PREDICTIVE CORRELATION FOR BINARY DIFFUSION COEFFICIENTS OF LIPIDS IN SUPERCRITICAL CARBON DIOXIDE

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In supercritical fluid extraction of natural products, and enzymatic reactions in oil industries diffusion coefficients D12 of lipids and their derivatives are required for designing reactors, in particular, estimating mass transfer rates. Although diffusion coefficient data are available in the literature, they are not sufficient. Moreover, various predictive correlations and methods are proposed, but these are based on the limited number of data, and/or are not covered over a wide range of temperature, pressure and molecular weight.

Recently, the authors found that hydrodynamic equation, $D12/T=\alpha\eta^{\beta}$ where η is the solvent viscosity, and α and β the constants for a specific solute irrespective of solvent species in supercritical state, CO2+hexane and liquid organic solvents. Both the parameters involved in the equation were individually determined for 12 solutes [1]. To develop the accurate correlations, D12 data of lipids are required over a wide range of solvent viscosity in supercritical and liquid states.

In this study, the measurements of lipids in supercritical carbon dioxide were reviewed, and D12 data on lipids in various organic solvents were measured by the Taylor dispersion method. The values were firstly affected by molecular size or molecular weight (MW), and secondly by the polarity, or functional groups. Moreover, the values were proportional to the power of MW to -0.5 up to 1134 for trinevonin. The hydrodynamic equation was generalized, and the constants α and β were expressed as a function of molecular weight, or solute molar volume at its normal boiling point for various lipids such as free fatty acids, methyl and ethyl esters, and mono-, di- and triglycerides. Moreover, the validities of the equations were discussed for diffusion coefficients in SC CO2 with an entrainer, CO2 expanded liquids, and liquid organic solvents. The accuracies were also compared with those proposed in the literature.

References

[1] T. Funazukuri, et al., J. Supercrit. Fluids., 46 (2008) 280-284.