A note on effective phase stability calculations using a Gradient-Based Cuckoo Search Algorithm

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A note on effective phase stability calculations using a Gradient-Based Cuckoo Search algorithm

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Abstract

Stochastic global optimization methods have been successfully used to perform phase stability calculations. However, these methods may show some drawbacks in challenging phase stability problems. In this study, we made use of the gradient of the tangent plane distance function to improve the performance of Cuckoo Search (CS) algorithm, which is a promising nature-inspired stochastic global optimization method, for the calculation of phase stability analysis. The new modified algorithm, Gradient-Based Cuckoo Search (GBCS), was evaluated for solving several challenging phase stability problems. Its performance at different numerical effort levels and the effect of stopping criterion have been analyzed. GBCS was found to perform better than the original CS algorithm. In comparison with other stochastic optimization methods using an improvement objective function-based stopping criterion, GBCS proved to be the most reliable without any reduction in efficiency.

1. Introduction

The prediction of phase behavior of a mixture involves the solution of phase stability (PS) analysis. This PS test involves the determination of whether a system will remain in one phase at the given conditions or split into two or more phases [1]. During the analysis of separation processes, PS problems need to be solved numerous times and the wrong estimation of the thermodynamic state may have negative impacts on the process design, analysis and operation. Solving this type of thermodynamic problems can be performed with global optimization methods [1]. It requires the minimization of the tangent plane distance function (TPDF) [2]. For PS problems, finding a local minimum for TPDF is not sufficient; and the global minimum must be identified for determining the correct stability condition. In general, the high non-linearity of thermodynamic models, the non-convexity of TPDF function and the presence of local optimal values that are very comparable to the global optimum value and the trivial solution in the search space make PS problems difficult to solve [1]. Since the solution of phase stability problems is an essential component of process simulators, the search for better methods and techniques to solve these often-difficult thermodynamic problems is still ongoing. Current methods have their own deficiencies and sometime fail to find the correct solutions for difficult PS problems [1,3]. Hence, PS problems require a reliable and efficient global optimization algorithm.

Stochastic global optimization techniques can be used to solve challenging global optimization problems such as those that formulate the phase thermodynamic behavior of multicomponent systems. These techniques are more advantageous compared to deterministic optimization techniques in terms of numerical implementation and computational time [1,4]. The stochastic optimization techniques do not require good starting points and can easily move out of local minima in their path to the global minimum. In particular, the sophisticated decision making process that swarms of living organisms exhibit has inspired many meta-heuristic stochastic optimization techniques [5]. Examples of those meta-heuristics are based on the decision making process of fireflies, ants, bees or birds [5,6]. Note that the phase stability problem has been solved using some of these novel bio-inspired optimization techniques and they include, e.g., Firefly Algorithm (FA) [7], Cuckoo Search (CS) [8], Ant Colony Optimization (ACO) [9] and Charged System Search (CSS) [10].

It is convenient to remark that newly developed techniques often offer improvements in reliability and efficiency of the stochastic algorithm. The authors as well as others have contributed
to this active field of study by evaluating alternative methods and comparing their performance with other methods, e.g. [8–11]. Based on the results of these studies, the Cuckoo Search (CS) algorithm has proven to be superior for PS analysis when compared to other algorithms [8]. Cuckoo Search (CS) [12,13] is a novel nature-inspired stochastic optimization method that is gaining popularity in finding the global minimum of diverse science and engineering application problems, including the resolution of combinatorial [14] and multi-objective optimization problems [15]. For interested readers, Yang and Deb [16] have reviewed the latest developments, applications and potential topics for further research of this stochastic method.

