Critical point calculations of multi-component reservoir fluids using nature-inspired metaheuristic algorithms

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A B S T R A C T

This study introduces the application of nature-inspired metaheuristic algorithms for performing critical point calculations in multicomponent reservoir fluids. These algorithms are Monkey – Krill Herd Hybrid (MAKHA), Intelligent Firefly Algorithm (IFA), Covariance Matrix Adaptation Evolution Strategy (CMAES), Artificial Bee Colony (ABC), Cuckoo Search (CS), Bare Bones Particle Swarm Optimization (BBPSO) and Flower Pollination Algorithm (FPA). Capabilities and limitations of these optimizers have been analyzed using black oil, volatile oil, and condensate reservoir fluids with fifty components. Results showed that BBPSO, IFA and FPA outperformed other nature-inspired methods for critical point calculations in tested fluids. In particular, BBPSO offered the best efficiency-reliability tradeoff for the accurate prediction of critical points in multicomponent mixtures.

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1. Introduction

In the petroleum industry, the use of reservoir simulation tools is a vital step for the prediction of the types of fluids and number of hydrocarbon phases flowing through porous media. These data are essential to facilitate the design of the equipment used for the production and treatment of these fluids. The reservoir simulation process includes the calculation of the critical point(s) and the phase envelope of the fluid to allow the determination of the flowing phase (liquid or gas, or mixed phase) based on the operating conditions of the reservoir (above or below the critical point) [1]. Simulation software can be used to calculate the critical point of the different streams at different points of the process including production and upstream field operations. The design of the treating facilities is based on whether the flowing fluid is in liquid, gas or mixed phase. Consequently, the critical points of multicomponent mixtures need to be accurately and efficiently calculated for a reliable simulation of oil and gas reservoirs.

Critical point calculation is a relevant and very challenging thermodynamic problem. The rigorous thermodynamic criterion for the critical state was formulated by Gibbs [2]. Since then different methods have been reported for performing critical point calculations [1,3–11] and several authors have reported that the computation of critical points is difficult by the complex nonlinear form of the criticality conditions especially for multicomponent systems. Therefore, current methods can not offer a guarantee for reliably solving critical point problems. In particular, to minimize the complexity of the computational calculations, Heidemann and Khalil [6] proposed equivalent forms of the criticality criteria based on the stability of homogeneous phases, which were defined in terms of a Taylor expansion of the Helmholtz energy. This procedure avoids differentiation of determinants and requires, during each iteration, the evaluation of only one determinant, the evaluation of a set of non-linear simultaneous equations, and the evaluation of a triple summation function. This problem formulation is the most widely used for critical points calculations. It is convenient to remark that the Heidemann and Khalil method [6] employs two nested single-variable iteration loops using a local equation solver (i.e., Newton–Raphson), which may fail if a poor initialization is used. In addition, this method involves the resolution of a system of \( r + 2 \) nonlinear equations where \( r \) is the number of components of the mixture under analysis. Therefore, the problem dimensionality is high especially for reservoir fluids, which impacts on both efficiency and reliability of solvers used for critical point calculations.

One of the numerical approaches used for calculating the critical points of multicomponent mixtures using equations of state is to
formulate the problem as a minimization problem where reliable global optimizers must be employed for finding the global minimum, which represents the critical point [5,12,13]. This approach has been applied by some authors for predicting critical points in multicomponent systems [5,12–16]. Since optimization problems derived from thermodynamic applications, including the calculation of critical states, generally feature local minima that are comparable to the global minimum, the need for reliable global optimization methods is accentuated [17]. Recent advances in the development of reliable and efficient stochastic global optimizers [18] suggest that the procedure for the calculation of the critical point in multicomponent systems can be significantly enhanced with novel metaheuristics. For example, Henderson et al. [12] have compared the performance of the stochastic global optimization against the deterministic method of Stradi et al. [13] and they showed that the final results were comparable and that the computational time was significantly reduced when stochastic methods were employed.

In particular, stochastic global optimization methods show high probabilities to locate the global minimum within reasonable computational costs, and thus they offer a desirable balance between reliability and efficiency for finding the global optimum solution. Furthermore, these methods do not require any assumption for the optimization problem at hand, are capable of addressing the non-linearity and non-convexity of the objective function involved in thermodynamic calculations, and are relatively easier to program and implement, among other advantages [17]. The application of stochastic global optimization methods for solving thermodynamic problems has been an active area of research [17]. To date, the most popular stochastic global optimization methods (e.g., Simulated Annealing, Genetic Algorithms, Tabu Search, Differential Evolution, Particle Swarm Optimization, and Ant Colony Optimization) have been used and applied for solving phase equilibrium thermodynamic problems [19–26]. On the other hand, recent studies have reported the application of emerging nature-inspired optimizers such as Bare-Bones Particle Swarm Optimization, Firefly Algorithm, Covariance Matrix Adaptation Evolution Strategy, Shuffled Complex Evolution Algorithm, Cuckoo Search, Monkey – Krill Herd Hybrid Algorithm, Bat algorithm, Artificial Bee Colony and Magnetic Charged System Search for solving phase stability and phase equilibrium problems [27–32].

