

عنوان مقاله:

Application of Genetic Algorithm to Calculate the Binary Interaction and Non-Randomness Parameters of the NRTL model for Ternary Ionic Liquid Systems

محل انتشار:

هفتمین کنگره ملی مهندسی شیمی (سال: ۱۳۹۰)

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خلاصه مقاله:

One of the most important applications of thermodynamics is the accurate prediction of fluid phase equilibria problems related to the real chemical engineering processes. Various equation of states as well as activity coefficient models have been developed for such calculations with a lot of interaction, size or randomness parameters which should be optimized based on the powerful and effective computational methods. To lead to globally optimal values, genetic algorithm (GA) has been established to predict the binary interaction parameters for multi-component liquid-liquid equilibrium data. GA requires only the lower and upper bounds for the interaction parameters and needs no initial guess. Ionic liquids (ILs) are being regarded favorable solvents for liquid-liquid extraction because of unique properties. In this work, a global optimization procedure based on the GA was developed to calculate the binary interaction and non-randomness parameters of the NRTL activity coefficient model for ۳۰ ternary aromatic extraction systems containing the ionic liquids at various temperatures. The values of binary interaction parameters and root mean square deviation (rmsd) are reported. Comparison of the obtained results with other estimation methods shows that GA is generally more effective and reliable. In order to confirm the accuracy of the results, the values of rmsd were compared with those reported in the literature.

کلمات کلیدی:

Binary Interaction Parameters, NRTL, Liquid-Liquid Extraction, G.A, Ionic Liquids

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