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Correlation of Solubilities in Mixed-Solvents with Local-composition-Regular Solution Theory

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Abstract (less than 300 words)

The dissolution of a solute in solvent is a common protocol in industries that process food and active pharmaceutical ingredients (API). Therefore, there is great demand to improve the processing of active components with desirable solvents and to reduce the use of organic solvents that can contaminate the product. Solid-liquid equilibrium data are necessary for addressing the forementioned challenges. However, determination of suitable solvent systems can complex because processing requirements involve multicomponents. In a previous study [1], local-composition-regular solution theory (LC-RST) was developed to correlate the solubility data of API in mixed-solvents for ternary systems. LC-RST can be extended to predict the phase behavior of non-polarity or non-specific interactions solutions [2, 3]. The objective of this study was to correlate solubility data of active pharmaceutical ingredients in mixed-solvents with LC-RST model and to study its generalization. The selected mixed-solvent were water-acetone, water- isopropanol and water- ethanol at 273 K to 313 K. In this study, the number of fitting parameters for ternary solid-liquid equilibrium data could be reduced from 12 to 6 with the sum of the solubility errors being in the range of 1.62×10^{-4} to 7.85×10^{-4}. Fitting parameters could be generalized with the properties of paracetamol and mixed-solvent systems. In the model two parameters had a linear relationship with the molecular weight of system; two parameters were related to the number of hydrogen donors and heat of fusion of the system; one parameter was related to the number of hydrogen accepters and donors of system; and one parameter was related to the solubility parameters of compounds in system. The potential application of correlation is for selection of vegetable oil based mixed-solvents for a separation process in supporting green and sustainable development.

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