In particular, nature-inspired metaheuristics mimic natural phenomena, especially biological systems, and they often use multiple interacting agents. These methods are considered as emerging algorithms, which have gained a significant attention in engineering applications including thermodynamics [29,32]. However, the use of these methods for solving the critical point criteria has not been studied. Note that the first methodology used for performing the critical points via stochastic global optimization was developed by Henderson et al. [12]. This formulation has the capability of determining more than one critical point and allows visualization of the critical phenomenon from the analysis of a two-variable (T and P) objective function, which helps to understand the complexity involved in the determination of the critical points. These authors applied the Simulated Annealing [12] and Differential Evolution algorithms [15] to perform the global minimization of the proposed objective function for critical point calculations in multicomponent systems (up to twenty nine components). It is clear that the numerical performance of a limited number of stochastic optimizers has been studied in critical point calculations [12,14–16] and, to the best of our knowledge, state-of-the-art nature-based metaheuristics have not been assessed for the resolution of this relevant thermodynamic problem. Therefore, there is a lack of knowledge on the efficiency and reliability of these metaheuristics for predicting critical points in multicomponent mixtures.

The aim of this study is to apply and assess a set of nature-inspired metaheuristics in the calculation of critical points of multicomponent reservoir fluids. In particular, seven of the most promising and most recent nature-inspired optimization methods have been studied in critical point calculations. These algorithms are: Bare Bones Particle Swarm Optimization (BBPSO) [27], Cuckoo Search (CS) [33], Intelligent Firefly (IFA) [34], Artificial Bee Colony (ABC) [35], Monkey and Krill Herd Hybrid (MAKHA) [36], Covariance Matrix Adaptation Evolution Strategy (CMAES) [37] and Flower Pollination Algorithm (FPA) [38]. Performance of these methods have been systematically analyzed using difficult critical point problems, specifically, multicomponent petroleum reservoir fluids from real oil fields with 50 components. These reservoir fluids have been useful to identify the effectiveness of tested nature-inspired stochastic methods in critical point calculations. Results show the potential application of this type of metaheuristics for critical point prediction in reservoir fluids and the opportunity areas to improve their performance are highlighted.

The remainder of this manuscript is organized as follows. A brief description of the critical point problem, the tested nature-inspired methods and the petroleum reservoir fluids used as cases of study are briefly presented in Section 2. Section 3 presents the results and discussion of the optimizer’s performance in solving multicomponent critical point calculations. Finally, the conclusions of this study are summarized in Section 4.

2. Problem formulation for critical point calculations and description of the nature-inspired metaheuristics

2.1. Objective function used for critical point calculations

The criticality criteria and the objective function reported by Henderson et al. [12] were used in this study. These authors reported a modified stability test function to develop the criticality conditions. Assume that, in the presence of a small perturbation, an r-component mixture with global molar composition \( z = (z_1, z_2, ..., z_r) \) is divided in two phases, i.e., the original phase and a hypothetical phase. Then, the modified stability test function can be defined as [12]

\[
\begin{align*}
    d(x) &= \sum_{i=1}^{r-1} x_i \left[ \left( \mu_i(x) - \mu^o_i(z) \right) - \left( \mu_i(x) - \mu^o_i(z) \right) \right] \\
    &+ \left[ \mu_i(x) - \mu^o_i(z) \right] \geq 0
\end{align*}
\]  

(1)

where \( x_i \) and \( \mu_i(x) \) are the molar fraction and the chemical potential for each component in the hypothetical phase, and \( \mu^o_i(z) \) is the chemical potential for component \( i \) in the original phase \( z \), respectively. Now, considering two intervals \((T_{min}, T_{max})\) and \((P_{min}, P_{max})\), where the critical temperature and pressure of the mixture are located, the calculation of the critical point can be formulated as the following optimization problem

\[
\begin{align*}
    \text{Min} \ f(T, P) &= q^2 \left( \frac{\partial^2 C}{\partial T \partial P} \right) + C^2 \left( \frac{\partial^2 C}{\partial T \partial P} \right) \\
    \text{subject to} \ T_{min} < T < T_{max} \text{ and } P_{min} < P < P_{max}. \text{ Note that} \\
    q &= \frac{1}{2} \nabla^2 d(z) \cdot u^2
\end{align*}
\]  

