## Contents

1 Basic Models of Computational Mass Transfer .......................... 1
   1.1 Equation of Mass Conservation and Its Closure .............. 3
   1.2 Turbulent Mass Diffusivity Model ........................... 6
   1.3 Conventional Turbulent Mass Diffusivity Model .............. 6
      1.3.1 Turbulent Schmidt Number Model .................... 6
      1.3.2 Inert Tracer Model ............................. 7
   1.4 $\overline{c^2} - \varepsilon_c$ Model (Two-Equation Model) .... 7
      1.4.1 The $\overline{c^2}$ and $\varepsilon_c$ Equations ........... 8
      1.4.2 The $\overline{c^2} - \varepsilon_c$ Model Equation Sets .. 17
      1.4.3 Determination of Boundary Conditions ............... 21
      1.4.4 Experimental Verification of Model Prediction ...... 24
      1.4.5 Analogy Between Transport Diffusivities ............. 26
      1.4.6 Generalized Equations of Two-Equation Model ...... 28
   1.5 Reynolds Mass Flux Model .................................. 29
      1.5.1 Standard Reynolds Mass Flux Model .................. 29
      1.5.2 Hybrid Reynolds Mass Flux Model .................... 37
      1.5.3 Algebraic Reynolds Mass Flux Model ................. 38
   1.6 Simulation of Gas (Vapor)–Liquid Two-Phase Flow ........... 39
   1.7 Model System of CMT Process Computation ................... 45
   1.8 Summary .................................................. 46
   References .................................................. 47

2 Application of Computational Mass Transfer (I) Distillation
   Process .................................................... 51
   2.1 Tray Column .............................................. 54
      2.1.1 $\overline{c^2} - \varepsilon_c$ Two-Equation Model .......... 54
      2.1.2 Reynolds Mass Flux Model .......................... 69
      2.1.3 Prediction of Multicomponent Point Efficiency ..... 78
2.2 Packed Column ................................................................. 90
  2.2.1 \( \overline{c^2} - \varepsilon_c \) Two-Equation Model .................. 90
  2.2.2 Reynolds Mass Flux Model ........................................... 95
2.3 Separation of Benzene and Thiophene by Extractive Distillation .................................................. 103
2.4 Summary ................................................................. 108
References ........................................................................ 109

3 Application of Computational Mass Transfer (II) Chemical Absorption Process ................................................. 111
  3.1 \( \overline{c^2} - \varepsilon_c \) Two-Equation Model ................................ 113
    3.1.1 Absorption of CO₂ by Aqueous MEA in Packed Column .................................................. 118
    3.1.2 Absorption of CO₂ by Aqueous AMP in Packed Column .................................................... 125
    3.1.3 Absorption of CO₂ by Aqueous NaOH in Packed Column ..................................................... 128
  3.2 Reynolds Mass Flux Model .................................................... 134
    3.2.1 Absorption of CO₂ by Aqueous MEA in Packed Column ..................................................... 137
    3.2.2 The Absorption of CO₂ by Aqueous NaOH in Packed Column ........................................... 144
  3.3 Summary ................................................................. 148
References ........................................................................ 148

4 Application of Computational Mass Transfer (III) Adsorption Process ................................................................. 151
  4.1 \( \overline{c^2} - \varepsilon_c \) Two-Equation Model for Gas Adsorption .............. 154
    4.1.1 \( \overline{c^2} - \varepsilon_c \) Model Equations .......................................................... 154
    4.1.2 Boundary Conditions ......................................................... 157
    4.1.3 Evaluation of Source Terms ................................................ 158
    4.1.4 Simulated Results and Verification ........................................ 160
    4.1.5 Simulation for Desorption (Regeneration) and Verification .......... 165
  4.2 Reynolds Mass Flux Model .................................................... 167
    4.2.1 Model Equations .............................................................. 167
    4.2.2 Simulated Results and Verification ........................................ 169
    4.2.3 Simulation for Desorption (Regeneration) and Verification .......... 171
  4.3 Summary ................................................................. 173
References ........................................................................ 173
### 5 Application of Computational Mass Transfer (IV)

