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Cuckoo Search: A new nature-inspired optimization method for phase equilibrium calculations

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ABSTRACT

In this study, Cuckoo Search is introduced for performing phase equilibrium and stability calculations for the first time. Cuckoo Search is a population-based method that mimics the reproduction strategy of cuckoos. This meta-heuristics have been successfully used for solving some engineering design and optimization problems with promising results. However, this emerging optimization method has not been applied in chemical engineering problems including thermodynamic calculations. This study reports the application of Cuckoo Search and its modified version for phase equilibrium and stability calculations in both reactive and non-reactive systems. Performance of this nature-inspired optimization method has been analyzed using several phase stability, phase equilibrium and reactive phase equilibrium problems. Results show that Cuckoo Search offers a reliable performance for solving these thermodynamic calculations and is better than other meta-heuristics previously applied in phase equilibrium modeling.

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1. Introduction

Phase equilibrium calculations are a relevant step in any simulator that aims to successfully design, develop and analyze an industrial process [1,2]. In particular, novel chemical industrial processes usually involve intensified operations like reactive distillation and supercritical fluid extraction, which may show a complex phase behavior at different operating conditions. Under these scenarios, accurate and reliable computations of phase property for any system are crucial due to their direct impact on process performance, costs and energy estimations.

Overall, the prediction of phase behavior in a mixture involves the solution of two relevant thermodynamic problems: phase stability (PS) and phase equilibrium (PE) calculations [2]. PS problems involve the determination of whether a thermodynamic system will remain at one phase at a given operating conditions (i.e., temperature, pressure and composition) or split into two or more phases [3]. This type of problems usually precedes the PE problems, which involve the identification and determination of the quantity and composition of the phases at equilibrium at specified conditions [2,4]. If a chemical reaction is possible between the components of the mixture under analysis, then reactive phase equilibrium calculations (i.e., the simultaneous physical and chemical equilibrium) (rPE) are performed [5]. Basically, PS problems require the global optimization of tangent plane distance function (TPDF) [2,3], whereas PE and rPE calculations require the corresponding minimization of the Gibbs free energy function [2,4,6].

Available literature [1,2] has highlighted the numerical challenges for performing the global minimization of Gibbs free energy and TPDF. In particular, the characteristics (i.e., number and type) of phases at equilibrium are unknown a priori and the non-convexity of thermodynamic functions, caused by high non-linearity of thermodynamic models, implies the presence of both trivial and local optimal solutions for PE, rPE and PS problems. Objective functions used for phase equilibrium calculations may have comparable local optimal values with the global optimum (e.g., when the mixture operating conditions are near to the phase boundaries or critical conditions), which increases the global optimization complexity [7].

To date, a number of deterministic and stochastic global optimization methods [2,4,6–38] have been proposed and applied to solve PS, PE and rPE problems but they all have their own capabilities and demerits. In particular, most deterministic methods may require large computational time (e.g., branch and bound methods and homotopy continuation approaches) [8–11], complex calculations (e.g., Jacobian matrix calculations in Newton Interval method) [12–15], mathematical reformulation and certain assumptions about the nature of the optimization problem
in order to obtain a reasonable chance of success. On the other hand, stochastic optimization methods require no prior assumptions or transformation of the objective function and can find the global minimum with high probability in less computational time [2]. Different meta-heuristics have been applied to perform PE, rPE and PS calculations in multicomponent and multireactive systems [4,7,23–38]. They include a variety of point-to-point and population-based meta-heuristics, e.g., Simulated Annealing [4,26,28,32], Genetic Algorithms [4,7], Tabu Search [24,35], Random Tunneling [27], Differential Evolution [7,30,31,35], Particle Swarm Optimization [33,34,36], Evolutionary Algorithms [29,37], Harmony Search [38], Firefly Algorithm [37] and other hybrid methods [37]. These stochastic algorithms have been found more promising than the deterministic global optimization methods but they too have their own limitations for finding the global optimum in very challenging problems. In addition, they often enforce a trade-off between speed and reliability in both phase stability and equilibrium calculations. To date, there is no single stochastic method capable of solving all optimization problems of different types and structures [39]. This situation implies that the requirement to develop new meta-heuristics is still a hot research topic in current literature of phase equilibrium modeling.