(2)

where \( \nabla^2 d(z) \) is the second order tensor of the derivative of Eq. (1) and \( u = 1 \), respectively. Suppose that \( q \) is the minimum value reached by the quadratic form \( q \) and it occurs when \( u = u^* \). Therefore, the eigenvector associated with the smallest eigenvalue \( \lambda_{min} \) of the Hessian matrix \( \nabla^2 d(z) \) is given by

\[
\lambda_{min} \]
\[ q^* = \frac{1}{2} \nabla_z^2 d(z) \cdot u^z_* \leq \frac{\lambda_{\min}}{2} \]  

Therefore, at the critical point, the first criticality condition is that \( \lambda_{\min} = 0 \). Consequently, the second criticality condition is

\[ c_* = \frac{1}{6} \nabla_z^3 d(z) \cdot u^z_* = 0 \]  

where \( \nabla_z^3 d(z) \) is the third order tensor of the derivative of Eq. (1). This form can be approximated to the following expression

\[ c_* = \frac{1}{6} \nabla_z^3 d(z) \cdot u^z_* = \frac{1}{6 \delta} \left[ u^z_* \nabla d(z + \delta u_s) + u^z_* \nabla d(z - \delta u_s) \right] = 0 \]  

where \( \delta = 0 \) is a sufficiently small scalar number. The value \( \delta = 10^{-4} \) proposed by Henderson et al. [12] was used in the critical point calculations performed in this study. Details for the calculation of \( q^*, c_* \) and all the used set of equations are given in the appendix of this paper. For a critical point, the global minimum for Eq. (2) is zero. So, \( T \) and \( P \) shall be the critical temperature and pressure, respectively, when the value of the objective function approaches zero [11,15]. This objective function was coded in the MATLAB technical computing environment.

2.2. Description of nature-inspired metaheuristics used for critical point calculations

Seven nature-inspired metaheuristics were selected for performing the minimization of Eq. (2). As stated, these methods are: CS, IFA, ABC, MAKHA, CMAES, FPA and BBPSO. Note that a screening process was performed to select these methods. This process depended mainly on the results of solving phase stability and phase equilibrium problems using global optimization methods as reported in the literature. For example, BBPSO was selected as it showed a better performance than that of Particle Swarm Optimization in solving VLE parameter estimation problems [27]. CMAES is better than Shuffled Complex Evolution [37], CS outperformed Integrated Differential Evolution [29], and IFA performed better than Firefly Algorithm [34]. On the other hand, phase equilibrium calculations showed that MAKHA performed better than Monkey Algorithm and Krill Herd Algorithm and ABC performed better than Firefly Algorithm [31]. In addition, results of preliminary critical point calculations using the multicomponent systems reported by Henderson et al. [12] were considered in this stage for supporting this algorithm selection.

Brief introductions of selected methods are reported in this manuscript. Interested readers are referred to the primary sources of those algorithms for more details [27,33–38]. Specifically, BBPSO [27] is based on the original Particle Swarm Optimization but without tuning parameters and with the incorporation of mutation and crossover operators of Differential Evolution to enhance the global search capability. CS is an optimization algorithm inspired by the obligate brood parasitism of some cuckoo species by laying their eggs in the nests of other host birds [33]. IFA [34] is a variant of Firefly Algorithm and it is an algorithm inspired by the flashing behavior of fireflies to attract other fireflies. ABC [35] is an optimization algorithm based on the intelligent foraging behavior of honey bee swarm. MAKHA [36] is a hybrid between Monkey Algorithm, which is inspired by the simulation of the climbing processes of monkeys to find the highest mountaintop, and Krill-Herd Algorithm that is based on the simulation of the herding behavior of krill individuals. CMAES [37] is a stochastic and derivative free method for numerical optimization of non-linear non-convex problems. Finally, FPA is inspired by the pollination of flowers [38]. MATLAB® codes of these algorithms were used in this study. Some codes were obtained from MATLAB® file exchange server and others were developed by the authors or obtained from their developers. Table 1 shows the values selected for the parameters of the seven optimization algorithms, which were determined using preliminary critical point calculations using the mixtures reported in Refs. [11,15].

