Computational Toolbox for Synthesis of Products and Processes using Supercritical Fluids

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Abstract
Supercritical fluids are becoming increasingly popular as green solvents with minimum adverse environmental impact. However, our understanding of highly non-ideal and complex phase behavior of resulting mixtures at elevated pressures are in part responsible for less wide spread usage then the potential. A computational toolbox in matlab is developed which not only predicts the high-pressure phase equilibrium correctly and consistently but also resolves the synthesis problem of supercritical products and processes. The computational tools are based on global solvers for solving highly non-linear equations. We utilize the Interval Analysis based global solvers to compute the phase behavior and stability issues of supercritical systems. Homotopy continuation based algorithm is used to compute the thermodynamic landmarks at elevated pressures followed by integration of Differential Algebraic Equations (DAEs). The computed information is utilized to develop a synthesis tool for supercritical systems. The highly non-ideal phase equilibrium is computed using Peng-Robinson-Stryjek-Vera equation of state with Wong-Sandler mixing rules. The toolbox is also utilized in synthesis of Carbon Dioxide based refrigerants as alternatives to CFCs as well as development of process schemes for separation of alcohol-water systems.

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