Nature-inspired meta-heuristic methods are considered as an emerging computing paradigm, which are becoming increasingly popular and promising to solve challenging global optimization problems involved in several real-world applications [40]. These methods are defined as those algorithms derived by mimicking natural phenomena and biological models; they are capable of outperforming other optimization techniques by providing a better numerical performance. In particular, Yang and Deb [41,42] introduced a new nature-inspired stochastic method called Cuckoo Search (CS). It is a population-based method that mimics the reproduction strategy of cuckoos. This novel meta-heuristics have been used for solving some engineering design and optimization problems with promising results [43,44]. Recently, a modification of this method called Modified Cuckoo Search (MCS) was introduced by Walton et al. [45] to enable faster convergence without losing the attractive features of traditional CS method. Both strategies have shown improved convergence characteristics with respect to the results obtained for other traditional stochastic optimization methods. Despite these findings, it appears that there are no studies on the solution of optimization problems from chemical engineering, including thermodynamic applications, using this meta-heuristic. In this article, Cuckoo Search is introduced as a new stochastic optimization method for phase equilibrium modeling. The performance of this novel stochastic method has been studied in solving PS, PE and rPE optimization problems. To the best of our knowledge, the application of CS to these thermodynamic calculations has not been reported and for the first time this topic is investigated in the literature. The aim of our study is to identify the relative strengths of CS for phase equilibrium calculations with and without chemical equilibrium. This study shows that CS offers a reliable performance and is better than other metaheuristics for solving these thermodynamic calculations.

2. Cuckoo Search for continuous global optimization

2.1. Cuckoo Search (CS)

Cuckoo Search is a nature-inspired meta-heuristic introduced by Yang and Deb [41,42]. It has been conceptualized from the brood parasitism behavior of the cuckoo bird. Specifically, brood parasitism is a reproductive strategy followed by cuckoos in which they lay their eggs in the nests of other birds, which are usually other species. If these eggs are discovered by the host bird, it may abandon the nest completely or throw away the alien eggs. This natural phenomenon has led to the evolution of cuckoo eggs to mimic the egg appearance of local host birds. For the implementation of these concepts, Yang and Deb [41,42] have employed the following rules: (1) one egg is laid by each cuckoo in a random nest and it represents a set of solution co-ordinates, (2) the best eggs (i.e., solutions) are contained in a fraction of the nests and will carry over to the next generation, and (3) the number of nests is fixed and a host bird can find an alien egg with a specified probability \( p_n \in [0,1] \). If this condition occurs, the host bird can discard the egg or abandon the nest, and a new nest will be built elsewhere. For algorithm simplicity, this condition has been implemented in CS assuming that a fraction \( p_n \) of \( n \) nests is replaced by new nests. Pseudo code of CS is reported in Fig. 1a and details of this meta-heuristic are reported in [41,42].

Note that Lévy flights are used in CS for performing effectively both local and global searches in the solution domain. A Lévy flight is a random walk (i.e., a trajectory that consists of taking successive random steps) and is characterized by a sequence of sudden jumps, which are chosen from a probability density function that has a power law tail. In fact, Lévy flight is considered as the optimum random search pattern and has been useful in stochastic simulations of random natural phenomena including applications of astronomy, physics and biology. To generate a new egg in CS, a Lévy flight is performed using the coordinates of an egg selected randomly. This step can be represented by

\[
x_{i+1} = x_i + \alpha \cdot \text{Lévy}(\lambda)
\]

where \( \theta \) denotes entrywise multiplication, \( \alpha \) is the step size and \( \text{Lévy}(\lambda) \) is the Lévy distribution. Egg is displaced to this new position if the objective function value is found better than another randomly selected egg. The step size \( \alpha \) controls scale of random search and depends on scales of the optimization problems under analysis. According to results reported in literature [45], this parameter can be set to 1 for most optimization problems. So, \( \alpha = 1 \) has been used in all our calculations. An advantage of CS over GA, PSO and other stochastic optimization methods is that there is only one parameter to be tuned namely the fraction of nests to be abandoned \( p_n \). However, Yang and Deb [41,42] found that the results obtained for a variety of optimization problems were not so dependent on the value of \( p_n \) and suggested using \( p_n = 0.25 \). This fact has been confirmed in preliminary calculations performed in this study and, as a consequence, we have used this value of \( p_n \) for phase equilibrium calculations with and without chemical equilibrium.

2.2. Modified Cuckoo Search (MCS)

Modified Cuckoo Search (MCS) was proposed by Walton et al. [45] to improve the convergence rate of traditional CS. Specifically, they proposed the following modifications:

(a) First modification was focused on the step size \( \alpha \). Unlike the use of constant \( \alpha \) values as in CS [41,42], the value of this parameter in MCS decreases as the iterations (or function evaluations) increases. This improvement was performed to promote more localized searching when the eggs are getting closer to solution. In MCS, the initial Lévy flight step size is defined as \( A = 1 \) and this parameter decreases at each iteration using \( \alpha = A/\text{Iter}^{0.5} \) where Iter is the iteration number. Note that this stage is only carried out on the fraction of nests to be abandoned.