2.3. Description of reservoir fluids used in critical point calculations

Six petroleum reservoir fluids obtained from different real production wells located in the western desert in Egypt was used in this study. The physical properties of pure components and the binary interaction parameters used in all the problems were obtained from Aspen HYSYS® simulation software. Peng–Robinson equation of state was employed as thermodynamic model. The composition of each mixture is listed in Table 2. Note that C31−C35 and C36, were added in HYSYS as hypothetical components. Twu model [39] was used to estimate their critical properties andacentric factor. The application of Twu model in HYSYS requires the knowledge of the molecular weight and the ideal liquid density (base properties). These base properties for C31−C35 were obtained from Ref. [40]. For each reservoir fluid used in this study, the base properties of C36, were obtained from the analysis of these fluids done by the Egyptian Petroleum Research Institute (EPRI). The binary interaction parameters for the hypo-components were estimated by HYSYS using Chueh–Prausnitz correlation [41]. For interested readers, the properties used for C33−C35 and C36, are listed in Table S1 of Supporting Information. It is important to note that small deviations from the estimated properties of each component might affect the quality of critical point prediction.

The reservoir fluid problems are arranged, in ascending order, in terms of increasing the mole fraction of methane. Table 2 shows that the mole fraction of methane in fluid R1 is very small (black oil), while in fluid R6 is relatively large (condensate) and the values in the other problems are intermediate. Therefore, mixtures R1 and R2 can be considered as black oil problems, R3- R5 are volatile oil problems and R6 is a condensate problem. These fluids were selected in order to analyze the performance of global optimizers in a wide range of chemical composition. Although, the critical point calculation is a two dimensional problem with only two decision
variables (temperature and pressure), these fluids make the calculation of critical point challenging because of their large number of components (i.e., 50 components) and thermodynamic characteristics, which generate high non-linearities in the objective function. It is important to remark that the number of components of the fluids selected in this study is higher than those used in other papers involving stochastic optimization methods (up to 29 components) [11,14–16]. For illustration, Fig. 1 shows the corresponding surfaces of the objective function Eq. (2), with amplification of the critical point region for fluids R1 – R6. As expected, the surfaces may show complex geometries near the critical point and the value of the objective function is very high over all the search region and drops suddenly to the global minimum when the critical point is approached. In fact, the global minimum of Eq. (2) is located in a narrow valley. This geometric behavior explains the problem complexity of critical point calculations in these reservoir fluids.

### 2.4. Numerical implementation of stochastic methods and performance metrics

For all the problems, the critical point calculation (i.e., the minimization of objective function) was performed using the same lower and upper bounds for the pressure and temperature (i.e., the decision variables). The values of the lower bounds for T and P were the pseudo critical temperature ($T_{pc}$) and pressure ($P_{pc}$), which were obtained from

$$T_{pc} = \sum_{i=1}^{l} T_{c,i}$$

(7)
Fig. 1. Surface plots of the objective function Eq. (2) used for the calculation of critical points.

Value of objective function Eq. (2) for the calculation of critical points

Optimization variables (i.e., temperature and pressure) used for critical point calculation

Fig. 1. Surface plots of the objective function Eq. (2) used in critical point calculations of reservoir fluids.
where $T_{ci}$ is the critical temperature of pure component $i$ in K, $P_{ci,j}$ is the critical pressure of pure component $i$ in Pa units, and $z_i$ is the mole fraction of component $i$ in the reservoir fluid. The values of the upper bounds were 750 K and 6.0E07 Pa, respectively.

Each critical point problem was solved 30 times, with different random initial seeds, to determine the reliability of the optimization algorithms. All calculations were performed using 1000 iterations as the stopping condition for the metaheuristics. The nature-inspired optimizers were evaluated according to their reliability and efficiency for finding the global optimum (i.e., for finding the critical point). The efficiency was determined by recording the number of function evaluations (NFE) for each optimization algorithm, where a low value of NFE means a higher algorithm efficiency. Note that NFE is an unbiased indicator of the computational costs required by a certain algorithm and is independent on the host hardware. The reliability of stochastic methods was measured via the success rate (SR) for finding the critical point. This metric is defined as the percentage of successful calculations that finds the critical point out of a certain number of trials performed (30 trials in this case). For algorithm comparison, a critical point calculation is considered successful if Eq. (2) ≤ $\epsilon$ where $\epsilon$ is the precision (or tolerance value) for the solution found by the stochastic method. Algorithm analysis was performed using different tolerance values (i.e., from 1E-03 to 1E-07). Note that the objective function Eq. (2) is very sensitive for any small change in the values of the pressure and temperature, and the tested values $\epsilon$ differ in the decimal place of the calculated critical conditions.

3. Results and discussion

Results of critical point calculations using tested metaheuristics are summarized as follows. First, the success rate (SR, %) and the minimum NFE required for the successful runs to reach a certain tolerance $\epsilon$ in critical point calculations for all fluids are reported in Table 3. The highest SR for each mixture among the seven optimizers has been highlighted in this table and these results are useful to determine the most reliable solver for each critical point problem, while the most efficient algorithm was identified using NFE. On the other hand, Table 4 shows a comparison between the critical point calculations obtained from this study and the results obtained from Aspen HYSYS, which employs a local solver for calculating critical points based on Michelsen method [10]. The highest relative difference (RD) in all problems between the results of this study and Aspen HYSYS is 3.98%; see Table 4. A detailed discussion of the performance of stochastic solvers is given below.