#### Fixed-Bed Catalytic Reaction

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.1 $\overline{c}^2 - \overline{c}_e$ Two-Equation Model for Catalytic Reactor</td>
<td>178</td>
</tr>
<tr>
<td>5.1.1 Model Equation</td>
<td>178</td>
</tr>
<tr>
<td>5.1.2 Boundary Conditions</td>
<td>182</td>
</tr>
<tr>
<td>5.1.3 Determination of the Source Terms</td>
<td>182</td>
</tr>
<tr>
<td>5.1.4 The Simulated Wall-Cooled Catalytic Reactor</td>
<td>183</td>
</tr>
<tr>
<td>5.1.5 Simulated Result and Verification</td>
<td>185</td>
</tr>
<tr>
<td>5.2 Reynolds Mass Flux Model for Catalytic Reactor</td>
<td>191</td>
</tr>
<tr>
<td>5.2.1 Model Equations</td>
<td>191</td>
</tr>
<tr>
<td>5.2.2 Simulated Result and Verification</td>
<td>194</td>
</tr>
<tr>
<td>5.2.3 The Anisotropic Mass Diffusivity</td>
<td>197</td>
</tr>
<tr>
<td>5.3 Summary</td>
<td>200</td>
</tr>
</tbody>
</table>

#### References

201

### 6 Application of Computational Mass Transfer (V) Fluidized Chemical Process

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.1 Flow Characteristics of Fluidized Bed</td>
<td>205</td>
</tr>
<tr>
<td>6.2 $\overline{c}^2 - \overline{c}_e$ Two-Equation Model for Simulating Fluidized Process</td>
<td>208</td>
</tr>
<tr>
<td>6.2.1 The Removal of CO$_2$ in Flue Gas in FFB Reactor</td>
<td>208</td>
</tr>
<tr>
<td>6.2.2 Simulation of Ozone Decomposition in the Downer of CFB Reactor</td>
<td>219</td>
</tr>
<tr>
<td>6.3 Reynolds Mass Flux Model for Simulating Fluidized Process</td>
<td>223</td>
</tr>
<tr>
<td>6.3.1 Model Equations</td>
<td>223</td>
</tr>
<tr>
<td>6.3.2 Simulation of the Riser in CFB Ozone Decomposition</td>
<td>227</td>
</tr>
<tr>
<td>6.3.3 Simulation of the Downer in CFB Ozone Decomposition</td>
<td>237</td>
</tr>
<tr>
<td>6.4 Summary</td>
<td>239</td>
</tr>
</tbody>
</table>

#### References

240

### 7 Mass Transfer in Multicomponent Systems

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.1 Mass Transfer Rate in Two-Component (Binary) System</td>
<td>245</td>
</tr>
<tr>
<td>7.2 Mass Transfer in Multicomponent System</td>
<td>251</td>
</tr>
<tr>
<td>7.2.1 Generalized Fick’s Law</td>
<td>252</td>
</tr>
<tr>
<td>7.2.2 Maxwell–Stefan Equation</td>
<td>252</td>
</tr>
<tr>
<td>7.3 Application of Multicomponent Mass Transfer Equation</td>
<td>256</td>
</tr>
<tr>
<td>7.3.1 Prediction of Point Efficiency of Tray Column</td>
<td>256</td>
</tr>
<tr>
<td>7.3.2 Two-Regime Model for Point Efficiency</td>
<td>257</td>
</tr>
<tr>
<td>7.3.3 Example of Simulation</td>
<td>261</td>
</tr>
</tbody>
</table>
7.4 Verification of Simulated Result .................................. 263
  7.4.1 Experimental Work ........................................... 263
  7.4.2 Comparison of Simulation with Experimental ............. 265
  7.4.3 The Bizarre Phenomena of Multicomponent System .......... 265
7.5 Determination of Vapor–Liquid Equilibrium Composition ...... 268
  7.5.1 Thermodynamic Relationship of Nonideal Solution ......... 268
  7.5.2 Prediction of Activity Coefficient: (1)
    Semi-empirical Equation ......................................... 271
  7.5.3 Prediction of Activity Coefficient (2) Group Contribution Method ........................................... 275
  7.5.4 Experimental Measurement of Activity Coefficient ........ 278
7.6 Results and Discussion ........................................... 280
  7.6.1 Correlation of the Phase Equilibrium ...................... 280
7.7 Summary ......................................................... 284
References ......................................................................... 284

