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Chemical Equilibria with Two or More EquationsMultiple Equations, Few Unknowns Using MATLAB; Method 1 Using the 'fsolve' Command; Method 2 Using the 'fminsearch' Function; Variations in MATLAB; Chemical Equilibria Using Aspen Plus; Chapter Summary; Problems; 5 Mass Balances With Recycle Streams; Mathematical Formulation; Example Without Recycle; Example With Recycle; Comparison of Sequential and Simultaneous Solution Methods; Example of Process Simulation Using Excel for Simple Mass Balances; Example of Process Simulation With Excel Including Chemical Reaction Equilibrium
Example of Process Simulation With Excel Including Phase EquilibriumDid Iterations Converge?; Extensions; Chapter Summary; Class Exercises; Class Discussion; Problems; 6 Simulation of Mass Transfer Equipment; Thermodynamics; Example: Multicomponent Distillation With Shortcut Methods; Mathematical Development; Multicomponent Distillation With Rigorous Plate-to-Plate Methods; Example: Packed Bed Absorption; Example: Gas Plant Production Separation; Chapter Summary; Class Exercise; Problems (Using Aspen Plus); 7 Process Simulation; Model Library; Example: Ammonia Process; Utility Costs
Convergence HintsOptimization; Chapter Summary; Class Exercise; Problems; 8 Chemical Reactors; Mathematical Formulation of Reactor Problems; Example: Plug Flow Reactor and Batch Reactor; Example: Continuous Stirred Tank Reactor; Using MATLAB to Solve Ordinary Differential Equations; Simple Example; Use of the 'Global' Command; Passing Parameters; Example: Isothermal Plug Flow Reactor; Example: Nonisothermal Plug Flow Reactor; Using FEMLAB to Solve Ordinary Differential Equations; Simple Example; Example: Isothermal Plug Flow Reactor; Example: Nonisothermal Plug Flow Reactor
Reactor Problems with Mole Changes and Variable Density

Sommario/riassunto

An innovative introduction to chemical engineering computingAs chemical engineering technology advances, so does the complexity of the problems that arise. The problemsthat chemical engineers and chemical engineering students face today can no longer be answered with programs written on a case-by-case basis. Introduction to Chemical Engineering Computing teaches professionalsand students the kinds of problems they will have to solve, the types of computer programs needed to solvethese problems, and how to ensure that the problems have been solved correctly.Each chapter