Overall, the performance of nature-based metaheuristics is poor for critical point calculations in black oil fluids (R1 and R2). These mixtures are the most challenging critical point problems analyzed in this study. SR ranged from 0 to 73.3% for R1 and from 0 to 76.7% for R2, respectively. As expected, SR values decreased with tolerance $\epsilon$; see Table 3. In particular, MAKHA, CMAES and ABC failed in all critical point calculations performed in these fluids. CS showed a 0% SR in R1 and improved its performance in R2, but it still exhibited a poor reliability (i.e., SR < 30%). IFA, FPA and BBPSO offered the best performance for critical point calculation in these mixtures where their SR ranged from 10 to 43.3, from 6.7 to 70.0 and from 0 to 73.3%, respectively. For these fluids, BBPSO and IFA were the most reliable methods especially at low $\epsilon$ values. It is interesting to remark that IFA has the highest SR at $\epsilon$ ≤ 1.0E-05, which suggests that this metaheuristics is capable of finding critical points with a high precision in these mixtures. NFE ranged from 14,221 to 19,920 in all calculations performed in these fluids; see Table 3. This numerical effort increased with the precision in the critical point condition. In general, minor differences in the numerical effort of tested optimizers have been identified.

Performance of nature-based solvers improved in critical point calculations of volatile oil fluids (examples R3 – R5). For illustration, Fig. 2 shows the convergence profile of the mean best values of Eq. (2) versus NFE for these reservoir fluids and all nature-inspired metaheuristics. It is clear that the reliability of optimizers increased with NFE and some methods may reach a high precision (i.e., low value of objective function) in the solution obtained for critical point conditions. Table 3 shows that SR of stochastic methods in R3 – R5 is: MAKHA = 0%, CMAES = 0%, ABC = 0–63.3%, CS = 13.3–100%, IFA = 43.3–96.7%, FPA = 40–100% and BBPSO = 90–100%. In particular, MAKHA and CMAES were not able to locate the critical point at tested tolerance values, which showed a 0% SR in all calculations performed in these fluids. On the other hand, the reliability of ABC improved with respect to the results obtained in black oil fluids but its SR was still lower than 60%. CS performed satisfactorily especially in fluids R4 and R5, while IFA, BBPSO and FPA outperformed other optimizers for critical point calculations in volatile oil fluids. However, BBPSO is the best method for critical point calculations in these reservoir fluids especially at lower tolerance values. Note that IFA also showed the better SR at tolerance values ≥ 1.0E-05 especially in fluids R4 and R5. With respect to algorithm efficiency, the average NFE of BBPSO was lower (up to 134%) than those obtained for other metaheuristics at all tested $\epsilon$ values. Numerical effort of BBPSO ranged from 5153 to 12,066 NFE, while remaining optimizers showed NFE from 11,663 to 19,930, see Table 3. In summary, BBPSO is the most reliable and efficient stochastic solver for critical point prediction in the volatile oil reservoir fluids.

For the condensate reservoir fluid R6, five solvers (i.e., BBPSO, IFA, FPA, CS, and ABC) showed a high SR (>87%) for finding the critical point at $\epsilon$ from 1E-03 to 1E-05, see Table 3. At these tolerance values, MAKHA failed for solving this critical point problem, while CMAES showed a SR from 6.7 to 10%. However, BBPSO, FPA and IFA showed the best reliability for finding the critical point at $\epsilon$ ≤ 1E–06 where only BBPSO had 100% SR at this tolerance condition. It is clear that BBPSO is the fastest solver in this problem at all tolerance values where NFE ranged from 3029 to 9305. This numerical effort is lower up to 240% than those obtained for other stochastic methods. With the exception of CMAES, NFE of other stochastic methods ranged from 7401 to 17,657. Note that CMAES is an efficient method at $\epsilon$ ≥ 1.0E-05 (NFE = 994–1121) but its reliability is very poor (i.e., SR < 10%). In general, BBPSO is the best solver in terms of efficiency and reliability for this reservoir fluid. Overall, results suggested that as the mole fractions of the light components increase (e.g., methane), the effectiveness of stochastic optimizers improves for performing critical point calculations. Therefore, the critical point calculation in condensate mixtures appears to be easier than that in black oil fluids.

