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Measurement and correlation of diffusion coefficients of $Cr(acac)_3$ in high temperature supercritical carbon dioxide

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Abstract (less than 300 words)

Over the last 40 years, the chemical processes with supercritical carbon dioxide ($scCO_2$) has been intensively studied from the early stages in many applications such as supercritical fluid extraction, separation/fractionation, cleaning, supercritical fluid deposition, polymer dyeing, nano/micropore formation, atmosphere or solvent for chemical reactions, and mobile phase for supercritical fluid chromatography. As the applications have expanded, the data on both equilibrium and transport properties for supercritical fluids/mixtures have been required and vigorously measured. However, they are not yet sufficient [1], and the diffusivity data on organometallic complexes, especially in high temperature $scCO_2$, are not sufficiently enough and demanded for determining kinetics and designing processes for supercritical fluid deposition. In this study, extending to our previous study in which diffusion coefficients of $Cr(acac)_3$ in $scCO_2$ were measured up to 343K [2], the measurements were carried out at temperatures up to 423 K and pressures up to 20 MPa by the chromatographic impulse response (CIR) method, which provides diffusion coefficient and retention factor. The new D_{12} data more deviated at CO_2 viscosities lower than 40 μPa s from the hydrodynamic equation, in which D_{12}/T vs. CO_2 viscosity can be represented by a straight line in logarithmic plot, and is effective for many organic compounds measured in liquid-like density region of $scCO_2$ [1-4], and the deviation becomes more at lower CO_2 viscosities. To the contrary, retention factors were expressed by a single equation as a function of temperature and CO_2 density over at entire conditions studied. The accuracies for various predictive correlations are examined, and a modified Schmidt number correlation is proposed. As a result, the modified Schmidt number correlation was effective with average relative deviation of 6.10 % for 282 data points over an entire range of temperature and pressure studied.

References

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