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Phase stability analysis of multicomponent systems using alternative stochastic optimization methods

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The thermodynamic behavior of mixtures is fundamental for the process systems engineering. Phase stability analysis is a key step for process design and it implies the global minimization of Tangent Plane Distance Function (TPDF). This thermodynamic calculation is challenging and effective global optimization methods are required. In this paper, two novel stochastic global optimization techniques, namely Gray Wolf Optimization (GWO) and Water Cycle Algorithm (WCA), were tested and compared for solving phase stability problems of non-reactive mixtures. A set of benchmark problems with different thermodynamic models was considered and the numerical performance of tested optimization methods have been discussed. Hybridization of the GWO stochastic methods have been analyzed to improve its ability to find the global minimum of TPDF. Results showed that that WCA has a better performance compared to the GWO method even using the hybridized algorithm.

Key words: Phase stability analysis, Water Cycle Algorithm, Gray Wolf Optimization, Thermodynamic modeling.

INTRODUCTION

Phase equilibrium behavior of pure compounds and mixtures plays an important role in process systems engineering [1]. The knowledge and analysis of the phase equilibrium is important for the design, simulation and optimization of process units such as distillation and extraction columns, reactors and absorbers. The characterization of the phase equilibrium behavior can be performed experimentally with its subsequent modeling and prediction using appropriate thermodynamic tools.

The modeling and prediction of the phase equilibrium for a mixture imply solving a fundamental problem: the phase stability analysis [2]. The problem of phase stability is solved to establish whether a multicomponent system, with a given composition at given temperature and pressure, will show phase-split [3]. The phase stability can be determined by analyzing the Gibbs free energy surface [4]. Michelsen [5] developed the Tangent Plane Distance Function (TPDF) to evaluate numerically the phase stability of mixtures. The global minimization of TPDF is used to identify the thermodynamic stability of a system. This thermodynamic calculation can be handled via the application of different mathematical tools like global optimization methods including stochastic optimizers [3,6].

Numerous global stochastic optimization methods have been reported in the literature, which can be useful for the resolution of the phase stability problem [3,7]. These methods require a very limited information about the nature of the optimization problem and can handle the discontinuity of objective functions and the presence of several local optima. The computational time of these methods is reasonable and their convergence to the global optimum is highly probable. Genetic Algorithm and Simulated Annealing, Tabu Search, Differential Evolution, Adaptive Random Search, Particle Swarm Optimization, Harmony Search and Cuckoo Search are examples of stochastic optimization methods used for this thermodynamic calculation. However, it is important to remark that stochastic optimizers still have limitations to resolve the phase equilibrium stability problem of highly non-ideal systems [3,7]. It is desirable to decrease the computational effort and to increase the effectiveness of available stochastic optimization methods that are applied in phase stability analysis [7].

The aim of this work was to test new optimization methods for resolving phase stability problems. Two new stochastic methods, Gray Wolf Optimization (GWO) [8] and Water Cycle Algorithm (WCA) [9], have been used in this study. GWO and WCA have been recently introduced to solve global a wide range of optimization problems optimization problems in engineering with promising results [8-11]. To best of the author's knowledge, these methods have not been applied in thermodynamic calculations including the modeling of phase behavior of mixtures. Therefore, these optimization

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strategies have been studied and evaluated to perform the phase stability analysis of non-reactive mixtures. Some alternatives to hybridize and improve the numerical performance of these metaheuristics are analyzed and discussed in this manuscript.

DESCRIPTION OF OPTIMIZATION METHODS GWO AND WCA

GWO is inspired from the hierarchy leadership and hunting behavior of the grey wolves. This algorithm imitates the form of the wolves hunting that is based on the persecution, surrounding and attacking of the preys, which has been adapted to resolve global optimization problems [8]. GWO is classified as an alternative swarm intelligence optimization algorithm and, according to literature [10], it may offer several advantages such as simplicity, flexibility and derivation-free mechanism. It has also fewer control parameters to be adjusted and has a fast convergence. Some authors have concluded that GWO has better numerical properties to avoid local optima in comparison to other conventional optimization techniques and has been suggested as a suitable stochastic method for solving highly non-linear, multivariable and multimodal optimization problems [10]. On the other hand, WCA was derived by observing and emulating the water cycle process. This metaheuristic algorithm emulates the behavior of the raindrops, river and sea during the water cycle. WCA also requires few tuning parameters and it is capable of handling nonconvex objective functions with several decision variables. The advantages of WCA include its simplicity in terms of coding and implementation. Therefore, it has been applied to solve a wide range of optimization problems [11]. Results reported in different studies have shown that this novel metaheuristic is a reliable optimizer and may outperform other classical stochastic optimization methods [11]. For illustration, the flowcharts of both algorithms are reported in Figures 1 and 2.