Herein, it is convenient to remark that nature-inspired methods may require a significant computational effort for improving the precision of decision variables $X$ and $P$ during critical point calculations because they explore randomly the search space. This behavior is illustrated in Fig. 2, where several NFE are required to reduce the value of objective function Eq. (2). Therefore, the application of a local optimization strategy for enhancing the accuracy of solution obtained by stochastic solvers has been also explored in this study. MATLAB® function fmincon was used in these calculations where the local optimizer started its iterations from the last value that was reached by stochastic solvers in each numerical run. Fig. 3 shows the global success rate (GSR, %) of all
improved the performance of ABC, CS and FPA for respectively. The application of local optimization method GSR at tolerance values for obtaining an accurate solution of the critical conditions in a rough calculation of the critical point and BBPSO is the best choice the solvers (with the local optimization method) in all the critical

<table>
<thead>
<tr>
<th>Metaheuristic</th>
<th>( \varepsilon )</th>
<th>Performance of nature-inspired metaheuristic for critical point calculation of reservoir fluid (^a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAKHA</td>
<td>1E-3</td>
<td>R1: 93.33 14684 46.67 14221 46.67 11683 80.00 11872 96.67 11663 100.00 10991</td>
</tr>
<tr>
<td>ABC</td>
<td>1E-3</td>
<td>100.00 19607 16.67 18892 43.33 17999 80.00 17746 93.33 17320 76.67 17653</td>
</tr>
<tr>
<td>FPA</td>
<td>1E-5</td>
<td>100.00 16053 46.67 13443 80.00 13087 96.67 12958 100.00 12165</td>
</tr>
<tr>
<td>MAKHA</td>
<td>1E-5</td>
<td>100.00 16053 46.67 13443 80.00 13087 96.67 12958 100.00 12165</td>
</tr>
<tr>
<td>CS</td>
<td>1E-3</td>
<td>93.33 14651 40.00 15773 93.33 8018 100.00 6297 93.33 5153 100.00 3029</td>
</tr>
<tr>
<td>ABC</td>
<td>1E-4</td>
<td>93.33 15885 33.33 17318 93.33 8674 100.00 6871 93.33 5681 100.00 3459</td>
</tr>
<tr>
<td>FPA</td>
<td>1E-5</td>
<td>50.00 17471 23.33 18734 93.33 9499 100.00 7474 93.33 6416 100.00 4235</td>
</tr>
<tr>
<td>MAKHA</td>
<td>1E-6</td>
<td>26.67 18520 80.00 15493 96.67 13817 100.00 12179 100.00 10532</td>
</tr>
<tr>
<td>CS</td>
<td>1E-6</td>
<td>0.00 18360 33.33 17360 83.33 15730 93.33 14919 96.67 14172</td>
</tr>
<tr>
<td>FPA</td>
<td>1E-7</td>
<td>0.00 18360 33.33 17360 83.33 15730 93.33 14919 96.67 14172</td>
</tr>
</tbody>
</table>

\(^a\) Values in bold font indicate the highest SR at certain tolerance value.

Table 3
Success rate (SR, %) and number of function evaluations (NFE) of nature-inspired metaheuristics in critical point calculations of reservoir fluids.

Table 4
Critical points calculated for reservoir fluids using Aspen HYSYS® and nature-inspired metaheuristics.

<table>
<thead>
<tr>
<th>Fluid</th>
<th>Critical point conditions ( T_c, K ) ( (\text{HYSYS}) )</th>
<th>( T_c, K ) ( (\text{this study}) )</th>
<th>( P_c, \text{KPa} ) ( (\text{HYSYS}) )</th>
<th>( P_c, \text{KPa} ) ( (\text{this study}) )</th>
<th>RD, %</th>
<th>Tc</th>
<th>Pc</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>637.15</td>
<td>635.79</td>
<td>5745</td>
<td>5673.70</td>
<td>0.21</td>
<td>1.26</td>
<td></td>
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<tr>
<td>R2</td>
<td>601.85</td>
<td>600.08</td>
<td>7746</td>
<td>7600.09</td>
<td>0.29</td>
<td>1.92</td>
<td></td>
</tr>
<tr>
<td>R3</td>
<td>518.75</td>
<td>518.25</td>
<td>16979.31</td>
<td>16604.76</td>
<td>0.10</td>
<td>2.26</td>
<td></td>
</tr>
<tr>
<td>R4</td>
<td>488.25</td>
<td>489.21</td>
<td>19540.87</td>
<td>18948.81</td>
<td>0.20</td>
<td>3.12</td>
<td></td>
</tr>
<tr>
<td>R5</td>
<td>452.75</td>
<td>452.98</td>
<td>22393.22</td>
<td>22045.77</td>
<td>0.05</td>
<td>1.58</td>
<td></td>
</tr>
<tr>
<td>R6</td>
<td>388.75</td>
<td>400.06</td>
<td>31847.15</td>
<td>30626.42</td>
<td>2.83</td>
<td>3.98</td>
<td></td>
</tr>
</tbody>
</table>

