CONTENTS

PREFACE xi
ACKNOWLEDGMENTS xiii
NOMENCLATURE xvii

I FUEL CELL PRINCIPLES

1 Introduction 3
  1.1 What Is a Fuel Cell? / 3
  1.2 A Simple Fuel Cell / 6
  1.3 Fuel Cell Advantages / 8
  1.4 Fuel Cell Disadvantages / 11
  1.5 Fuel Cell Types / 12
  1.6 Basic Fuel Cell Operation / 14
  1.7 Fuel Cell Performance / 18
  1.8 Characterization and Modeling / 20
  1.9 Fuel Cell Technology / 21
  1.10 Fuel Cells and the Environment / 21
  1.11 Chapter Summary / 22
      Chapter Exercises / 23
## 2 Fuel Cell Thermodynamics

2.1 Thermodynamics Review / 25
2.2 Heat Potential of a Fuel: Enthalpy of Reaction / 34
2.3 Work Potential of a Fuel: Gibbs Free Energy / 37
2.4 Predicting Reversible Voltage of a Fuel Cell under Non-Standard-State Conditions / 47
2.5 Fuel Cell Efficiency / 60
2.6 Thermal and Mass Balances in Fuel Cells / 65
2.7 Thermodynamics of Reversible Fuel Cells / 67
2.8 Chapter Summary / 71
   Chapter Exercises / 72

## 3 Fuel Cell Reaction Kinetics

3.1 Introduction to Electrode Kinetics / 77
3.2 Why Charge Transfer Reactions Have an Activation Energy / 82
3.3 Activation Energy Determines Reaction Rate / 84
3.4 Calculating Net Rate of a Reaction / 85
3.5 Rate of Reaction at Equilibrium: Exchange Current Density / 86
3.6 Potential of a Reaction at Equilibrium: Galvani Potential / 87
3.7 Potential and Rate: Butler–Volmer Equation / 89
3.8 Exchange Currents and Electrocatalysis: How to Improve Kinetic Performance / 94
3.9 Simplified Activation Kinetics: Tafel Equation / 97
3.10 Different Fuel Cell Reactions Produce Different Kinetics / 100
3.11 Catalyst–Electrode Design / 103
3.12 Quantum Mechanics: Framework for Understanding Catalysis in Fuel Cells / 104
3.13 The Sabatier Principle for Catalyst Selection / 107
3.14 Connecting the Butler–Volmer and Nernst Equations (Optional) / 108
3.15 Chapter Summary / 112
   Chapter Exercises / 113

## 4 Fuel Cell Charge Transport

4.1 Charges Move in Response to Forces / 117
4.2 Charge Transport Results in a Voltage Loss / 121
4.3 Characteristics of Fuel Cell Charge Transport Resistance / 124
4.4 Physical Meaning of Conductivity / 128
4.5 Review of Fuel Cell Electrolyte Classes / 132
CONTENTS

4.6 More on Diffusivity and Conductivity (Optional) / 153
4.7 Why Electrical Driving Forces Dominate Charge Transport (Optional) / 160
4.8 Quantum Mechanics–Based Simulation of Ion Conduction in Oxide Electrolytes (Optional) / 161
4.9 Chapter Summary / 163
    Chapter Exercises / 164

5 Fuel Cell Mass Transport
5.1 Transport in Electrode versus Flow Structure / 168
5.2 Transport in Electrode: Diffusive Transport / 170
5.3 Transport in Flow Structures: Convective Transport / 183
5.4 Chapter Summary / 199
    Chapter Exercises / 200

6 Fuel Cell Modeling
6.1 Putting It All Together: A Basic Fuel Cell Model / 203
6.2 A 1D Fuel Cell Model / 206
6.3 Fuel Cell Models Based on Computational Fluid Dynamics (Optional) / 227
6.4 Chapter Summary / 230
    Chapter Exercises / 231

