THERMODYNAMICS OF THE GAS – LIQUID – SOLID EQUILIBRIUM. FORMATION OF NANOPARTICLES FROM A SUPERCRITICAL SOLVENT

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Abstract

A thermodynamic model is suggested for calculating the phase states and equilibrium of the fluid – solid systems over a wide range of temperature, pressure and composition. A system including ethanol, carbon dioxide and phenanthrene was analyzed. The calculations allowed determining the boundaries of the parameter region where phenanthrene is evolved as a solid phase depending on the chemical composition of initial mixture, amount and ratio of solvent and antisolvent.

Rapid expansion of supercritical solution (RESS) comprising ethanol, carbon dioxide and phenanthrene was simulated to establish the conditions of the solid phase formation, which underlies the formation of nanoparticles. It was shown that the choice of initial parameters of supercritical state of the mixture is decisive for the optimal conditions of the solid phase formation during expansion of the fluid.