The purpose of this study is to take CS a step further using a straightforward algorithm modification that significantly improves the reliability and efficiency of the algorithm for phase stability analysis. One of the important features of the use of a stochastic global optimizer is the lack of the need for information about the gradient of the objective function. Gradient-free optimization methods can be either deterministic or stochastic, but their applications can be found in several disciplines [17]. In different applications, however, the gradient of the objective function is already available or easily obtainable. Yet, this valuable piece of information is entirely ignored by stochastic optimization methods. In particular, the gradient of the TPDF objective function can be easily obtained as explained in the following sections. The purpose of this study is to illustrate that the use of the gradient of TPDF, which is readily available with insignificant additional computational cost, may improve the performance of CS algorithm for phase stability calculations. Therefore, we propose a straightforward modification to the CS algorithm to make use of the gradient information and enhance its reliability and efficiency in the global minimization of TPDF. Our results illustrate the benefits of using the gradient as a source of new information that guide cuckoos in their search of the global minimum of TPDF. The remainder of this communication is divided as follows: Section 2 summarizes the phase stability problem using TPDF and its corresponding formulation as an optimization problem. The Cuckoo Search algorithm and the proposed modification are presented in Section 3. The results of the phase stability calculations, including the evaluation of the performance of the modified algorithm in comparison with the original CS, are presented and discussed in Section 4. Section 5 summarizes the conclusions of this study.

2. Description and formulation of the phase stability problem

Phase stability analysis states that a phase is stable if the tangent plane generated at the feed (or initial) composition lies below the molar Gibbs energy surface for all compositions. The common implementation of this stability criterion is to minimize the tangent plane distance function (TPDF), defined as the vertical distance between the molar Gibbs energy surface and the tangent plane at the given phase composition [2]. This thermodynamic function is given by

\[
TPDF = \sum_{i=1}^{c} y_i (\mu_i|_y - \mu_i|_z)
\]

where \(\mu_i|_y\) and \(\mu_i|_z\) are the chemical potentials of component \(i\) calculated at compositions \(y\) and \(z\), respectively. For performing a stability analysis of a phase/mixture of composition \(z\), TPDF must be globally minimized with respect to the composition of a trial phase \(y\). If the global minimum value of TPDF is negative, the phase is not stable at the given conditions, and phase split calculations are necessary to identify the compositions of each phase [1,2]. The decision variables for minimizing TPDF in phase stability problems are mole fractions, \(y_i\) for \(i = 1, 2, \ldots, c\), each in the range \([0,1]\), and the constraint is that the summation of these mole fractions is equal to 1. This constrained global optimization of TPDF can be transformed into an unconstrained problem by using decision variables \(\beta_i\) instead of \(y_i\) as follows [1]:

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

\[
n_{iy} = \sum_{j=1}^{c} n_{ijy} \quad \text{and} \quad y_i = \frac{n_{iy}}{n_{T}} \quad i = 1 \cdots c
\]

where \(n_T\) is the total moles in the feed mixture used for stability analysis, and \(n_{iy}\) are the conventional mole numbers of component \(i\) in trial phase \(y\). The number of decision variables is \(c\) for the unconstrained minimization of TPDF. Thus, the unconstrained global optimization problem for phase stability analysis becomes:

\[
\min_{\beta_i} TPDF(\beta_i)
\]

\[
TPDF = f(\beta_i) = \sum_{i=1}^{c} y_i (\beta_i|_y - \mu_i|_z)
\]

\[
0 \leq \beta_i \leq 1, \quad i = 1, \ldots, c
\]

The gradient of the objective function given by Eq. (5) can be easily derived as follows:

\[
\frac{\partial f}{\partial \beta_k} = \sum_{i=1}^{c} \left[ \mu_i|_y - \mu_i|_z \right] \frac{\partial y_i}{\partial \beta_k} + \sum_{i=1}^{c} y_i \frac{\partial \mu_i|_y}{\partial \beta_k}
\]

The second term is identical to zero based on the Gibbs–Duhem equation. The derivative of the mole fraction with respect to the decision variables \(\beta_k\) is

\[
\frac{\partial y_i}{\partial \beta_k} = \left\{ \begin{array}{ll}
-\frac{z_n y_i (\beta_i z_n T)}{n_{T}^2 y} , & i \neq k \\
\frac{z_n y_i (n_{T} - \beta_k z_n T)}{n_{T}^2 y} , & i = k
\end{array} \right. \quad (7)
\]