the solvers (with the local optimization method) in all the critical point problems at tested tolerance values. GSR of all optimizers is: MAKHA = 0%, CMAES = 0–1.7%, ABC = 1.1–29.4%, CS = 7.8–70%, IFA = 53.3–68.9%, FPA = 21.1–95.6% and BBPSO = 65–83.3%, respectively. The application of local optimization method improved the performance of ABC, CS and FPA for \( \varepsilon = 1.0E-03 \) and 1.0E-04, while MAKHA and CMAES are the worst even after using the local optimization method. Overall, BBPSO is the most reliable method at tolerance values < 1.0E-04, while FPA showed the best GSR at tolerance values > 1.0E-04. So, FPA can be used for obtaining a rough calculation of the critical point and BBPSO is the best choice for obtaining an accurate solution of the critical conditions in multicomponent systems.

Based on these results, the ranking for the nature-inspired optimizers for critical point calculations in reservoir fluids is given by: BBPSO > IFA > FPA > CS > ABC > CMAES > MAKHA. In general, BBPSO is the most effective (i.e., efficient and reliable) nature-inspired method for critical point calculations in reservoir fluids, while MAKHA and CMAES are the worst methods and they should not be used in these calculations. Numerical experience of the authors suggested that a tolerance value \( \varepsilon < 1.0E-04 \) is sufficiently small to accurately determine the critical points in reservoir fluids. Under this scenario, BBPSO may offer a SR > 80% for critical point calculations in multicomponent systems.

Finally, the efficiency of selected nature-inspired methods has been compared, in terms of NFE, with respect to the results reported by Henderson et al. [15] using different versions of Differential Evolution. For illustration, Table 5 shows the results of BBPSO, IFA and FPA for critical point calculations of ternary system ethane (1) + n-pentane (2) + n-heptane (3). Critical properties and
acentric factors of pure components were taken from Poling et al. [42], while binary interaction coefficients are $k_{12} = 0.009$, $k_{13} = 0.007$ and $k_{23} = 0.01$ [11,15]. All nature-inspired optimizers showed 100% reliability for critical point calculations independent of the tolerance value used and their NFE ranged from 5097 to 15,721. Note that DE and its variants showed a NFE of 1960–5880 for solving this problem [15]. Overall, Henderson et al. [15] solved several critical point problems of multicomponent systems (from ternary up to twenty-nine components) where NFE of DE algorithms ranged from 1960 to 12,680. Table 3 shows that NFE of BBPSO, IFA and FPA may range from 5153 to 19,920 for critical point calculations of mixtures with 50 components. Therefore, these results suggest that emerging nature-inspired optimizers may offer a good performance for critical point calculations especially in multicomponent systems and they can be effective as the traditional stochastic optimization methods.

### 4. Conclusions

This study has introduced the application of emerging nature-inspired optimizers for critical point calculations in black oil, volatile oil and condensate reservoir fluids. The effectiveness of these stochastic optimizers was analyzed and results showed that Bare Bones Particle Swarm Optimization, Intelligent Firefly Algorithm and Flower Pollination Algorithm offered the best performance for solving critical point problems in multi-component oil reservoir fluids. However, Bare Bones Particle Swarm Optimization is the method with the best efficiency-reliability tradeoff for obtaining accurate solutions of the critical conditions in multicomponent systems. On the other hand, Monkey and Krill Herd Hybrid, Covariance Matrix Adaptation Evolution Strategy and Artificial Bee Colony were the worst optimizers and these methods are not suitable for critical point calculations in these fluids. Cuckoo Search showed an acceptable success rate for critical point calculations especially in volatile oil fluids. In summary, this study illustrates the potential applications of nature-inspired metaheuristics for challenging thermodynamic calculations in real multi-component systems.
A brief description of these equations is provided in Appendix A. Supplementary data containing the tables and figures for the critical point calculations of the ternary mixture ethane (1) + n-pentane (2) + n-heptane (3).

**Table 5**

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<th>NFE</th>
<th>SR, %</th>
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</table>

Success rate (SR, %) and number of function evaluations (NFE) of nature-inspired metaheuristics in critical point calculations of the ternary mixture ethane (1) + n-pentane (2) + n-heptane (3).

