World Academy of Science, Engineering and Technology
International Journal of Mathematical and Computational Sciences
Vol:14, No:12, 2020

Prediction of the Solubility of Benzoic Acid in Supercritical CO2 Using the PC-SAFT EoS

Authors : Hamidreza Bagheri, Alireza Shariati

Abstract : There are many difficulties in the purification of raw components and products. However, researchers are seeking better ways for purification. One of the recent methods is extraction using supercritical fluids. In this study, the phase equilibria of benzoic acid-supercritical carbon dioxide system were investigated. Regarding the phase equilibria of this system, the modeling of solid-supercritical fluid behavior was performed using the Perturbed-Chain Statistical Association Fluid Theory (PC-SAFT) and Peng-Robinson equations of state (PR EoS). For this purpose, five PC-SAFT EoS parameters for pure benzoic acid were obtained using its experimental vapor pressure. Benzoic acid has association sites and the behavior of the benzoic acid-supercritical fluid system was well-predicted using both equations of state, while the binary interaction parameter values for PR EoS were negative. Genetic algorithm, which is one of the most accurate global optimization algorithms, was also used to optimize the pure benzoic acid parameters and the binary interaction parameters. The AAD% value for the PC-SAFT EoS, were 0.22 for the carbon dioxide-benzoic acid system.

Keywords : supercritical fluids, solubility, solid, PC-SAFT EoS, genetic algorithm
Conference Title : ICSRD 2020 : International Conference on Scientific Research and Development
Conference Location : Chicago, United States
Conference Dates : December 12-13, 2020