement and Prediction of Thermophysical Properties for Dimethyl Ether with Liquefied Petroleum Gas Components (Part 2). J JPN PETROL INST, 63 (2020) 172-183.
[28] R.W. Crain Jr and R.E. Sonntag, Nitrogen constants for the Benedict-Webb-Rubin equation of state. J CHEM ENG DATA, 12 (1967) 73-75.
[29] F.S. Acton, Analysis of straight-line data. (No Title), (1959).

[30] P.R. Bevington, D.K. Robinson, J.M. Blair, A.J. Mallinckrodt, and S. McKay, Data reduction and error analysis for the physical sciences. Comput. Phys., 7 (1993) 415-416.
[31] M. Gomez-Nieto and G. Thodos, Benedict-webb-rubin parameters for ethanol. Can. J. Chem. Eng., 54 (1976) 438-440.
[32] H. Brough, W. Schlinger, and B. Sage, Evaluation of Equation of State Constants with Digital Computers. Ind. Eng. Chem. Res., 43 (1951) 2442-2446.
[33] D.K. Grozdanić, B. Djordjević, and A. Tasić, Calculation of some thermodynamic properties of gaseous water by means of BWR equation of state. Can. J. Chem. Eng., 66 (1988) 697-700.
[34] W. Huang and J. Xu, Particle Swarm Optimization, in Optimized Engineering Vibration Isolation, Absorption and Control. Springer (2023) 15-24.
[35] P. Du, N. Liu, H. Zhang, and J. Lu, An improved ant colony optimization based on an adaptive heuristic factor for the traveling salesman problem. J. Adv. Transp., 2021 (2021) 1-16.
[36] S.K. Nayak, P. Parida, and A. Kumar, A study of 3 μ th-order of convergence of Chebyshev–Halley family method and its convergence plane. SeMA Journal, (2023) 1-22.