Thus, the gradient of the unconstrained objective function becomes

\[
\frac{\partial f}{\partial \beta_k} = \frac{z_n y_i}{n_{T}^2 y} \left[ \sum_{i=1}^{c} \left( \mu_i|_y - \mu_i|_z \right) (-\beta_k z_n T) \right] + \left( \mu_k|_y - \mu_k|_z \right) (n_T)
\]

Based on the Gibbs–Duhem equation, this gradient does not involve any derivatives of the chemical potential function. Thus, it can be easily implemented without the need to perform any model-specific differentiation. The computational cost associated with the calculation of the gradient is insignificant. Then, we have incorporated the use of this gradient in the search algorithm of CS to improve its performance for phase stability calculations. In the next section, we describe this modified CS algorithm.

3. Description of Gradient-Based Cuckoo Search algorithm

3.1. Cuckoo Search algorithm

The concept of CS [12,13] originates from the brood parasitism behavior of the cuckoo birds, which lay their eggs in the nests of other species. The eggs that are discovered by the host bird are abandoned. Thus, cuckoo eggs evolved to mimic the egg appearance
of local host birds. To implement those concepts, the CS algorithm employ the following rules:

1. Each cuckoo lay an egg in a random nest. The egg represents a set of solution coordinates.
2. The best eggs (i.e., solutions) are contained in a fraction of the nests and are carried over to the next generation.
3. The number of nests does not change. A host bird can find an alien egg with a specified probability \( p_a \in [0,1] \).

If an alien egg is found, the host can abandon the nest or discard the egg, and then build a new nest elsewhere. This condition was implemented in CS with the assumption that a fraction \( p_a \) of \( n \) nests is replaced by new nests. The pseudocode of CS is reported in Fig. 1. The reader is referred to the primary references of CS [12,13] for more information. The use of Lévy flights in CS makes its local and global search quite effective. A Lévy flight is a trajectory that consists of taking successive random steps. This sequence of sudden jumps, which are chosen from a power-law tail probability density function, is a characteristic of the Lévy flight, which is considered as the optimum random search pattern. To generate a new egg, a Lévy flight is performed using the coordinates of a randomly selected egg. This step can be represented by

\[
X_i^{t+1} = X_i^t + \alpha \odot \text{Lévy} (\lambda) \tag{9}
\]

where \( \odot \) denotes entry-wise multiplication, \( \alpha \) is the step size and \( \text{Lévy} (\lambda) \) is the Lévy distribution. The condition for displacing an egg to the new position is that the value of the objective function is found better than another randomly selected egg. The step size \( \alpha \), which depends on the scale of the problem, controls the scale of random search.

A fraction \( (1 - p_a) \) of the nests selected at random is abandoned and replaced by new ones at new locations via a local random walk. The local random walk can be written as

\[
X_i^{t+1} = X_i^t + \alpha (X_{i'}^t - X_i^t) \tag{10}
\]

where \( X_i^t \) and \( X_{i'}^t \) are two different solutions selected randomly by random permutation and \( \alpha \) is a random number drawn from a uniform distribution. The only parameter to be tuned is the fraction of nests to be abandoned \( (1 - p_a) \). However, it was found [12,13] that its value is not critical for the optimization results. Yang and Deb [12,13] suggested using \( p_a = 0.25 \).

3.2. Incorporation of the gradient information in CS algorithm: Gradient-Based Cuckoo Search algorithm

The purpose of this section is to introduce the modification of the original CS algorithm to incorporate information about the gradient of the objective function. Any modification to algorithm should not change its stochastic nature so as not to negatively affect its performance. A modification was made to the local random walk in which a fraction \( (1 - p_a) \) of the nests are replaced, see Eq. (10). In the original algorithm, when new nests are generated from the replaced nests via a random step, the magnitude and the direction of the step are both random. In the modified algorithm, the randomness of the magnitude of the step is reserved. However, the direction is determined based on the sign of the gradient of the function. If the gradient is negative, the step direction is made positive. If the gradient is positive, the step direction is made negative. Thus, new nests are generated randomly from the worse nests but in the direction of the minimum as seen from the point of view of the old nests. Thus, Eq. (10) is replaced by

\[
\text{step}_i = \alpha (X_{i'}^t - X_i^t) \tag{11}
\]

\[
X_i^{t+1} = X_i^t + \text{step}_i \odot \text{sign} \left( \frac{\text{step}_i}{d_{fi}} \right) \tag{12}
\]

where the sign function obtains the sign of its argument and \( d_{fi} \) is the gradient of the objective function at each variable, i.e. \( df_i/\partial X_i \).