To evaluate the partial derivatives $\partial \ln \phi / \partial x_i$, using the Peng Robinson equation of state, the logarithm of fugacity coefficient is written in the following form

$$
\ln \phi_i = \frac{b_i}{Z} (Z - 1) - \ln Z - \frac{bP}{RT} - \frac{a}{2\sqrt{2}hRT} \left( \frac{\sum x_i a_{ij}}{a} - \frac{b_i}{b} \right) - \frac{\sum x_i a_{ij}}{a} - \frac{b_i}{b} \left( Z(1 - \sqrt{2}) - b_j - b_r \right)
$$

and

$$
\ln \phi_i = \frac{b_i}{Z} (Z - 1) - \frac{bP}{RT} - \frac{a}{2\sqrt{2}hRT} \left( \frac{\sum x_i a_{ij}}{a} - \frac{b_i}{b} \right) - \frac{\sum x_i a_{ij}}{a} - \frac{b_i}{b} \left( Z(1 - \sqrt{2}) - b_j - b_r \right)
$$

where

$$
\frac{\partial \ln \phi_i}{\partial x_j} = \frac{\partial \ln \phi_i}{\partial x_j} - \frac{\partial \mu_i}{\partial x_j}
$$

and

$$
\frac{\partial \mu_i}{\partial x_j} = RT \left[ \frac{\ln \phi_i}{x_j} - \frac{\ln (x_i P)}{x_j} \right]
$$

Thus, the following equations apply.

Further studies should focus on improving the diversification and intensification stages of BBPSO, IFA and FPA for enhancing their global optimization capabilities in the modeling of black oil fluids, which appear to be challenging critical point problems.

**Appendix A. Supplementary data**

Supplementary data related to this article can be found at http://dx.doi.org/10.1016/j.fluid.2015.10.002.
\[ E_4 = \frac{b_i}{Z^2} \left[ \frac{A}{bB} \frac{\partial}{\partial x_j} \left( \ln \left( \frac{Z + (1 + \sqrt{2}) B}{Z + (1 - \sqrt{2}) B} \right) \right) + \ln \left( \frac{Z + (1 + \sqrt{2}) B}{Z + (1 - \sqrt{2}) B} \right) \frac{\partial}{\partial x_j} \left( \frac{A}{bB} \right) \right] \]  

(A11)

In Eqs. (A6) – (A11), Z is the compressibility factor calculated using PR equation. The cubic form of the compressibility factor is given by

\[ Z^3 - (1-B)Z^2 + (A - 2B - 3B^2)Z - (AB - B^2 - B^3) = 0 \]  

(A12)

Consequently, the following equation can be used

\[ \frac{\partial Z}{\partial x_j} = \frac{2A(B-Z^2)}{a} \sum_{k=1}^{r} x_k (a_{ij} - a_{ik}) + \frac{b}{Z^2 - 2(1 - B)Z + A - 2B - 3B^2} \left( b_j - b_i \right) \]  

(A13)

Another set of partial derivatives for evaluation of Eqs. (A1) and (A2) are given by the following expressions

\[ \frac{\partial}{\partial x_j} \left[ \frac{A}{bB} \sum_{k=1}^{r} x_k a_{ik} \right] = \frac{A}{bB} \left( a_{ij} - a_{ik} \right) - \frac{b_j - b_i}{b} \sum_{k=1}^{r} x_k a_{ik} \]  

(A14)

\[ \frac{\partial}{\partial x_j} \left[ \ln \left( \frac{Z + (1 + \sqrt{2}) B}{Z + (1 - \sqrt{2}) B} \right) \right] = \frac{2\sqrt{2}B}{b(Z^2 + 2BZ - B^2)} \left( b_j - b_i \right) \]  

(A15)

In the present work, a and b are obtained by classical mixing rules as follows

\[ a = \sum_{i=1}^{r} \sum_{j=1}^{r} x_i x_j a_{ij} \quad b = \sum_{i=1}^{r} x_i b_i \]  

(A17)

where

\[ b_i = 0.077796 \frac{RT_i}{P_i} \]  

\[ a_{ij} = (1 - k_{ij})(a_{ij})^{0.5} \]  

\[ a_i = a_c \alpha_i \]  

(A18)

\[ a_c = 0.457235 \left( \frac{RT_c}{P_c} \right)^2 \]  

\[ \alpha_i = \left[ 1 + m_i \left( 1 - \frac{T}{T_c} \right)^{0.5} \right]^2 \]  

(A19)

\[ m_i = 0.37646 + 1.54226\omega_i - 0.26992\omega_i^2 \]  

(A20)

where \( T_c, P_c \), and \( \omega_i \) are critical temperature, critical pressure, and acentric factor for pure component i, respectively; and \( A = \frac{aP(RT)^2}{b}\) and \( B = \frac{bpR}{RT} \).

References