(b) Other improvement added information exchange between eggs to speed up the convergence. Top eggs are introduced, which are obtained from a fraction of the eggs with the best fitness. For each of these top eggs, a second egg is randomly selected in this group and a new egg is then generated on the line connecting these two top eggs. The inverse of the golden ratio
\( \psi_r = (1 + 5^{1/2})/2 \) is used to calculate the location of the new egg along this line. Using this approach, the new egg is located closer to the egg with the best fitness. Note that the new egg is generated at the midpoint if both eggs have the same fitness. If the same egg is selected twice, a local Lévy flight search is performed using a random nest with step size \( \alpha = A/\text{iter}^2 \). These steps are illustrated in the pseudo code given in Fig. 1b. Note that two parameters of MCS must be tuned: the nest fraction to make up the top nests and the fraction of nests to be abandoned. However, Walton et al. [45] suggested fixing \( p_b = 0.75 \) and the nest fraction of top nests = 0.25. We have used the same parameter values in our calculations.

3. Formulation of optimization problems for phase equilibrium and stability calculations

Details and characteristics (i.e., objective function, constraints and decision variables) of global optimization problems for PE, rPE and PS are provided in the following sections. It is convenient to remark that a proper description of these thermodynamic problems has been covered in several references, e.g. [2,4,34,36,37]. However, an overview of these thermodynamic problems is provided in this section with the intention of making the result and discussion easier to follow.

3.1. Phase stability

As stated, solving the PS problem is usually the starting point for the phase equilibrium calculations. The theory used to solve this problem was first formulated by Gibbs [46] and it states that a stable phase implies that the tangent plane generated at the feed (or initial) composition lies below the molar Gibbs energy surface for all compositions. Michelsen [3] formulated the tangent plane distance function (TPDF) to perform this phase stability analysis. TPDF is defined as the vertical distance between the molar Gibbs energy surface and the tangent plane at the given phase composition [3] and is given by

\[
\text{TPDF} = \sum_{i=1}^{c} y_i (\mu_i |y| - \mu_i |z|)
\]

where \( c \) is the number of components of the mixture, \( \mu_i |y| \) and \( \mu_i |z| \) are the chemical potentials calculated at trial composition \( y \) and feed composition \( z \), respectively. Stability analysis is performed via the global minimization of TPDF with respect to the trial phase composition \( y \). If TPDF \( \geq 0 \) at the global optimum, the mixture is not stable at these conditions and phase split calculations must be attempted to identify the compositions of each phase. In fact, phase stability analysis is a constrained optimization problem but the global minimization of TPDF can be performed using an unconstrained approach if the following variable transformation is applied [2]

\[
n_{iy} = \beta_i z_i n_F \quad i = 1, \ldots, c
\]

\[
y_i = \frac{n_{iy}}{\sum_{j=1}^{c} n_{ij}} \quad i = 1, \ldots, c
\]

where \( \beta_i \) are the decision variables of the unconstrained problem, \( n_{iy} \) are the mole numbers of component \( i \) in phase \( y \) and \( n_F \) is the
Table 1
Description, thermodynamic models and feed conditions of selected phase equilibrium (PE) and phase stability (PS) problems.

<table>
<thead>
<tr>
<th>No.</th>
<th>System</th>
<th>Feed conditions</th>
<th>Thermodynamic models</th>
<th>Global optimum for</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>PE</td>
</tr>
<tr>
<td>1</td>
<td>n-Butyl acetate + water</td>
<td>$n_F = (0.5, 0.5)$ at 298 K and 101.325 kPa</td>
<td>NRTL model</td>
<td>-0.020198</td>
</tr>
<tr>
<td>2</td>
<td>Toluene + water + aniline</td>
<td>$n_F = (0.29989, 0.20006, 0.50005)$ at 298 K and 101.325 kPa</td>
<td>NRTL model</td>
<td>-0.352957</td>
</tr>
<tr>
<td>3</td>
<td>$N_2 + C_1 + C_2$</td>
<td>$n_F = (0.3, 0.1, 0.6)$ at 270 K and 7600 kPa</td>
<td>SRK EoS with classical mixing rules</td>
<td>-0.547791</td>
</tr>
<tr>
<td>4</td>
<td>$C_1 + H_2 S$</td>
<td>$n_F = (0.9813, 0.0187)$ at 190 K and 4053 kPa</td>
<td>SRK EoS with classical mixing rules</td>
<td>-0.019892</td>
</tr>
<tr>
<td>5</td>
<td>$C_2 + C_4 + C_5 + C_6$</td>
<td>$n_F = (0.401, 0.293, 0.199, 0.0707, 0.0363)$ at 390 K and 5583 kPa</td>
<td>SRK EoS with classical mixing rules</td>
<td>-1.183653</td>
</tr>
<tr>
<td>6</td>
<td>$C_1 + C_2 + C_3 + C_4 + C_5 + C_6 + C_7:16 + C_{17},$</td>
<td>$n_F = (0.7212, 0.09205, 0.0455, 0.03123, 0.01273, 0.01361, 0.07215, 0.01248)$ at 353 K and 38,500 kPa</td>
<td>SRK EoS with classical mixing rules</td>
<td>-0.838783</td>
</tr>
<tr>
<td>7</td>
<td>$C_1 + C_2 + C_3 + C_4 + C_5 + iC_6 + C_{17} + C_{2}, C_{12}, C_{14}, C_{15},$</td>
<td>$n_F = (0.614, 0.10259, 0.04985, 0.008989, 0.02116, 0.00722, 0.01187, 0.01435, 0.16998)$ at 314 K and 2010.288 kPa</td>
<td>SRK EoS with classical mixing rules</td>
<td>-0.769772</td>
</tr>
<tr>
<td>8</td>
<td>$C_1 + C_2 + C_3 + C_4 + C_5 + C_6 + C_7 + C_8 + C_9 + C_{10}$</td>
<td>$n_F = (0.6436, 0.0752, 0.0474, 0.0412, 0.0297, 0.0138, 0.0303, 0.0371, 0.0415, 0.0402)$ at 435.35 K and 19,150 kPa</td>
<td>SRK EoS with classical mixing rules</td>
<td>-1.121176</td>
</tr>
</tbody>
</table>

