

RESEARCH PAPERS

苯乙烯/二氧化碳/聚苯乙烯三元混合物的相平衡预测

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摘要 A lattice fluid model, Sanchez-Lacombe equation, is used to predict the phase behavior for a styrene/CO₂/polystyrene ternary system. The binary parameters involved in the equation were optimized using experimental data. Phase diagrams and the distribution coefficients of styrene between polymer phase and fluid phase are obtained over a wide range of pressure, temperature and composition. The analysis of ternary phase diagrams indicates that this system at relatively high pressure or low temperature may display two-phase equilibrium, and at low pressures or high temperatures three-phase equilibrium may appear. The distribution coefficients of styrene between the fluid phase and the polymer phase increase asymptotically to unity when the concentration of styrene increases. The results provide thermodynamic knowledge for further exploitation of supercritical carbon dioxide assisted devolatilization and impregnation.

关键词 [ternary phase diagram](#) [distribution coefficient](#) [polystyrene](#) [supercritical fluid](#)

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Prediction of Phase Behavior for Styrene/CO₂/Polystyrene Mixtures

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Abstract A lattice fluid model, Sanchez-Lacombe equation, is used to predict the phase behavior for a styrene/CO₂/polystyrene ternary system. The binary parameters involved in the equation were optimized using experimental data. Phase diagrams and the distribution coefficients of styrene between polymer phase and fluid phase are obtained over a wide range of pressure, temperature and composition. The analysis of ternary phase diagrams indicates that this system at relatively high pressure or low temperature may display two-phase equilibrium, and at low pressures or high temperatures three-phase equilibrium may appear. The distribution coefficients of styrene between the fluid phase and the polymer phase increase asymptotically to unity when the concentration of styrene increases. The results provide thermodynamic knowledge for further exploitation of supercritical carbon dioxide assisted devolatilization and impregnation.

Key words [ternary phase diagram](#); [distribution coefficient](#); [polystyrene](#); [supercritical fluid](#)

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