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

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ABSTRACT

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.

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

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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. Moreover, these methods do not require any assumptions 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 $\boldsymbol{z} = (z_1, z_2, \ldots, z_r)$ 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]

$$d(\boldsymbol{x}) = \sum_{i=1}^{r-1} x_i \left\{ \left[\mu_i(\boldsymbol{x}) - \mu_i^o(\boldsymbol{z})\right] - \left[\mu_r(\boldsymbol{x}) - \mu_r^o(\boldsymbol{z})\right] \right\} + \left[\mu_r(\boldsymbol{x}) - \mu_r^o(\boldsymbol{z})\right] \geq 0 \tag{1}$$

where x_i and $\mu_i(\boldsymbol{x})$ are the molar fraction and the chemical potential for each component in the hypothetical phase, and $\mu_i^o(\boldsymbol{z})$ is the chemical potential for component i in the original phase $\boldsymbol{z}$, 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

$$Min\, f(T,P) = q_*^2(\boldsymbol{z},T,P) + c_*^2(\boldsymbol{z},T,P) \tag{2}$$

subject to $T_{\min} < T < T_{\max}$ and $P_{\min} < P < P_{\max}$. Note that

$$q = \frac{1}{2}\nabla^2 d(\boldsymbol{z}) \cdot \boldsymbol{u}^2 \tag{3}$$

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