The constraints of PS problems used in this study are

$$\sum_{i=1}^{c} n_{ij} = \text{total moles in the mixture under analysis.}$$

Thus, the unconstrained TPDF minimization is stated as

$$\min \beta \quad \text{TPDF} \quad i = 1, \ldots, c$$

$$0 \leq \beta_i \leq 1$$

(5)

It is convenient to remark that the thermodynamic properties for the evaluation of TPDF and Gibbs free energy are calculated using

$$\frac{\mu_i - \mu_i^0}{R_g T} = \ln \left( \frac{x_i \phi_i}{\varphi_i} \right) = \ln(x_i g_i)$$

(6)

where $\mu_i^0$ and $\phi_i$ are the pure component chemical potential and fugacity coefficient, $\mu_i, \varphi_i$, and $g_i$ are the chemical potential, fugacity coefficient and activity coefficient of component $i$ at the mixture, and $R_g$ is the universal gas constant, respectively. Table 1 contains the characteristics of PS problems used in this study.

3.2. Phase equilibrium

At given conditions of $P$, $T$ and feed composition $z$, a mixture of substances may separate into two or more phases if PS indicates that it is unstable. If chemical equilibrium is not present, this thermodynamic problem is termed a phase equilibrium calculation. Gibbs free energy minimization subject to mass balance equality constraints is the traditional approach to calculate the equilibrium state of a mixture as per classical thermodynamics [1,2]. Usually, Gibbs free energy of mixing ($g$) is used as objective function for PE calculations and is defined as

$$g = \sum_{i=1}^{c} \sum_{j=1}^{\pi} n_{ij} \ln(x_i g_{ij}) = \sum_{j=1}^{\pi} \sum_{i=1}^{c} n_{ij} \ln \left( \frac{x_i \phi_i}{\varphi_i} \right)$$

(7)

where $\pi$ is the number of phases at equilibrium and $\theta_i$ denotes the composition (i.e., $x$ or $n$) or thermodynamic property of component $i$ in phase $j$. Global minimization of $g$ must be performed with respect to $n_{ij}$ and subject to the mass balance constraints

$$\sum_{j=1}^{\pi} n_{ij} = z_i n_F \quad i = 1, \ldots, c$$

(8)

$$0 \leq n_{ij} \leq z_i n_F \quad i = 1, \ldots, c \quad j = 1, \ldots, \pi$$

(9)

The unconstrained global minimization of $g$ is defined using the decision variables $\beta_{ij} \in (0,1)$ and the optimization problem can be defined as [2]

$$\min_{\beta} g$$

$$0 \leq \beta_{ij} \leq 1 \quad i = 1, \ldots, c \quad j = 1, \ldots, \pi - 1$$

(10)

where

$$n_{1i} = \beta_{1i} z_i n_F \quad i = 1, \ldots, c$$

(11)

$$n_{ij} = \beta_{ij} \left( z_i n_F - \sum_{m=1}^{j-1} n_{im} \right) \quad i = 1, \ldots, c; \quad j = 2, \ldots, \pi - 1$$

(12)

$$n_{i\pi} = z_i n_F - \sum_{m=1}^{\pi-1} n_{im} \quad i = 1, \ldots, c$$

(13)
Table 2
Description, thermodynamic models and feed conditions of selected reactive phase equilibrium (rPE) problems.

