

Lower Critical Solution Temperature (LCST) of Binary Polymeric Solutions: A Chemical Engineering Point of View

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The phase behavior of (binary) polymeric solutions such as lower critical solution temperature (LCST) has an important role in many polymeric processes. For theoretical investigation on the prediction of LCST, a substantial data points on LCST of binary polymeric solutions were collected from literatures and used to (i) develop an efficient and accurate empirical correlation for LCST estimation through statistical modeling using matrix algebra (namely M1) and also (ii) to present a reliable calculation routine through chemical engineering thermodynamic approach (namely M2). To develop the statistical model (M1), the connectivity indices of polymer and solvent were used as the independent variables in M1. The thermodynamic models of Nonrandom Two Liquids (NRTL), Universal Quasi-Chemical (UNIQUAC), Flory-Huggins (FH), Modified Separation of Cohesive Energy Density Model (MOSCED) and Compressible Regular Solution (CRS) were studied in presentation of chemical engineering thermodynamic approach (M2). Four statistical parameters i.e. Sum of Squares due to Error of the fit (SSE), the Square of the correlation (R²), adjusted R-square (R²-adj) and Standard Error of the Regression (RMSE) were defined as criteria to evaluate the models and convergence of calculations. The minimization of errors and objective functions was done by applying Particle Swarm Optimization (PSO) algorithm. The reliability and accuracy of proposed approaches discussed in-details and the results were compared to the available experimental data and the reported results of quantitative structure–property relationship (QSPR) approach.