NIST ThermoData Engine: Solvent Design and Propagation of Uncertainties for Process Simulation

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Benefits of the Dynamic Data Evaluation concept implemented in the NIST ThermoData Engine software (TDE) have been extended to two new areas: solvent design and estimation of uncertainties for properties of process streams. Solvent design covers three most common tasks: search for the best solvent for a solid solute, for separation of two solid solutes, and for extraction. While providing traditional prediction-based solutions, the procedure includes features specific to TDE: use of the array of critically evaluated experimental data for binary mixtures, automated analysis of molecular structures, and recently generated NIST-KT-UNIFAC parameters. Estimation of the uncertainties for properties of process streams is important in order to reduce traditional "overdesign" in chemical technology. It is based on the covariance method and propagates critically re-assessed experimental uncertainties and model deviations to most common calculations of properties of multi-component streams at bubble, dew, and two-phase VLE conditions. Verification of the uncertainty assessment has been done using experimental data for ternary mixtures. Results and computational times have been compared with the alternative approach of stochastic sampling.