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Performance analysis of stopping criteria of population-based metaheuristics for global optimization in phase equilibrium calculations and modeling

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ABSTRACT

This paper investigates the numerical behavior of several stochastic optimization methods in phase equilibrium modeling and calculations using different stopping (also known as termination and convergence) criteria. Several optimization methods, namely, Ant Colony Optimization, Particle Swarm Optimization, Differential Evolution and Harmony Search, and some of their variants, were used to compare the capabilities and limitations of different stopping criteria in phase stability problems, phase equilibrium calculations, reactive phase equilibrium calculations and parameter estimation for local composition models. The termination conditions included improvement-, movement- and distribution-type stopping rules that track the values of objective function and/or decision variables. Drawbacks and implications of tested stopping criteria were analyzed, and results showed that the selection of the stopping condition is a key factor for reliable thermodynamic calculations via global optimization using these metaheuristics. In particular, improvement-type criteria based on the tracking of the objective function values are recommended for identifying the convergence of stochastic methods in solving new phase equilibrium problems, where the global optimum is unknown.

1. Introduction

The phase equilibrium modeling of multi-component systems is essential in the design, optimization and control of separation schemes [1]. Phase equilibrium calculations are the core of the modeling of separation process performance, and they must be conducted, reliably and efficiently, to avoid uncertainties and errors in process design. Overall, many thermodynamic calculations are involved in phase equilibrium modeling, and they can be formulated as global optimization problems. Both deterministic and stochastic optimization methods play a major role in thermodynamic calculations in process engineering software [1,2]. Stochastic global optimization methods have attractive characteristics for phase equilibrium calculations and their advantages have been documented in several studies, e.g. Refs. [3–8].

Stochastic optimization methods involve probabilistic elements and use random numbers in the search for the global optimum [9]. They employ heuristics for exploring (diversification) and exploiting (intensification) the search space, and learning strategies are used to find near-optimal solutions [10]. When applying these strategies to the solution of any optimization problem, the main concern is to determine the algorithm capability for finding the global optimum. The desirable feature of an effective optimization method is a high success rate (i.e., probability) for finding the global solution at the expense of the lowest computational effort. Herein, it is important to remark that stochastic methods require, theoretically, an infinite number of objective function evaluations to guarantee the convergence to the global optimum [11]. The numerical behavior of stochastic optimizers is determined by the parameters employed for controlling the search process (via the diversification and intensification stages) and the termination

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criterion. The selection of a stopping criterion impacts both efficiency and reliability during global optimization. Under ideal circumstances, the implementation of a stopping criterion would be capable of identifying the following conditions: 1) the optimization method has located the global optimum, or 2) the optimization method is stagnant and it is preferable to terminate the search because no significant improvements on the solution can be obtained. In the literature of phase equilibrium modeling, three stopping conditions have been mainly used with the stochastic optimization methods. They are based on the measurement of the relative error to the known value of the global optimum, the improvement in the value of the objective function for a certain number of iterations or function evaluations, or a maximum allowable numerical effort that is defined in terms of the number of algorithm iterations or function evaluations [2–9]. These stopping conditions are suitable for the development and improvement of optimization methods and/or for the analysis of different algorithms. For the solution of new or real-life application problems, the main disadvantage of these criteria is the lack of knowledge of the objective function characteristics including the value of the global optimum. For example, the number of function evaluations that is necessary to reach convergence is unknown *a priori*. This scenario impacts the implementation of stochastic methods for solving global optimization problems involved in phase equilibrium calculations of any mixture or system under study.

Previous studies have highlighted the necessity of further research on stopping criteria in global optimization [12]. It has been pointed out that the statistical information from the global search should be considered for any development in this direction. Although the requirement of identifying proper convergence conditions for any optimization algorithm independent of the problem at hand is very important, only a few studies have focused on comparing different stopping rules for global optimization using stochastic methods, e.g. Ref. [13]. Results showed that considerable performance variations can be observed depending on the applied stopping criterion. In the area of phase equilibrium modeling, several papers have shown the dependence of the numerical performance of stochastic methods on the stopping rule used for solving phase stability, Gibbs free energy minimization and parameter identification problems in thermodynamic models [3]. The main conclusion of these studies is that the optimization algorithms must use an effective stopping criterion without compromising the reliability of finding the global optimum. Therefore, alternative stopping criteria should be identified and tested with stochastic optimization methods for performing reliable and efficient thermodynamic calculations for any kind of mixtures (e.g., reactive, non-reactive and electrolytes). To the best of author's knowledge, efforts in this direction have not been reported.