This modification does not change the structure of the CS algorithm, as indicated by the pseudocode of GBCS in Fig. 1, but it makes an important usage of the available information about the gradient of the objective function. No additional parameter is needed to implement this change in the stochastic optimization method, which was called Gradient-Based Cuckoo Search algorithm (GBCS).
Table 1
Description, thermodynamic models and feed conditions of selected phase stability (PS) 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>n-Butyl acetate + water</td>
<td>(n_r = (0.5, 0.5)) at 298 K and 101.325 kPa</td>
<td>NRTL model</td>
<td>-0.032466</td>
</tr>
<tr>
<td>2</td>
<td>Toluene + water + aniline</td>
<td>(n_r = (0.29889, 0.20006, 0.50005)) at 298 K and 101.325 kPa</td>
<td>NRTL model</td>
<td>-0.294540</td>
</tr>
<tr>
<td>3</td>
<td>(N_2 + C_1 + C_2)</td>
<td>(n_r = (0.3, 0.1, 0.6)) at 270 K and 7600 kPa</td>
<td>SRK EoS with classical mixing rules</td>
<td>-0.015767</td>
</tr>
<tr>
<td>4</td>
<td>(C_1 + H_2S)</td>
<td>(n_r = (0.9813, 0.0187)) at 190 K and 4053 kPa</td>
<td>SRK EoS with classical mixing rules</td>
<td>-0.003932</td>
</tr>
<tr>
<td>5</td>
<td>(C_1 + C_2 + C_3 + C_4)</td>
<td>(n_r = (0.40, 0.293, 0.199, 0.0707, 0.0363)) at 390 K and 5583 kPa</td>
<td>SRK EoS with classical mixing rules</td>
<td>-0.000002</td>
</tr>
<tr>
<td>6</td>
<td>(C_1 + C_2 + C_3 + C_4 + C_5 + C_6 + C_{16} + C_{17})</td>
<td>(n_r = (0.7212, 0.09205, 0.04455, 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>-0.002688</td>
</tr>
<tr>
<td>7</td>
<td>(C_1 + C_2 + C_3 + iC_4 + C_5 + iC_6 + C_7 + C_{10})</td>
<td>(n_r = (0.614, 0.10259, 0.040985, 0.008985, 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>-1.486205</td>
</tr>
<tr>
<td>8</td>
<td>(C_1 + C_2 + C_3 + C_4 + C_5 + C_6 + C_7 + C_8 + C_{10})</td>
<td>(n_r = (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>-0.000002</td>
</tr>
</tbody>
</table>

Both CS and GBSC were coded in MATLAB. These codes were modified to allow for the two stopping criteria used in this study as discussed below. A value of 0.25 was given to \(p_{\text{ns}}\), the only parameter needed to tune the CS and GBCS algorithms. Further, \(NP = 5D\) for both methods where \(D\) is the number of decision variables.

4. Results and discussion

4.1. Description of implementation conditions and performance metrics for comparison of CS and GBCS

Eight PS problems were used for testing the performance of both CS and GBCS, whose details can be found in Table 1. These PS problems correspond to benchmark problems reported in other studies on stochastic global optimization [4,7–10]. These problems were solved 100 times independently with a different random number seed. The performances of stochastic algorithms were compared based on these calculations and the following metrics:

(a) Success rate (%) of the algorithm to locate the global optimum within an accuracy of 1.0E−5 from the known global optimum.

(b) Average number of function evaluations (NFE), which is an indicator of computational efficiency since the function evaluation involves extensive computations in application problems. This metric is independent of the computer and software platform used.