The numerical performance of GWO and WCA was tested for the resolution of phase stability analysis using mixtures with different thermodynamic properties. Several binary and multicomponent systems were used where these problems are characterized by their non-convex and non-linear objective functions [4,7].

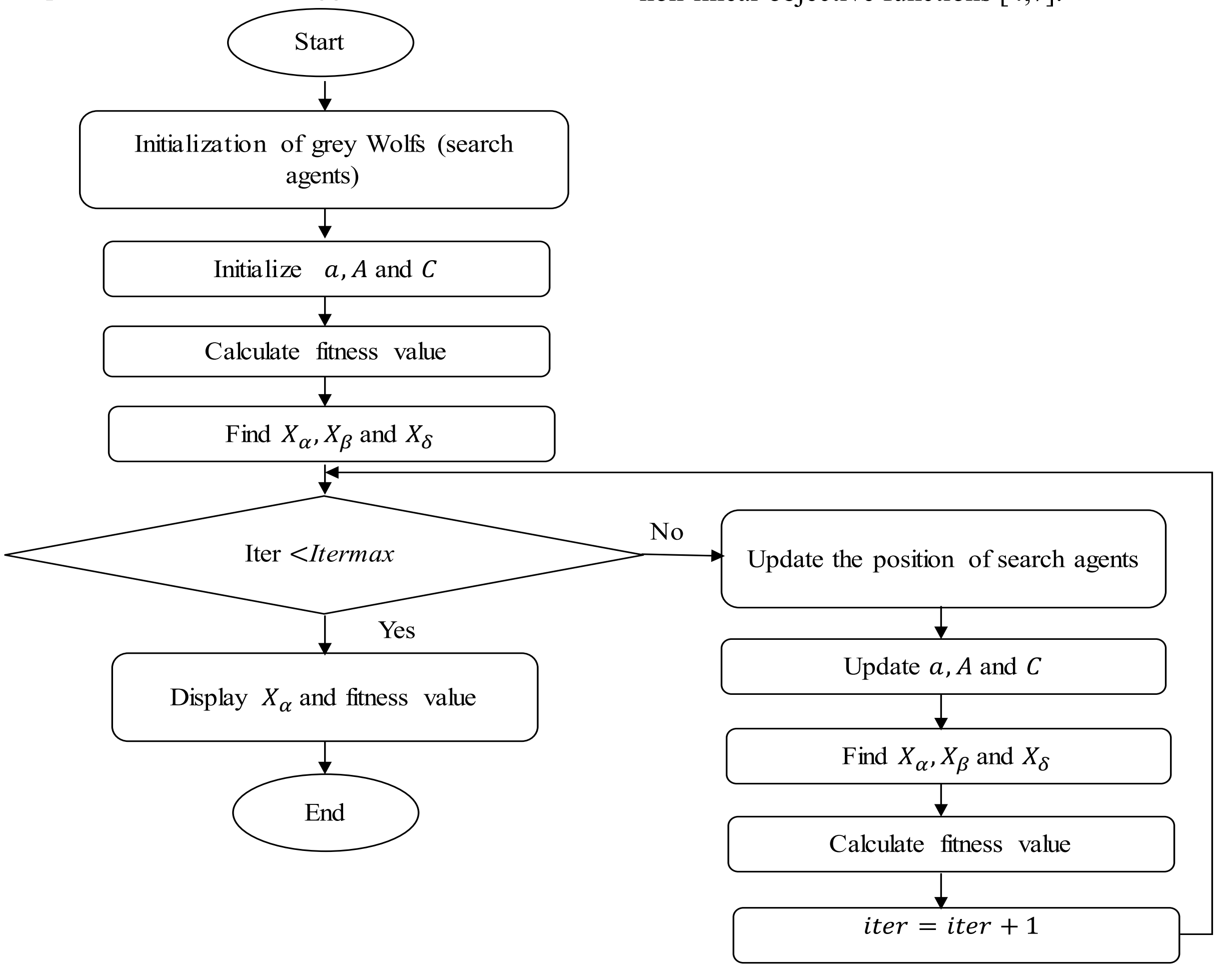

Fig. 1. Flowchart of Grey Wolf Optimization (GWO) method.