<table>
<thead>
<tr>
<th>No.</th>
<th>System</th>
<th>Feed conditions</th>
<th>Thermodynamic models</th>
<th>Global optimum</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>A1 + A2 ↔ A3 + A4 (1) Ethanol (2) Acetic acid (3) Ethyl acetate (4) Water</td>
<td>( n_T = (0.5, 0.5, 0.0, 0.0) ) at 355 K and 101.325 kPa</td>
<td>NRTL model and ideal gas. ( K_{eq} = 18.670951 )</td>
<td>−2.05812</td>
</tr>
<tr>
<td>2</td>
<td>A1 + A2 ↔ A3, and A4 as an inert component (1) Isobutene (2) Methanol (3) Methyl tert-butyl ether (4) n-Butane</td>
<td>( n_T = (0.3, 0.3, 0.0, 0.4) ) at 373.15 K and 101.325 kPa</td>
<td>Wilson model and ideal gas. ( \Delta G_{sys}/R = -4205.05 + 10.0982T - 0.2667T \ln T )</td>
<td>−1.434267</td>
</tr>
<tr>
<td>3</td>
<td>A1 + A2 ↔ 2A3 ↔ 2A4 (1) 2-Methyl-1-butene (2) 2-Methyl-2-butene (3) Methanol (4) Tert-amy methyl ether</td>
<td>( n_T = (0.354, 0.183, 0.463, 0.0) ) at 355 K and 151.95 kPa</td>
<td>Wilson model and ideal gas. ( K_{eq} = 10.057 + 10^{-04} e^{4273.5T}/T ) where ( T ) is in K</td>
<td>−1.226367</td>
</tr>
<tr>
<td>4</td>
<td>A1 + A2 ↔ A3 + A4 (1) Acetic acid (2) n-Butanol (3) Water (4) n-Butyl acetate</td>
<td>( n_T = (0.3, 0.4, 0.3, 0.0) ) at 298.15 K and 101.325 kPa</td>
<td>UNIQUAC model and ideal gas. ( \ln K_{eq} = 450/T + 0.8 )</td>
<td>−1.10630</td>
</tr>
<tr>
<td>5</td>
<td>A1 + A2 ↔ A3</td>
<td>( n_T = (0.6, 0.4, 0.0) )</td>
<td>Margules solution model ( g^f/R g_T = 3.6x_1 x_2 + 2.4 x_1 x_3 + 2.3 x_2 x_3 ) ( K_{eq} = 0.9825 )</td>
<td>−0.144508</td>
</tr>
<tr>
<td>6</td>
<td>A1 + A2 ↔ 2A3 ↔ 2A4 with A5 as inert component (1) 2-Methyl-1-butene (2) 2-Methyl-2-butene (3) Methanol (4) Tert-amyl methyl ether (5) n-Pentane</td>
<td>( n_T = (0.1, 0.15, 0.7, 0.0, 0.05) ) at 335 K and 151.3875 kPa</td>
<td>Wilson model and ideal gas. ( K_{eq} = 10.057 + 10^{-04} e^{4273.5T}/T ) where ( T ) is in K</td>
<td>−0.872577</td>
</tr>
<tr>
<td>7</td>
<td>A1 + A2 ↔ A3</td>
<td>( n_T = (0.52, 0.48, 0.0) ) at 323.15 K and 101.325 kPa</td>
<td>Margules solution model ( K_{eq} = 3.5 )</td>
<td>−0.653756</td>
</tr>
<tr>
<td>8</td>
<td>A1 + A2 ↔ A3 + A4</td>
<td>( n_T = (0.048, 0.2, 0.45, 0.0) ) at 360 K and 101.325 kPa</td>
<td>NRTL model ( K_{eq} = 4.0 )</td>
<td>−0.311918</td>
</tr>
</tbody>
</table>

For this optimization problem, the quantity and identity of phases at the equilibrium are assumed to be known beforehand and the decision variables are \( \bar{P}_{ij} = c(\pi - 1) \). Description of PE problems used in this study is also given in Table 1.

3.3. Reactive phase equilibrium

In rPE problems, the composition and distribution of phases at equilibrium of reacting mixtures are also determined via Gibbs free energy minimization, which is subject to both chemical equilibrium and mass balance constraints [5,14]. In this study, rPE calculations have been performed using a constrained approach for Gibbs free energy minimization, which is defined in terms of the reaction equilibrium constants [7]. Specifically, for a multicomponent and multiphase system with \( r \) independent chemical reactions, the objective function is given by [7]

\[
g_R = g - \sum_{j=1}^{\pi} \ln K_{eq}^{-1}n_{ref,j} \tag{14}
\]

where \( g \) is given by Eq. (7), \( N \) is a square and invertible matrix obtained from the stoichiometry of a set of selected reference components, \( \ln K_{eq} \) is a vector of logarithms of chemical equilibrium constants for \( r \) independent reactions, and \( n_{ref} \) is also a vector with the molar composition of the reference components. Eq. (14) is globally minimized subject to the following restrictions obtained from the rearrangement of the mass balance equations

\[
n_{ij} = n_{ij} - \bar{v}_i N^{-1}(n_{ref,i} - n_{ref,j}) - \sum_{j=1}^{\pi-1} (n_{ij} - \bar{v}_i N^{-1} n_{ref,j}) \quad i = 1, \ldots, c - r \tag{15}
\]

where \( n_{ij} \) is the initial moles of component \( i \) in the feed. In summary, Eq. (14) is minimized with respect to \( c(\pi - 1) + r \) decision variables \( n_{ij} \) and the remaining \( n_{ix} \) are calculated using Eq. (15), subject to \( n_{ix} > 0 \). rPE calculations are performed using the penalty function method according to the procedure reported by [7,37]. Finally, Table 2 provides the details of the selected rPE problems.

