Ant Colony Optimization: A New Stochastic Solver for Modeling Vapor-Liquid Equilibrium Data

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In this study, a new stochastic global optimization method based on Ant Colony Optimization (ACO) has been developed and used to solve the parameter estimation problem in vapor-liquid equilibrium data modeling. ACO is a relatively novel stochastic optimization method that mimics foraging behavior of ant colonies. We have developed a new version of ACO, which employs feasible region selection, for performing global optimization in problems with continuous decision variables. The performance of this new ACO has been tested in the modeling of vapor-liquid equilibrium data using both the classical least squares and error-in-variable formulations. Our results show that this new ACO is a suitable optimization method for parameter estimation problems with several decision variables. In addition, the proposed ACO is more reliable than other meta-heuristics used for the modeling of phase equilibrium data.

1. Introduction

The modeling of phase equilibrium plays an important role in the design, development, operation, optimization and control of separation processes for the chemical and petrochemical industries. In particular, the correct thermodynamic processing of experimental data using reliable numerical strategies and thermodynamic models is crucial for process system engineering (Graczová et al., 2009). A common problem in the modeling phase equilibrium is to determine the parameters of a thermodynamic model used to represent a specific set of experimental information such as vapor-liquid or liquid-liquid equilibrium data. Specifically, the task is to establish the values of model parameters that provide the best fit to measured data using a proper objective function, which can be formulated using either the least squares or maximum likelihood criterion (Englezos and Kalogerakis, 2001). For the case of vapor-liquid equilibrium (VLE) data, the parameter estimation problems usually have non-linear and non-convex spaces even using simple thermodynamic models (Gau et al., 2000; Bonilla-Petriciolet et al., 2010). This optimization problem is complex in nature and difficult to solve employing traditional local optimization methods due to: a) the presence of several local minima for the objective function used as the optimization criterion, b) several models may be used to represent phase properties causing discontinuities in the objective function in some regions of solution domain, and c) the model parameters may vary

over a wide range of the solution domain. Therefore, the development of reliable methods for the modeling of phase equilibrium is still a challenge.

In the literature, several studies have shown the potential of stochastic optimization methods to solve parameter estimation problems for the VLE modeling (Bonilla-Petriciolet et al., 2010). Specifically, stochastic global optimization methods offer several advantages for solving global optimization problems such as generality, reliability and robust performance, little information requirement for the optimization problem to be solved, easy implementation, and reasonable computational requirements. To date, different stochastic methods have been studied and tested for parameter estimation using VLE data, and they include simulated annealing, genetic algorithms, differential evolution, harmony search and particle swarm optimization. These strategies usually show a suitable performance but, in some challenging problems, they fail to locate the global optimum (Bonilla-Petriciolet et al., 2010). It is important to remark that the failure to find the globally optimal parameters for a thermodynamic model may cause errors and uncertainties in process system design (Gau et al., 2000). Therefore, alternative optimization strategies should be studied to identify a better approach for parameter estimation in VLE modeling.

In particular, Ant Colony Optimization (ACO) is a promising solver for phase equilibrium modeling and, to the best of our knowledge; there are no studies in the literature on the phase equilibrium modeling using this stochastic method. ACO is a relatively novel meta-heuristic that mimics foraging behavior of ant colonies (Blum, 2005). These ants deposit pheromone on the ground for making some favorable paths that should be followed by other members of the colony. ACO algorithm exploits this mechanism for solving global optimization problems. In this study, a new version of ACO with feasible region selection, namely ACO-FRS, has been developed for performing global optimization in problems with continuous decision variables. The performance of ACO-FRS has been tested using several parameter estimation problems that include binary VLE data and local composition models. In summary, our results are useful to identify the capabilities and limitations of this new ACO method for this thermodynamic application.

2. Description of Ant Colony Optimization with feasible region selection

As stated, ACO is inspired by the foraging behavior of ants. At the core of this behavior is the indirect communication between the ants by means of chemical pheromone trails, which enables them to find short paths between their nest and food sources. This characteristic of real ant colonies is exploited in ACO algorithms in order to solve global optimization problems (Blum, 2005). The meta-heuristic of ACO consists of three algorithmic components: ant-based solution construction, pheromone update and daemon actions. The first ant algorithm was developed by Dorigo and since then several improvements of the ant system have been proposed (Blum, 2005). Until now, this stochastic optimization method has been successfully applied in several engineering and real world problems including some chemical engineering applications.

