## **Table of Contents**

- Preface
- 1 Introduction
- Differential Equations
- Organization
- Algebraic Equations
- Process Simulation
- Appendices
- 2 Equations of State
- Equation of state mathematical formulation
- Solving equations of state Using Excel
- Solution using 'Goal seek'
- Solution using 'Solver'
- Example of a chemical engineering problem solved using 'Goal Seek'
- Solving equations of state using MATLAB(r)
- 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
- 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
- Non-ideal liquids test of thermodynamic model
- Chapter summary
- Problems
- 4 Chemical Reaction Equilibrium
- Chemical equilibrium expression
- Example of hydrogen for fuel cells
- Solution with Excel
- Solution using MATLAB
- Chemical equilibria with two or more equations
- Multiple equations, few unknowns with MATLAB
- Method 1 using the 'fsolve' command
- Method 2 using the 'fminsearch' function
- Variations in MATLAB
- Chemical Equilibria with 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 using Excel including chemical reaction equilibrium
- Example of process simulation using Excel including phase equilibrium
- Chapter summary
- Class exercises
- Class discussion
- Problems
- 6 Simulation of Mass Transfer Equipment
- Thermodynamics
- Mathematical development
- Example: multicomponent distillation with rigorous plate-to-plate methods
- Example: packed bed absorption
- Example: gas plant product 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 (CSTR)
- Using MATLAB to solve ordinary differential equations
- Passing parameters
- Example: multicomponent distillation with shortcut methods
- Simple example
- Use of the 'global' command
- Simple example
- Example: isothermal plug flow reactor
- Example: non-isothermal flow reactor
- Using FEMLAB to solve ordinary differential equations
- Example: isothermal plug flow reactor
- Example: non-isothermal flow reactor
- Reactor problems with mole changes and variable density
- Chemical reactors with mass transfer limitations
- Continuous stirred tank reactors (CSTR)

- Solution using Excel Solution using MATLAB
- CSTR with multiple solutions
  Solutions to multiple equations using MATLAB
- Transient continuous stirred tank reactors (CSTR)
- Chapter summary Problems
- 9 Transport Process in One Dimension