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Hybrid Particle Swarm-Ant Colony Algorithm to Describe the Phase Equilibrium of Systems Containing Supercritical Fluids with Ionic Liquids

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Abstract. Based on biologically inspired algorithms, a thermodynamic model to describe the vapor-liquid equilibrium of binary complex mixtures containing supercritical fluids and ionic liquids, is presented. The Peng-Robinson equation of state with the Wong-Sandler mixing rules are used to evaluate the fugacity coefficient on the systems. Then, a hybrid particle swarm-ant colony optimization was used to minimize the difference between calculated and experimental bubble pressure, and calculate the binary interaction parameters for the excess Gibbs free energy of all systems used. Simulations are carried out in nine systems with imidazolium-based ionic liquids. The results show that the bubble pressures were correlated with low deviations between experimental and calculated values. These deviations show that the proposed hybrid algorithm is the preferable method to describe the phase equilibrium of these complex mixtures, and can be used for other similar systems.

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1 Introduction

Phase equilibrium data of mixtures containing ionic liquids are necessary for further development of some separation processes [1]. Blanchard *et al*. [2] described several potential applications of supercritical fluids with ionic liquids. The gas solubility data provides important information for the characterization of solute-solvent interactions and so contribute to understand the mechanisms of dissolution. From a practical point of view, gas solubility can be useful in the calculation of vapor-liquid equilibrium [3].

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One of the common approaches used in the literature to correlate and predict phase equilibrium requires an equation of state that well relates the variables temperature, pressure and volume and appropriate mixing rules to express the dependence of the equation of state parameters on the concentration [1]. The existing methods to solve phase equilibrium systems obtain only local solutions. It has been demonstrated that for cases of systems containing supercritical fluids, the optimum values of the interaction parameters depend on the searching interval and on the initial value of used interaction parameters [4]. Then, the parameter optimization procedures are very important in engineering, industrial, and chemical process for development of mathematical models, since design, optimization and advanced control of bioprocesses depend on model parameter values obtained from experimental data [1].

The aim of optimization is to determine the best-suited solution to a problem under a given set of constraints. Mathematically, an optimization problem involves a fitness function describing the problem, under a set of constraints representing the solution space for the problem. The optimization problem, now-a-days, is represented as an intelligent search problem, where one or more agents are employed to determine the optimum on a search landscape [5]. Modern optimization techniques have aroused great interest among the scientific and technical community in a wide variety of fields recently, because of their ability to solve problems with non-linear and non-convex dependence of design parameters [6].

Thus, the use of heuristic optimization methods, such particle swarm optimization [7] and ant colony optimization [8], for the parameter estimation is very promising [1]. These biologically-deriver methods represent an excellent alternative to find a global optimum for phase equilibrium calculations.

In this work, nine binary vapor-liquid phase systems containing supercritical fluids and ionic liquids were evaluated using a hybrid algorithm based on particle swarm optimization and ant colony optimization. The complete program was used to calculate the binary interaction parameters of these complex mixtures by minimization of the difference between calculated and experimental data.

2 Thermodynamic model

As known, the phase equilibrium problem to be solved consists of the calculation of some variables of the set *T*-*P*-*x*-*y* (temperature, pressure, liquid-phase concentration and vapor-phase concentration, respectively), when some of them are known. For a vapor-liquid mixture in thermodynamic equilibrium, the temperature and the pressure are the same in both phases, and the remaining variables are defined by the material balance and the "$fundamental\ equation\ of\ phase\ equilibrium$". The application of this fundamental equation requires the use of thermodynamic models which normally include binary interaction parameters [9].

The classical thermodynamic models commonly used in the literature to treat these