4. Results and discussion

4.1. Implementation details of CS algorithms and performance metrics

All the optimization algorithms and objective functions were coded in Matlab®. The codes used for CS and MCS were those developed by Yang and Deb [41,42] and Walton et al. [45], respectively. As stated, parameter \( p_a \) was assigned to values of 0.25 and 0.75 for CS and MCS, respectively. All selected PS, PE and rPE problems
were solved by running each algorithm 100 times, using different random number seeds and random initial values of decision variables for each run, with the aim of carrying out a reliable and unbiased performance analysis. The performances of CS and MCS were compared on basis of the following metrics: Success Rate (SR) for finding the global minimum of the objective functions and the average number of objective function evaluations (NFE) in the trials performed. These performance metrics were calculated using two different stopping criteria. First stopping criterion (SC-1) is the maximum number of iterations of CS and MCS, which corresponds to a proportionate NFE depending on the number of decision variables (d). However, it is convenient to remark that this criterion provides different values of NFE for both CS and MCS, even using the same population size (NP), due to two main reasons. Firstly, NFE in these methods is dependent not only on the population size and number of iterations but also on the value of p0, which is different for both of these meta-heuristics. Secondly, the segregation of nests into ‘top nests’ and ‘discarded nests’ and the conditional loops used for the objective function evaluation imply that NFE for a fixed number of iterations is not fixed for MCS with different random number seeds, though the values are similar for each trial with a standard deviation of less than 3%. In fact, our preliminary calculations showed that for these problems, the performance of MCS improves more significantly with increase in NP than with increase in number of iterations. Thus, to allow both methods to perform to their potential, a population size of 5d and 10d was assigned to CS and MCS respectively where d is the number of decision variables. With these population sizes, both CS and MCS provide roughly the same NFE for a specified number of iterations. The best objective function values obtained by these methods were recorded at different iterations (i.e., from 10 to 1500 iterations of both CS and MCS). Also, a local optimization (i.e., intensification step) using SQP algorithm of MATLAB® was performed for each of these milestone iteration values using the best function value obtained by the stochastic method as the starting value for local optimizer. This intensification step was performed to improve the solution quality obtained by both CS and MCS. Second stopping criterion (SC-2) is the improvement based criterion SC-max, which is defined on the maximum number of iterations without improvement in the best objective function value. SC-max values of 10, 25 and 50 were used for PS and PE problems, and for rPE problems the values used were 6, 12 and 24. Similarly, the local optimization was used with this convergence criterion. Note that these stopping conditions are same as those used by Zhang et al. [36] and Fateen et al. [37], which have been used for comparison purposes.

Finally, SR is calculated as the number of times the algorithm returned the objective function value to specified level of accuracy (ε): |F_{glob} − F_{obj,loc}| ≤ ε where F_{glob} and F_{obj,loc} is the known global optimum and the local optimum found by the algorithm. For problems PS-5 and PS-8, ε was taken as 10^{-6}, while for all other problems the tolerance accuracy is 10^{-5}. Global success rate (GSR) for each class of thermodynamic problems (i.e., PS, PE, rPE) was calculated as

\[
\text{GSR} = \frac{\sum_{i=1}^{np} \text{SR}_i}{np}
\]

where SRi is the success rate for problem i and np is the total number of problems in that class. Typical convergence plots were generated using both methods and reported for selected problems after 1500 iterations.

4.2. Phase stability problems

Fig. 2a shows GSR of the two methods with local optimization using SC-1 as stopping condition for all PS problems. As expected, GSR increases with the increase in number of iterations for both CS and MCS but the trend of this improvement is different. Results show that the performance of MCS may reach a maximum GSR of 70.3%. On the other hand, CS shows a high reliability for finding the global optimum, which is nearly 100% GSR. It is interesting to note that MCS has a higher success rate at early iterations (iter < 100) but after that CS completely overpowers it delivering a SR of nearly 100% for all problems using iter ≥ 250. In fact, SR of CS remains almost constant at 95–100% after 500 iterations. With illustrative purposes, Fig. 3 shows the typical convergence plots of both CS and MCS, without local optimization, for selected PS problems. For example in problem PS-6 (Fig. 3c), MCS shows a higher initial rate of convergence but gets stuck at a local optimum well away from the global minimum resulting in SR0% even after an NFE of 100,000. However, CS is capable of finding the global optimum. It is convenient to remark that CS can find the global optimum with a high precision even without using the local optimization method. For instance, in PS-5 (Fig. 3b) the convergence performance of CS showed that the global solution found can be accurate up to 9 decimal places at iter = 1500. Problem PS-8 shows a similar trend with MCS unable to overcome the low tolerance barrier, while CS offers a better convergence performance. Overall, these results show that the performance of CS is better than that obtained for MCS. Hence, using SC-1 with 500 iterations could be a good option for solving PS problems using CS.

