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Predicting the solubilities of acetylacetonate-type metal precursors in supercritical CO_2: Thermodynamic modeling using PC-SAFT

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Abstract (less than 300 words)

The deposition of metal particles on porous supports such as mesoporous silica using supercritical CO_2 has attracted much attention as a method for preparing supported catalysts because the metal particles can be dispersed in the pore structure [1, 2]. Prediction methodology of the solubility of metal precursors in supercritical CO_2 is important to efficiently design the supported catalyst using the supercritical CO_2 deposition method.

In this study, a thermodynamic model using the PC-SAFT (perturbed-chain statistical associating fluid theory) equation of state [3] was used to predict the solubility of various acetylacetonate-type metal precursors in supercritical CO_2. The pure component parameters (the segments number, segment diameter, and dispersion energy) of the metal precursors were determined by considering the correlation with the solubility data of the metal precursors in various organic solvents that were newly measured in this study. The pure component parameters of the metal precursors determined using the correlations were applied to the prediction of the solubility data of metal precursors in supercritical CO_2 using PC-SAFT. The model could reproduce the solubility of various metal precursors over a wide range of temperatures and pressures in supercritical CO_2 without the binary interaction parameter (k_{ij}) for almost all conditions investigated.

References

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