(c) Global success rate (GSR) = \(\sum_{i=1}^{NP} S_{RI}/NP\) where \(NP\) is the number of PS problems and \(S_{RI}\) is the individual success rate for each PS problem.

These performance metrics were calculated for two stopping criteria: SC-1 based on the maximum number of iterations and SC-2 based on the maximum number of iterations without improvement in the best objective function value (SC\(_{\text{max}}\)). The local optimizer sequential quadratic program (SQP) was employed to improve the precision of solution obtained by the stochastic method. The best solution obtained by the stochastic algorithm was used as the initial guess for SQP.

Performance analysis of both GBCS and CS was complemented using the performance profile (PP) of Dolan and Moré [18]. Performance profiles of these methods were calculated using the following equations:

\[
r_{\text{ps}} = \frac{t_{\text{ps}}}{\min\{t_{\text{ps}} : 1 \leq sm \leq n_b\}}
\]

where \(n_b\) is the number of optimization methods to be tested, \(n_p\) is the number of problems used in this comparison, \(t_{\text{ps}}\) is the value of the performance metric for problem \(p\) and solver \(s\), \(t_{\text{ps}}\) is the performance ratio used to compare the performance on problem \(p\) by solver \(s\) with the best performance by any solver on this problem; and \(\rho(\xi)\) is the fraction of the total number of problems for which solver \(s\) has a performance ratio \(t_{\text{ps}}\) within a factor of \(\xi\) of the best possible ratio. Under this scenario, \(t_{\text{ps}} = 1\) for the stochastic method that performs the best on a specific problem \(p\).

In our study, the efficiency of the bio-inspired optimization method in accurately finding the global minimum of the objective function is considered as the principal goal, and hence the performance metric \(t_{\text{ps}}\) is defined as the minimum NFE required by the mean best value of 100 runs to achieve the problem’s global minimum with an acceptable tolerance of 1E-5. Note that each run is different because of random number seed used and the stochastic nature of the method. So, the focus is on the average performance of both stochastic optimization methods. The performance analysis using PP was done via a plot of \(\rho(\xi)\) versus \(\xi\). The best stochastic method has been identified comparing the values of \(\rho(\xi)\) for both CS and GBCS, and selecting the highest one. In our case, the PP plot compares how efficiently the stochastic methods can find the global optimum value relative to one another, and so the best algorithm refers to the stochastic method that provides the smallest number of NFE needed to reach the global minimum in the phase stability problems used.

4.2. Numerical performance of GBCS and CS

On PS problems, similar numerical tests using the CS and GBCS stochastic algorithms were performed. The results were collected at different iteration levels, starting from 10-iteration level, and after local optimization at each of these iteration levels. As expected, GSR of CS and GBCS for all PS problems using SC-1 improves with increasing the number of iterations, see Fig. 2a. Without local optimization, GBCS outperformed CS up to 250 iteration, suggesting superior exploration capabilities. At higher iterations, the performance of the two algorithms was similar. Although the selected PS problems were somewhat difficult to optimize, both algorithms performed well reaching a GSR of above 99% at 1500 iteration without the need of a local optimizer. Fig. 2b shows the improvements in GSR with the use of a local optimization technique at the end of the stochastic techniques. The use of the local
optimizer blurred the difference between the two algorithms resulting in similar performance when SC-1 was used as the stopping criterion.

In stochastic global optimization, it is necessary to use a suitable stopping criterion for the optimization algorithm to stop at the right time incurring least computational resources without compromising reliability of finding the global optimum. Results on the effect of stopping criterion, SC-2 with $SC_{\text{max}} = 10$, 25 and 50 on CS and GBCS are presented in Fig. 3. GSR and NFE/1000 reported in this figure are for the stochastic method with the use of local optimization. The plots show that, in general, reliability of the algorithms and NFE increase with increasing $SC_{\text{max}}$. The reliability of GBCS is significantly higher than that of CS when SC-2 is used at the different stopping values. The results for SC-2 are particularly important because the number of functions evaluation is considerably less than those needed when SC-1 is used as evident in Fig. 3b. In application problems where a balance of reliability and efficiency is sought, SC-2 may deem to be the stopping criterion of choice. In this case, GBCS outperformed CS in the PS problems studied.

