سیویلیکا - ناشر تخصصی مقالات کنفرانس ها و ژورنال ها
گواهی ثبت مقاله در سیویلیکا
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عنوان مقاله:

Application of NRTL, UNIQUAC and NRTL-NRF models for Ternary Liquid-Liquid Equilibrium Systems Including Ionic Liquids

محل انتشار:

هفتمین کنگره ملی مهندسی شیمی (سال: 1390)

تعداد صفحات اصل مقاله: 9

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خلاصه مقاله:

Ionic Liquids (ILs) with their limitless combination of cations and anions can offer an optimal solvent for a specific purpose especially separation processes. As alkyl-sulfate derivates are the most promising ILs to be applied in industrial processes, current work investigated the phase behavior of 7-ILs comprising sulfate-base anions , in 19-ternary liquid-liquid systems using three local composition models, namely Non-Random Two Liquid (NRTL), Non-Random Two Liquid Non-Random Factor (NRTL-NRF) and UNiversal QUAsi Chemical (UNIQUAC) activity coefficient models. All the interaction parameters are regressed using an optimization program based on Simplex method of Nelder and Mead. Comparison of the results is expressed by root mean square deviation (rmsd) between experimental and calculated compositions. The results demonstrate that the NRTL-NRF model is extremely satisfactory with rmsd values about 1.08 and that this model is highly appropriate to calculate the thermodynamic properties of ionic-liquid solution

کلمات کلیدی:

NRTL, UNIQUAC, NRTL-NRF, Ionic Liquid, Liquid-Liquid Equilibria

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