7 Fuel Cell Characterization
7.1 What Do We Want to Characterize? / 238
7.2 Overview of Characterization Techniques / 239
7.3 In Situ Electrochemical Characterization Techniques / 240
7.4 Ex Situ Characterization Techniques / 265
7.5 Chapter Summary / 268
    Chapter Exercises / 269

II FUEL CELL TECHNOLOGY

8 Overview of Fuel Cell Types
8.1 Introduction / 273
8.2 Phosphoric Acid Fuel Cell / 274
8.3 Polymer Electrolyte Membrane Fuel Cell / 275
8.4 Alkaline Fuel Cell / 278
8.5 Molten Carbonate Fuel Cell / 280
CONTENTS

8.6 Solid-Oxide Fuel Cell / 282
8.7 Other Fuel Cells / 284
8.8 Summary Comparison / 298
8.9 Chapter Summary / 299
Chapter Exercises / 301

9 PEMFC and SOFC Materials 303

9.1 PEMFC Electrolyte Materials / 304
9.2 PEMFC Electrode/Catalyst Materials / 308
9.3 SOFC Electrolyte Materials / 317
9.4 SOFC Electrode/Catalyst Materials / 326
9.5 Material Stability, Durability, and Lifetime / 336
9.6 Chapter Summary / 340
Chapter Exercises / 342

10 Overview of Fuel Cell Systems 347

10.1 Fuel Cell Subsystem / 348
10.2 Thermal Management Subsystem / 353
10.3 Fuel Delivery/Processing Subsystem / 357
10.4 Power Electronics Subsystem / 364
10.5 Case Study of Fuel Cell System Design: Stationary Combined Heat and Power Systems / 369
10.6 Case Study of Fuel Cell System Design: Sizing a Portable Fuel Cell / 383
10.7 Chapter Summary / 387
Chapter Exercises / 389

11 Fuel Processing Subsystem Design 393

11.1 Fuel Reforming Overview / 394
11.2 Water Gas Shift Reactors / 409
11.3 Carbon Monoxide Clean-Up / 411
11.4 Reformer and Processor Efficiency Losses / 414
11.5 Reactor Design for Fuel Reformers and Processors / 416
11.6 Chapter Summary / 417
Chapter Exercises / 419
12 Thermal Management Subsystem Design 423
12.1 Overview of Pinch Point Analysis Steps / 424
12.2 Chapter Summary / 440
Chapter Exercises / 441

13 Fuel Cell System Design 447
13.1 Fuel Cell Design Via Computational Fluid Dynamics / 447
13.2 Fuel Cell System Design: A Case Study / 462
13.3 Chapter Summary / 476
Chapter Exercises / 477

14 Environmental Impact of Fuel Cells 481
14.1 Life Cycle Assessment / 481
14.2 Important Emissions for LCA / 490
14.3 Emissions Related to Global Warming / 490
14.4 Emissions Related to Air Pollution / 502
14.5 Analyzing Entire Scenarios with LCA / 507
14.6 Chapter Summary / 510
Chapter Exercises / 511

A Constants and Conversions 517

B Thermodynamic Data 519

C Standard Electrode Potentials at 25°C 529

D Quantum Mechanics 531
D.1 Atomic Orbitals / 533
D.2 Postulates of Quantum Mechanics / 534
D.3 One-Dimensional Electron Gas / 536
D.4 Analogy to Column Buckling / 537
D.5 Hydrogen Atom / 538
D.6 Multielectron Systems / 540
D.7 Density Functional Theory / 540
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>E Periodic Table of the Elements</td>
<td>543</td>
</tr>
<tr>
<td>F Suggested Further Reading</td>
<td>545</td>
</tr>
<tr>
<td>G Important Equations</td>
<td>547</td>
</tr>
<tr>
<td>H Answers to Selected Chapter Exercises</td>
<td>551</td>
</tr>
<tr>
<td>BIBLIOGRAPHY</td>
<td>555</td>
</tr>
<tr>
<td>INDEX</td>
<td>565</td>
</tr>
</tbody>
</table>