In this paper, we introduce a new ACO algorithm for solving global optimization problems with continuous decision variables. Specifically, our algorithm, namely ACO-FRS, creates a set of search regions, where each region represents a solution of the optimization problem. An initial pheromone amount is deposited in every dimensional component of all the regions. Note that a key component of ACO method is the ant based solution construction activity. In simple ACO, the pheromone information is read by the ant and used in a stochastic way to decide its movements. In our algorithm, this step is performed for each dimension of solution vector and the transition rule represents the selection probability that a region component has when any ant explores it at any time. In this stage, a selection of feasible regions is performed and this process is different for each ant. Using this approach, the ACO algorithm is able to perform a global search due to the use of regions with low pheromone concentrations, thus diversifying the solution vectors obtained. This path search process allows the ant moves from the selected component to a nearby location. A solution is constructed only after finishing the selection of all region components and the path search process. The fitness is evaluated and the new solution will replace an existing region based on the comparison of function values. Pheromone is updated by intensification, where a discrete amount of pheromone is added. Thus, the algorithm carry outs an implicit evaluation because the pheromone intensification is not proportional to the quality of the solution and all ants deposit the same amount of pheromone. Finally, after all ants have performed region exploration, the pheromone of all regions is evaporated by subtracting a fixed value. This iterative process is repeated until the given termination criterion is satisfied. Figure 1 provides the corresponding flowchart of our ACO-FRS.

3. Nonlinear parameter estimation problem for modeling vapor-liquid equilibrium data

The objective functions commonly used for parameter estimation problem in VLE data modeling can be obtained from either the least squares principle or the maximum likelihood criterion (Gau et al., 2000; Englezos and Kalogerakis, 2001). In the first approach, the model parameters are determined whereas, in the second formulation, both the true values of state variables and model parameters are obtained. In this paper, we have considered both approaches to illustrate the performance of ACO-FRS in the modeling of VLE data. For the case of VLE data (i.e., x-y-P at constant T, or x-y-T at constant P), local composition models such as Wilson, UNIQUAC and NRTL are widely used for phase equilibrium modeling and data correlation. So, under these conditions, the least square formulation (LS) for VLE data correlation can be defined using activity coefficients

$$F_{obj} = \sum_{i=1}^{c} \sum_{j=1}^{ndat} \left(\frac{\gamma_{ij}^{\exp} - \gamma_{ij}^{calc}}{\gamma_{ij}^{\exp}} \right)^2 \qquad (1)$$

where γ^{exp} and γ^{calc} is the experimental and calculated values for the activity coefficients, $ndat$ is the number of experimental data, and c is the number of components in the mixture, respectively. At low pressure, γ_i can be calculated from VLE data and,

assuming an ideal gas behavior, the experimental activity coefficients can be determined from VLE measurements using the following expression

$$\gamma_i^{\exp} = \frac{y_i^{\exp}P}{x_i^{\exp}P_i^0} \quad i = 1,...,c \tag{2}$$

where x^{exp} and y^{calc} are respectively the experimental mole fractions in liquid and vapor phases at equilibrium, and P^0 is the vapor pressure at the system temperature T.
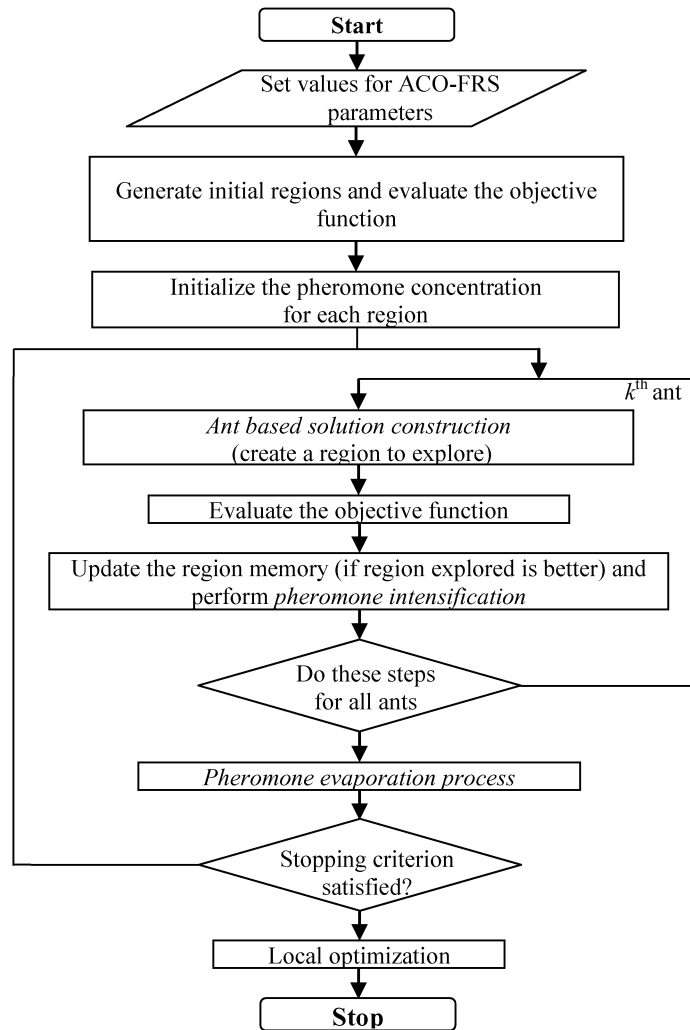
Figure 1: Flowchart of Ant Colony Optimization with feasible region selection.