Fig. 4 shows the evolution of the mean function values of the 100 runs with NFE for all problems considered. In such a way, the reliability and efficiency of the two algorithms, without the use of a local optimizer, can be easily compared. For problems 1 and 2, which are the two easiest PS problems to solve, CS was slightly more reliable and efficient than GBCS. For the rest of the problems, GBCS was more reliable and efficient than CS. The use of the gradient appeared to aid the convergence of the algorithm to the global minimum for the more difficult phase stability problems.

The performance profiles, shown in Fig. 5, summarize the results of the GBCS evaluation in comparison with CS, in terms of the efficiency of achieving the global minimum. GBCS was the better performing algorithm in the cases considered, as indicated by the cumulative highest performance ratio $\tilde{\rho}(f)$ in Fig. 5.

A study for the performance of GBCS when SC-2 was used, when compared with other algorithms for the same PS problems, was made. This study made use of published [7,19] and unpublished data to compare the reliability (i.e., GSR) and efficiency (i.e., NFE) for GBCS with other SGO methods. In addition to the original CS algorithm, the methods compared are Firefly Algorithm (FA), Intelligent Firefly Algorithm (IFA), Artificial Bee Colony (ABC), Bat Algorithm (BA), Shuffled Complex Evaluation (SCE), Covariance Matrix Adaptation Evolution Strategy (CMA-ES), and Bare-Bones Particle Swarm Optimization (BBPSO). The results of this comparative study are reported in Figs. 6 and 7 showing the reliability and efficiency, respectively. Since, the increase in reliability of a method usually comes at the expense of an increase in NFE (i.e., decrement of the algorithm efficiency), it is important to look closer at the interactions between reliability and efficiency of the
algorithms under study. Fig. 6 shows that GBCS has outperformed all other algorithms in terms of reliability, both with and without the use of a local optimizer. Nonetheless, some of the other algorithms use less number of function evaluations as depicted in Fig. 7. When the three most reliable algorithms (GBCS, CS, BBPSO) are considered, GBCS has the highest GSR and the lowest NFE. The improvement of performance achieved by GBCS in comparison with the original CS did not come at the expense of an increment of NFE. On the contrary, GBCS is more efficient than CS as shown in Fig. 7.
Fig. 5. Performance profile of the efficiency of GBCS and CS methods for the global optimization of phase stability problems used in this study.

Fig. 6. Global success rate (GSR) of GBCS for phase stability analysis in comparison with other stochastic methods (CS, BBPSO, ABC, CMA-ES, SCE, BA, IFA, FA) using SC-2 (SC_{max} = 10, SC_{max} = 25 and SC_{max} = 50). (a) Stochastic method only and (b) Stochastic method combined with local optimization.

Fig. 7. Number of Function Evaluations (NFE) of GBCS for phase stability analysis in comparison with other stochastic methods (CS, BBPSO, ABC, CMA-ES, SCE, BA, IFA, FA) using SC-2 (SC_{max} = 10, SC_{max} = 25 and SC_{max} = 50).

5. Conclusions

In this study, we made use of the gradient of the TPDF objective function to improve the performance of Cuckoo Search algorithm for phase stability calculations. The new modified algorithm, GBCS, was evaluated for solving difficult phase stability problems reported in literature. Its performance at different iteration levels and the effect of stopping criterion have been analyzed. GBCS was found to perform better than the original CS algorithm when both stopping criteria were used. In comparison with other SGO methods using the SC-2 stopping criterion, GBCS proved to be the most reliable for phase stability analysis without any reduction in efficiency. This alternative stochastic method can be used for solving other difficult optimization problems involved in applied thermodynamics, for which the gradient of the objective function is readily available. In further studies, we will apply GBCS for the global minimization of the Gibbs free energy and in the non-linear parameter estimation problem of thermodynamic models.

References