Chemical Engineering Calculations using Scilab

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Abstract

In this work we presented some Chemical Engineering and Materials Science calculations using Scilab 5.1.1 environment, particularly: (i) azeotrope calculations at low and high pressures; (ii) double retrograde vaporization; (iii) parameter estimation, applied to binary interaction parameters of equations of state mixing rules and (iv) multireactive chemical equilibria, with applications in biomimetic studies. Azeotrope and double retrograde calculations were investigated because these thermodynamic phenomena are characterized by nonlinear systems of algebraic equations which can be exhibit more than one solution. Thus, some deterministic and stochastic techniques were used in order to obtain all the solutions for these kind of nonlinear systems. Azeotrope calculations were conducted using equations of state with appropriated mixing rules (for high pressure calculations) and excess Gibbs free energy models (for low pressures). Numerical aspects of convergence were investigated, particularly in the cases with double azeotropy. Double retrograde vaporization is an interesting thermodynamic phenomenon where the dew point locus show three or four solutions for an specified vapor composition. Thus, in a nonlinear system sense, we are interested in numerical methodologies to obtain, in a reasonable computational time, all the solutions. This problem is more severe if we consider multicomponent systems (such as petroleum fractions). The third problem approached is the parameter estimation, applied to binary interaction parameters of mixing rules. This problem involves, in a inner loop, the bubble or dew point coexistence problem, in order to minimize the difference between experimental and calculated values. In this context, the surfaces of objective functions were obtained using Scilab, in order to show the neighborhood of the minimum. Finally, we analyze the multireactive chemical equilibrium problem, involving calcium and phosphate ions and their complexes. In this case, we obtain a nonlinear system with more than 20 equations (chemical equilibrium relations and material balances), which was solved using Newton's method, implemented in Scilab 5.1.1. The solution of this system is useful to predict the conditions of formation for some interesting calcium phosphates, such as hydroxyapatite. Thus, several linear algebra packages implemented in Scilab 5.1.1 were used, such as matrix inversions (necessary, for instance, in Newton-Raphson recurrence equation), matrix-vector products, matrix-matrix products and element-to-element calculations. Scilab graphical capability was also explored for visualization of contour curves of objective functions, dew/bubble point curves/surfaces and basins of attractions for roots of nonlinear systems.

Key words: Nonlinear systems, optimization, chemical engineering