

Experiment and a New Thermodynamic Model Based on Group Contribution for Correlation Liquid-Liquid Equilibria in Aqueous Two Phase Systems of PEG and (K₂HPO₄ or Na₂SO₄)

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Abstract

A new thermodynamic model based on group contribution has been proposed for studying the phase behavior of aqueous two phase polymer-salt systems. The assumptions of NRTL-NRF model and the activity coefficient equation of UNIQUAC-NRF model have been used for the groups. In this new model, UNIFAC-NRF, the nonrandom state of groups were selected as a reference state. The binary interaction parameters were adjusted using the data of binary salt-water systems and the ternary systems were correlated with only six binary adjustable parameters. The Debye-Huckel equation based on Fowler-Guggenheim equation was used to calculate the long range electrostatic interaction of the ions. The UNIFAC-NRF model was applied to correlate the experimental data of aqueous two phase systems: PEG-K₂HPO₄-water and PEG-Na₂SO₄-water for two different molecular weight of PEG at different pH. The results of the new model showed that it can be used to correlate the LLE in aqueous solution of polymer-salt very well.

Keywords: Aqueous two phase system, Activity coefficient, UNIFAC-NRF, Polyethylene glycol, Liquid-Liquid Equilibria

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Introduction

Aqueous two-phase extraction system has become an important emerging technique for separation, concentration and purification of proteins, cell organelles and other biological products. Aqueous two phase systems (ATPS) are particularly suited for separation and purification of proteins from crude material like cell extracts, down stream broth, culture filtrate, because insoluble cell debris often partitions in one of the two phases. The representation of phase diagrams in aqueous two-phase systems (ATPS) is of great importance for prediction of partitioning of proteins. As a consequence, some successful models in this specialised area have been developed. There are mainly three kinds of models were proposed in literature, either based on the osmotic virial expansion, or the local composition models. The osmotic virial expansions are derived from knowledge of the osmotic pressure of a solvent in the solution and were used by Kabiri Badr and Cabezas [3], Grossmann et al. [4], Wu et al. [5]. The models based on the lattice theories, the Flory-Huggins theory, and on the local composition concepts, the UNIQUAC and the UNIFAC models are among the most familiar ones used to represent LLE phase diagrams of polymer-salt ATPS. In the case of UNIQUAC and UNIFAC models the LLE of polymer-salt systems have been investigated by Gao [6,7] and Peng et al [8]. Wu et al. [9] investigated the LLE of ATPS using the NRTL model. The NRTL model is one of the most successful and practical models for electrolyte and nonelectrolyte systems of small molecules, but for electrolyte solution it is limited to a molality of 6 of salt in solution [10]. Haghtalab and Vera [11] modified the NRTL model, named NRTL-NRF based on the non-random state as a reference state. By using the assumptions of the NRTL-NRF model, Haghtalab and Asadollahi [12,13] developed a UNIQUAC-NRF model, which was applied to polymer-polymer systems. Recently Haghtalab and