Table 3 shows the performance of these methods with local optimization for all problems using SC-2. Overall, SR and NFE were found to improve with increase in value of SC-Max and MCS shows a better GSR (79%) than CS (65%) in this case but it generally requires
more NFE to achieve this purpose. It is interesting to remark that MCS with local optimization may provide competitive SR values for some examples even using SC-2 = 10 but it is still unable to overcome the premature convergence problems in those examples where it has failed using SC-1 (e.g., PS-8). Overall, results show that CS is the better of the two methods for performing the global minimization of TPDF, yielding a SR of nearly 100% for even the most challenging PS problems.

4.3. Phase equilibrium problems

Global success rates of both CS and MCS, with and without local optimization, for PE problems and using SC-1 are reported in Fig. 4. A two period moving average has also been plotted in Fig. 4a for each method to illustrate the pattern of change in the respective GSR. Without the local optimization method, MCS has a higher SR for smaller iteration values before being overwhelmed by sudden increase in performance of CS. Overall, the improvement in GSR for MCS was found to be almost linear reaching a maximum of 76.6% whereas CS showed a sudden jump to nearly 100% GSR at 250 iteration level, see Fig. 4a. In several PE examples, CS significantly outperformed the reliability of MSC with fewer NFE to converge. In fact, in some challenging problems (e.g., PE-6), MCS may fail to converge giving SR 0% after several NFE. On the other hand, the reliability of both methods was found to increase on combining with local optimizer, especially at low iteration values as shown in Fig. 4b but CS maintains the lead on GSR at tested conditions. Specifically, GSR of MCS with local optimization ranged from 67 to 91% whereas CS showed a GSR from 73 to 99%, respectively. Note that these performance patterns of both stochastic methods also occurred for PE and rPE problems. It appears that Iter ≥ 500 would be the best option for implementing CS in PE problems. In case of MCS, there is a steady increase in GSR with increase in number of iterations which creates the need for a high NFE for successful implementation.

Finally, GSR obtained by the two methods using SC-2 criteria for all PE problems are reported in Table 4. CS shows a better GSR especially at SC-max = 50 where its SR is nearly 100% for all problems. MCS seems to perform better than CS at lower values of SC-2 but only for some PE problems. Overall, CS shows a better reliability using only about half the NFE of MCS. In summary, the performance of the two methods for PE problems were found to be better than for PS problems and CS was found to be more effective for PE calculations.

4.4. Reactive phase equilibrium problems

rPE problems are generally considered as the most challenging global optimization functions to solve among the three types of thermodynamic problems that we have discussed in this manuscript. Fig. 2b shows GSR of CS and MCS using local optimization and SC-1 for rPE problems and Fig. 5 reports typical convergence plots for selected examples. Results indicate that both CS and MCS without local optimization show negligible success up to 100 iterations. Thereafter, CS improves its performance reaching a 90% GSR for 250 iterations and nearly 100% GSR at higher Iter. MCS shows a relatively poor reliability using few NFE and is able to cross the 50% GSR mark only after 750 iterations giving a maximum GSR of 70.2% without the local optimizer. Since SR for both methods is almost 0 for low iteration values, the convergence analysis

<table>
<thead>
<tr>
<th>Problem</th>
<th>SC-max</th>
<th>Performance for Cuckoo Search</th>
<th>Modified Cuckoo Search</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>SR (%)</td>
<td>NFE</td>
<td>SR (%)</td>
</tr>
<tr>
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<td>10</td>
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<td>25</td>
<td>71, 1911</td>
<td>100, 829</td>
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<tr>
<td></td>
<td>50</td>
<td>88, 4230</td>
<td>100, 1693</td>
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<td>10</td>
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<td>94, 4476</td>
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<td>25</td>
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<td>25</td>
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<td></td>
<td>50</td>
<td>22, 20,565</td>
<td>32, 97,481</td>
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</table>

GSR (%) and total NFE | 66 | 311,740 | 79 | 585,589
has been studied only after 1000 NFE. In particular, Fig. 5 shows that MCS may show a faster convergence at early NFE before being overtaken by CS. CS typically converges at around 10,000 NFE (i.e., 250 iterations) for all rPE problems. MCS takes longer numerical effort to converge as seen in the plots of Fig. 5 for rPE-2, rPE-4 and rPE-5. It is clear that MCS without local optimization is prone to quickly getting trapped at local optimum and may fail in terms of its ability to accurately locate the global solution to the specified level of accuracy in challenging global optimization problems. As expected, the performance of both methods improved significantly on combining with local optimization, especially at lower iteration levels. SR of MCS with local optimization improved slightly from about 74% with 10 iterations to about 80% with 100 iterations and remained almost constant thereafter. On the other hand, CS showed significant improvement in SR reaching from about 74% in 10 iterations to nearly 100% after 500 iterations (see Fig. 2b). Note that rPE-4 appears to be the most difficult problem to solve with both algorithms even using the local optimizer.

