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Simulation; Differential Equations; Appendices; 2 Equations of State; Equations of State - Mathematical Formulation; Solving Equations of State Using Excel (single equation in one unknown); Solution Using 'Goal Seek'; Solution Using Solver; Example of a Chemical Engineering Problem Solved Using 'Goal Seek'; Solving Equations of State Using MATLAB (single equation in one unknown); Example of a Chemical Engineering Problem Solved Using MATLAB

Another Example of a Chemical Engineering Problem Solved Using MATLAB

Equations of State with Aspen Plus; Example; Specific Volume of a Mixture; Chapter Summary; Problems; 3 Vapor-Liquid Equilibrium; Flash and Phase Separation; Isothermal Flash - Development of Equations; Example Using Excel; Thermodynamic Parameters; Example Using MATLAB; Example Using Aspen Plus; Nonideal Liquids - Test of Thermodynamic Model; Chapter Summary; Problems; 4 Chemical Reaction Equilibrium; Chemical Equilibrium Expression; Example of Hydrogen for Fuel Cells; Solution Using Excel; Solution Using MATLAB

Chemical Equilibria with Two or More Equations

Multiple 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 Equilibrium

Did 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 Hints

Optimization; 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 computing

As chemical engineering technology advances, so does the complexity of the problems that arise. The problems that 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 professionals and students the kinds of problems they will have to solve, the types of computer programs needed to solve these problems, and how to ensure that the problems have been solved correctly. Each chapter