On the other hand, if we assume that there are measurement errors in the state variables x, y, P and T with standard deviations (σ_x, σ_y, σ_P and σ_T), the optimization problem that must be solved is the error-in-variable (EIV) formulation, which is defined as

$$F_{obj} = \sum_{j=1}^{ndat} \sum_{i=1}^{c} \left[\frac{(x_{ij}^t - x_{ij})^2}{\sigma_x^2} + \frac{(y_{ij}^t - y_{ij})^2}{\sigma_y^2} + \frac{(T_j^t - T_j)^2}{\sigma_T^2} + \frac{(P_j^t - P_j)^2}{\sigma_P^2} \right] \tag{3}$$

where x^t, y^t, T^t and P^t are the unknown "true" values of state variables. Note that this optimization problem can be formulated as an unconstrained using the VLE equations to eliminate y^t and P^t in the objective function. Usually, Equations (2) and (3) are strongly non-linear, potentially non-convex with several local minima within the specified bounds (Bonilla-Petriciolet et al., 2010). Therefore, the VLE modeling involves solution of a global optimization problem. In this study, we have used the Wilson, NRTL and UNIQUAC models to calculate the liquid phase activity coefficients in the modeling of VLE data. The objective functions are optimized with respect to the energy parameters (*npar*) of these models for the case of LS formulation, while the EIV formulation is optimized with respect to *npar* + *c·ndat* decision variables. Note that the energy parameters of these thermodynamic models are defined as in the DECHEMA.

4. Results

We have tested and compared the performance of ACO-FRS using a number of binary VLE data and different local composition models. Details of all VLE examples are reported by Bonilla-Petriciolet et al. (2010). All selected examples have been used for testing other deterministic and stochastic optimization strategies (e.g., Gau et al., 2000; Bonilla-Petriciolet et al., 2010). All VLE examples are solved 100 times each, starting from a different, random point inside specified bounds on decision variables, and the performance of ACO-FRS is tested using the global success rate for finding the global optimum (SR, %), the mean number of function evaluations (NFE) and CPU time for different stopping criteria. With illustrative purposes, the results of solving the VLE parameter estimation problems for different iterations of ACO-FRS and using both LS and EIV are shown in Figure 2. In general, ACO-FRS may offer a better performance than those reported for other stochastic methods (e.g. particle swarm optimization or genetic algorithms) especially for optimization problems with several decision variables. However, ACO-FRS may fail in the global minimization of the objective functions involved in some challenging problems. In summary, our numerical experience indicates that ACO-FRS can be considered an alternative method for parameter estimation in VLE modeling.

5. Conclusions

The present study introduces the application of a new ACO with feasible selection region for solving the parameter estimation problem for modeling vapor-liquid equilibrium data with local composition models and both the classical least squares and error-in-variables approaches. Our results suggest that ACO-FRS is a promising direct-search method for solving global optimization problems in phase equilibrium modeling.
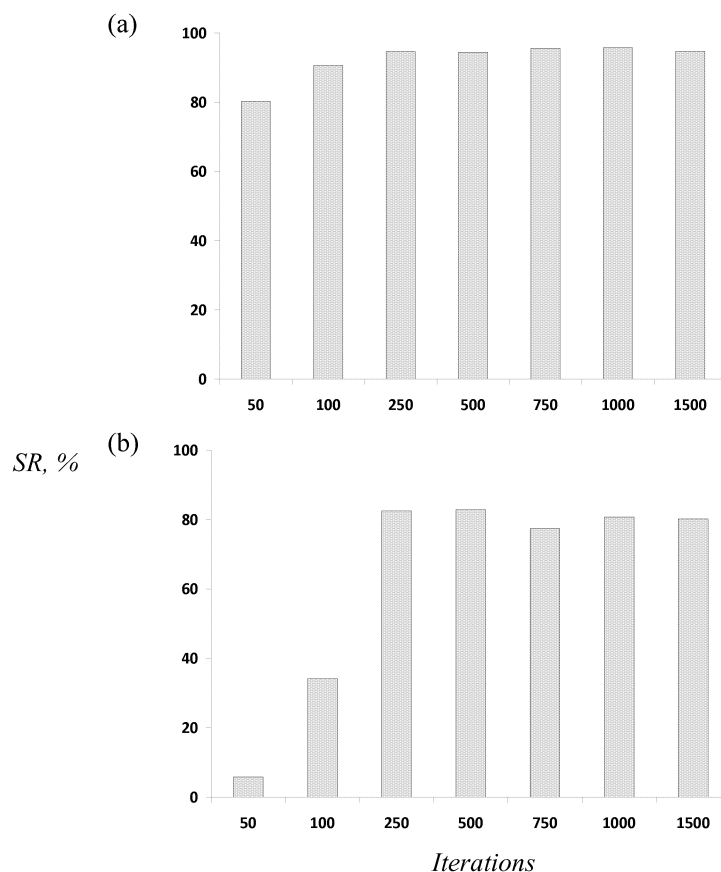
Figure 2: Global success rate of Ant Colony Optimization with feasible region selection for the modeling of binary VLE data using (a) LS and (b) EIV approaches.

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