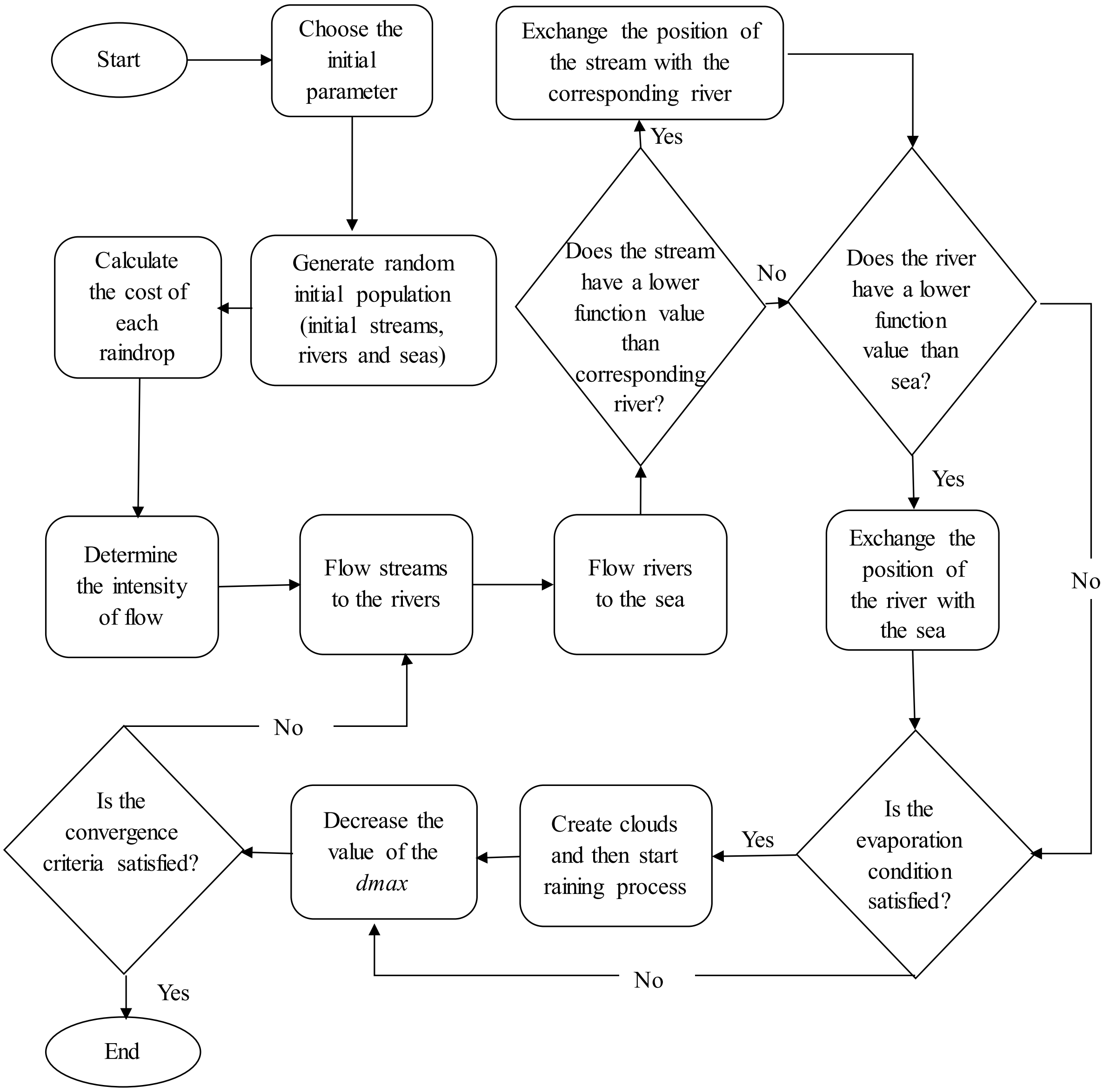

Fig. 2. Flowchart of Water Cycle Algorithm (WCA) method.

They include mixtures with vapor-liquid (VLE) and liquid-liquid (LLE) equilibria where the NRTL and UNIQUAC models was used for LLE and the SRK equation of state for VLE. The performance of each method in the unconstrained global minimization of TPDF has been analyzed using the success rate (SR, %), which was calculated for 100 independent trials performed for each phase stability problem with random initial values for the decision variables. Global success rate (GSR, %) was also calculated and the number of function evaluations (NFE) was employed as measure of the computational efficiency. Both stochastic methods were studied using the same stopping criterion, i.e., the maximum number of iterations *Itermax* = 100. Results of this numerical analysis were useful to identify the strengths and weaknesses of tested stochastics optimization methods in phase stability calculations.