With respect to stopping condition SC-2, the performance of CS with local optimization is better than that obtained for MCS, see Table 5. Both methods have almost the same GSR (≥80%) but CS takes only about 30% of the NFE as compared to MCS, being this method more effective for solving rPE problems. Our calculations also indicate that the performance of both CS and MCS without local optimization is in general unsatisfactory using SC-2 as stopping

### Table 4: Performance of Cuckoo Search and Modified Cuckoo Search for phase equilibrium problems using SC-max as stopping condition.

<table>
<thead>
<tr>
<th>Problem</th>
<th>SC-max</th>
<th>Performance for Cuckoo Search</th>
<th>Modified Cuckoo Search</th>
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<tr>
<td></td>
<td>SR (%)</td>
<td>NFE</td>
<td>SR (%)</td>
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<td>PE-1</td>
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<td>7743</td>
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<td>GSR (%) and total NFE</td>
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### Table 5: Performance of Cuckoo Search and Modified Cuckoo Search for reactive phase equilibrium problems using SC-max as stopping condition.

<table>
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<tr>
<th>Problem</th>
<th>SC-max</th>
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<th>Modified Cuckoo Search</th>
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</tr>
<tr>
<td></td>
<td></td>
<td>GSR (%) and total NFE</td>
<td>81</td>
</tr>
</tbody>
</table>
condition. Therefore, it is more convenient to employ the application of SC-1 as stopping criterion of CS for solving rPE problems. In particular, Iter = 500 appears to be a suitable convergence value. Finally, the poor performance of MCS calls for higher NFE to produce a significant SR. So, CS has emerged to be more reliable and efficient of the two methods for solving rPE problems.

4.5. Performance comparison of CS with other stochastic optimization methods

Recently, our research group has reported the performance of different meta-heuristics on PS, PE and rPE calculations [7,34–38]. These methods include Covariant Matrix Adaptation Evaluation Strategy, Shuffled Complex Evolution, Firefly Algorithm, Integrated Differential Evolution with and without tabu list, Unified Bare Bone Particle Swarm Optimization, among others traditional optimization strategies. These studies concluded that Firefly Algorithm (FA), Covariant Matrix Adaptation Evaluation Strategy (CMA-ES) and Integrated Differential Evolution (IDE) appear to be promising stochastic methods for phase equilibrium calculations. Hence, we have compared the results obtained in this study with those reported for these optimization methods [36,37]. Table 6 reports the comparison of GSR of each method across all PS, PE and rPE problems using different values of stopping condition SC-1 and the local optimization method. Overall, results show that CS offers a better numerical performance than other methods in terms of effectiveness for finding the global optimum of tested thermodynamic functions especially in PS and rPE problems when Iter > 250. Specifically, GSR of CS is nearly 100% using at Iter = 1500. We can conclude that it is the best method for phase equilibrium calculations in both reactive and non-reactive systems if a proper numerical effort is employed. Note that MCS appears to be the least reliable of all the above methods.

5. Conclusions

In this study, an emerging stochastic optimization method namely Cuckoo Search has been introduced for solving phase equilibrium and stability problems. In particular, the traditional algorithm of Cuckoo Search and its modified version has been used for solving challenging phase stability, phase equilibrium and reactive phase equilibrium problems. Overall, CS was found to be accurate and reliable for solving these thermodynamic problems if a proper numerical effort is used and offers a better performance than that obtained for its modified algorithm and other stochastic optimization methods such as Covariant Matrix Adaptation Evaluation Strategy, Firefly Algorithm and Integrated Differential Evolution. In fact, CS appears to be among the best stochastic methods for global optimization in phase equilibrium and stability calculations. Further studies should focus on improving the performance of CS at a reduced number of function evaluations. In particular, the hybridization of CS with other more effective meta-heuristics (e.g., tabu search) is a suitable option for improving the performance of CS at early iterations.

List of symbols

c number of components of the mixture
CS Cuckoo Search
d number of decision variables
g Gibbs free energy of mixing
Iter iteration number
$K_{eq}$ chemical equilibrium constant
MCS modified Cuckoo Search
n mole
NFE: number of function evaluations

\( \rho \): pressure

\( \rho_a \): probability of CS

\( \text{PE} \): phase equilibrium

\( \text{PS} \): phase stability

\( \text{rPE} \): reactive phase equilibrium

SC-1, SC-2: stopping condition of stochastic method

\( x, y, z \): mole fractions

\( T \): temperature

\( \text{TPDF} \): tangent plane distance function

\( \alpha \): step size of OS

\( \beta_i \): decision variable

\( \mu \): chemical potential

\( \varphi \): fugacity coefficient

\( \gamma \): activity coefficient

\( \pi \): number of phases at equilibrium

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References


