

Prediction of Solubility of Solids in Supercritical Solvents using a Combined Crossover Lattice Equation of State – Molecular Dynamics Approach

이용진, 신문삼, 김화용*
서울대학교
(hwayongk@snu.ac.kr*)

In the present study, the crossover lattice equation of state was employed to calculate the solubilities of solids in supercritical solvents over a wide range of pressure and temperatures. The characteristic parameters of the pure components, appearing in the original sanchez-lacombe equation of state, were estimated using a molecular dynamic procedure (MD). The theoretically calculated solubilities were found to be in excellent agreement with the corresponding experimentally measured values, demonstrating the capability of the xLF EOS to predict the solubility of solids in supercritical solvents.