RESULTS

Global success rate (GSR) of GWO and WCA in tested phase stability problems is given in Figure 3. GSR ranged from 18 to 78 % for WCA and from 12 to 76 % for GWO. Results show that WCA has the best numerical behavior for solving phase stability problems independently of the thermodynamic model used in the calculation of TPDF. This method showed highest GSR than that obtained for GWO. Note that the performance of both GWO and WCA was improved after increasing NFE. It was noted that both algorithms often improved the objective function values at early NFE. In some phase stability problems, GWO and WCA provided similar results for the mean and standard deviation of the corresponding objective function. The standard deviation of both methods was relatively large in the early values of NFE. Results also showed that these stochastic methods could be trapped in local optimal values (e.g., trivial solution). For these challenging problems, WCA could improve the values of TPDF after significantly increasing NFE. It was observed that the diversification stage should be enhanced in these methods, especially, in GWO.

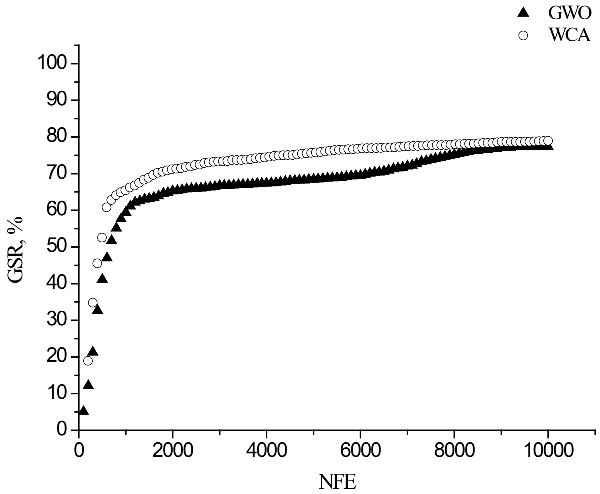

Fig. 3. Global success rate (GSR) of GWO and WCA for solving phase stability problems.

The performance of the GWO and WCA algorithms for locating the global minimum in phase stability problems was compared to the results reported for other metaheuristics used in the literature, see Table 1. This comparison included the next methods: Unified Bare-Bones Particle Swarm Optimization (UBBPSO), Firefly Algorithm (FA), Cuckoo Search (CS), Modified Cuckoo Search (MCS), Krill Herd algorithm (KH) and the modified Lévy-Flight Krill Herd algorithm (LKH). Results showed that the algorithm WCA was better than CS, MCS and UBBPSO and it showed a reliable performance with low NFE.

Table 1. Performances of WCA, GWO and other stochastic optimization methods used for phase stability analysis in nonreactive mixtures.

Method	*GSR, %*	*Average NFE*
WCA	88	25463
GWO	73	20512
UBBPSO	88	439100
FA	68	8461
CS	81	27166
MCS	76	41645
KH	89	1494
LKH	80	613

In summary, these results indicated that WCA showed a better numerical performance than GWO for solving tested thermodynamic problems. Overall, WCA could find the global minimum of TPDF with a low NFE in several non-reactive mixtures and can outperform other metaheuristics reported in other studies. Some improvements were made in GWO to strength its search mechanism. For this purpose, the operator of pitch adjustment of the Harmony Search Algorithm [12] was implemented in GWO to enhance its effectiveness in phase stability calculations. GSR of this modified GWO varied from 17 to 77 % at different numerical efforts. The combination of HS with GWO improved the diversification of original GWO allowing the exploration of more areas to find the global minimum of TPDF. Note that the convergence of this hybrid optimizer was fast in some phase stability calculations. However, this improvement was not significantly in comparison with WCA. Therefore, these results showed that WCA is the best stochastic method for the set of stability problems used in this study.

CONCLUSION

Grey Wolf Optimization and Water Cycle Algorithm were introduced to perform thermodynamic calculations related to the phase equilibrium modeling. Results showed that WCA was capable to solve several phase stability problems with an acceptable performance. WCA required the smallest number of function evaluations to obtain a success rate similar or higher than that obtained for GWO. The performance of GWO was improved via its hybridization with Harmony Search. This new algorithm HS-GWO presented a better convergence properties for the global minimization of TPDF. However, it was outperformed by WCA, which was the best stochastic method for solving phase stability problems. This study provides insights on the application of alternative stochastic optimization methods to solve challenging thermodynamic calculations. The performance of WCA and GWO should be improved with other numerical strategies to enhance their exploration and exploitation capabilities for phase stability analysis in nonreactive systems. These improvements should be focused on their convergence properties especially to increase the reliability at a low number of function evaluations.

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