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Short communication

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

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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

$$TPDF = \sum_{i=1}^{c} y_i \left(\mu_i\big|_y - \mu_i\big|_z \right) \tag{1}$$

where $\mu_i\big|_y$ and $\mu_i\big|_z$ 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 β_i instead of y_i as follows [1]:

$$n_{iy} = \beta_i z_i n_F \quad i = 1, \ldots, c \tag{2}$$

$$n_{Ty} = \sum_{j=1}^{c} n_{jy} \tag{3}$$

$$y_i = \frac{n_{iy}}{n_{Ty}}, \quad i = 1 \cdots c \tag{4}$$

where n_F 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:

$$\begin{gathered} \min TPDF(\beta_i) \\ TPDF = f(\beta_i) = \sum_{i=1}^{c} y_i(\beta_i)[\mu_i(\beta_i)|_y - \mu_i|_z] \\ 0 \le \beta_i \le 1, \quad i = 1, \ldots, c \end{gathered} \tag{5}$$

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

$$\frac{\partial f}{\partial \beta_k} = \sum_{i=1}^{c} [\mu_i\big|_y - \mu_i\big|_z] \frac{\partial y_i}{\partial \beta_k} + \sum_{i=1}^{c} y_i \frac{\partial \mu_i\big|_y}{\partial \beta_k} \tag{6}$$

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 β_k is

$$\frac{\partial y_i}{\partial \beta_k} = \begin{cases} \dfrac{-z_k n_f(\beta_i z_i n_f)}{n_{Ty}^2}, & i \neq k \\ \dfrac{z_k n_f(n_{Ty} - \beta_k z_k n_f)}{n_{Ty}^2}, & i = k \end{cases} \tag{7}$$

Thus, the gradient of the unconstrained objective function becomes

$$\frac{\partial f}{\partial \beta_k} = \frac{z_k n_f}{n_{Ty}^2} \{[\sum_{i=1}^{c} (\mu_i\big|_y - \mu_i\big|_z)(-\beta_i z_i n_f)] + (\mu_k\big|_y - \mu_k\big|_z)(n_{Ty})\} \tag{8}$$

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