

عنوان مقاله:

Calculation of the solid solubilities in supercritical carbon dioxide using a modified Wong-Sandler mixing rule

محل انتشار:

ششمین کنگره بین المللی مهندسی شیمی (سال: 1388)

تعداد صفحات اصل مقاله: 6

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خلاصه مقاله:

The Peng-Robinson (PR) and Soave-Redlich-Kwong (SRK) equations of state (EOS) and three mixing rules including: Co-volume-dependant (CVD), Wong-Sandler (WS) and Modified Wong-Sandler (MWS) mixing rules are applied in this study to calculate the solid solubilities of polar and non-polar solid mixtures such as aromatic hydrocarbons, aliphatic carboxylic acids, aromatic acids, heavy aliphatic and aromatic alcohols in supercritical carbon dioxide. The NRTL model is chosen as the Excess Gibbs Free Energy model (for WS and MWS mixing rules). The coefficients of the NRTL model and the binary interaction parameters of three mixing rules with two EOSs (PR and SRK EOSs) have been determined for 970 experimental data points of 100 CO₂ binary systems which are reported in the literature. The conclusion, after comparing the calculated errors for various models, was that the best results were obtained for the PR EOS and the MWS mixing rule proposed here. The regressed interaction parameters of the binary system, without any further modification, were then extended to ternary mixtures. The MWS mixing rule gives satisfactory results of the solid solubility in supercritical carbon dioxide for both the binary and ternary systems.

کلمات کلیدی:

Cubic equation of state; Mixing rules; Solid solubilities; Supercritical carbon dioxide

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