Hence, the present study investigates the numerical behavior of several stochastic optimization methods in phase equilibrium calculations using different stopping criteria. The numerical analysis has been performed using a set of population-based optimization methods (namely, Ant Colony Optimization, Particle Swarm Optimization, Differential Evolution and Harmony Search, and their variants), and the stopping conditions proposed by Zielinski et al. [13]. Thermodynamic calculations considered in this study are phase stability problems, phase equilibrium calculations, reactive phase equilibrium calculations and parameter estimation for local composition models. In the rest of this paper, the phrase: 'thermodynamic calculations' refers to these four types of problems. Drawbacks and implications of tested stopping criteria were analyzed, and results showed that the selection of the stopping condition is a key factor for reliable thermodynamic calculations via global optimization with these metaheuristics.

2. Description of stochastic optimization methods and stopping criteria

2.1. Stochastic optimization methods

Eight stochastic optimization methods were used to compare the capabilities and limitations of different stopping criteria in phase equilibrium calculations. Selected metaheuristics are based on the well-known population-based strategies: Differential Evolution (DE) [14], Particle Swarm Optimization (PSO) [15], Harmony Search (HS) [16] and Ant Colony Optimization (ACO) [17]. Fig. 1 shows the pseudo-codes of selected methods, and they are briefly described below.

Ant Colony Optimization (ACO_R). This metaheuristic is based on the behavior of ants in the search for food and finding their way back to the nest using a chemical trail, called pheromone. Pheromone trail guides the other ants toward the target point, and the ant selects its path based on the pheromone quantity. The collective behavior that results from this stage is a positive feedback response and, consequently, more ants will follow a specific path to the food source. By emulating the collective behavior of real ants, it is possible to solve optimization problems. ACO consists of three scheduled activities [17]: the solution construction that is a probabilistic process based on the pheromone levels, the update of pheromone trail (deposit and evaporation processes) and the daemon actions. Originally, ACO was proposed to solve combinatorial problems and its extension to real-variable (ACO_R) spaces was presented by Socha and Dorigo [18]. For illustration, Fig. 1a shows a simplified pseudo-code of ACO_R. Jayaraman et al. [19] described the application of ACO to the solution of continuous, combinatorial and multi-objective process optimization problems.

Ant Colony Optimization with feasible region selection (ACOFRS). This method is an alternative implementation of the ACO for the solution of optimization problems with continuous variables [20]. There are two main differences between ACOFRS and ACO_R. One difference is that the archive (memory of the algorithm, which can be considered as the population) is substituted by the concept of regions and the number of search agents (ants) is equal to the number of regions. Another difference is that, even though the solution construction process is based on the same probabilistic rule, the pheromone level is dimensionally assigned and then the dimensional elements of previous solutions (regions) are considered based on their pheromone levels. Main steps of ACOFRS code are summarized in Fig. 1b and algorithm details are available in Ref. [20].

Differential Evolution (DE). This evolutionary algorithm [14] starts with an initial population of individuals, which are potential solutions of the optimization problem. A mutant solution is generated by the mutation operator involving several individuals randomly selected from the current population. Then, in the crossover operation, a new trial solution is obtained by copying, with specified crossover probability, elements of the mutant solution obtained to a pre-determined target individual. Finally, in the selection operation, the better solution between the trial and target individuals is selected, based on their objective function values, for the next generation. This procedure is repeated for all solutions in the current population to complete an iteration. The iterations are repeated until the satisfaction of the specified termination criterion (Fig. 1c). DE used in this study corresponds to the algorithm DE/rand/1/bin from Ref. [14]. Sim et al. [21] reviewed developments in and applications of DE to chemical engineering.

Differential Evolution with Tabu list (DETL). This method is a hybrid evolutionary strategy that includes the tabu concept of Tabu Search (TS) in DE algorithm [22]. DETL also generates an initial population and the objective function for each individual is