8 Micro Behaviors Around Rising Bubbles ......................... 287
  8.1 Fluid Velocity Near the Bubble Interface ...................... 288
    8.1.1 Model Equation of Velocity Distribution
      Near a Rising Bubble ............................................ 290
    8.1.2 Experimental Measurement and Comparison
      with Model Prediction ............................................ 295
  8.2 Concentration Field Around a Bubble ...................... 298
    8.2.1 Concentration at Bubble Interface ......................... 298
    8.2.2 Interfacial Mass Transfer ..................................... 306
  8.3 Discussion ......................................................... 309
  8.4 Summary ......................................................... 309
References ......................................................................... 310

9 Simulation of Interfacial Effect on Mass Transfer ............. 311
  9.1 The Interfacial Effect ............................................. 313
  9.2 Experimental Observation of Interfacial Structure Induced by Marangoni Convection ................................. 315
    9.2.1 Stagnant Liquid and Horizontal Gas Flow ................ 316
    9.2.2 Horizontal Concurrent Flow of Liquid and Gas .......... 318
    9.2.3 Vertical (Falling Film) Countercurrent Flow
      of Liquid and Gas .................................................. 319
  9.3 The Condition for Initiating Marangoni Convection .......... 320
    9.3.1 Model Equations ............................................... 321
    9.3.2 Stability Analysis ............................................... 323
  9.4 Mass Transfer Enhancement by Marangoni Convection .... 327
9.5 Experiment on the Mass Transfer Enhancement by Interfacial Marangoni Convection ................. 330
  9.5.1 Absorption of CO₂ by Horizontal Stagnant Solvent .... 330
  9.5.2 Desorption of CO₂ by Falling Film Solvent ........... 332
9.6 The Transition of Interfacial Structure from Order to Disorder ........................................ 335
9.7 Theory of Mass Transfer with Consideration of Marangoni Effect ........................................ 338
9.8 Simulation of Rayleigh Convection ..................... 343
  9.8.1 Mathematical Model .................................. 343
  9.8.2 Result of Simulation and Analysis ................... 346
9.9 Experimental Measurement of Rayleigh Convection ......... 352
9.10 Simulation and Observation of Two-Dimensional Solute Convection at Interface ....................... 360
  9.10.1 Simulation of Two-Dimensional Interfacial Concentration .................................. 360
  9.10.2 Experimental Observation of Interfacial Concentration Gradient ............................ 365
9.11 Marangoni Convection at Deformed Interface Under Simultaneous Mass and Heat Transfer ............ 365
  9.11.1 Model Equations .................................... 366
  9.11.2 Generalization to Dimensionless ..................... 370
  9.11.3 Stability Analysis .................................. 372
9.12 Summary ................................................ 376
References ................................................................ 376

10 Simulation of Interfacial Behaviors by the Lattice-Boltzmann Method ........................................ 379
  10.1 Fundamentals of Lattice-Boltzmann Method .............. 381
    10.1.1 From Lattice Gas Method to Lattice-Boltzmann Method .................................. 381
    10.1.2 Basic Equations of Lattice-Boltzmann Method .................................. 382
    10.1.3 Lattice-Boltzmann Method for Heat Transfer Process ..................................... 389
    10.1.4 Lattice-Boltzmann Method for Mass Transfer Process ..................................... 391
  10.2 Simulation of Solute Diffusion from Interface to the Bulk Liquid .................................... 392
  10.3 Fixed Point Interfacial Disturbance Model ............... 394
    10.3.1 Single Local Point of Disturbance at Interface .................................. 394
    10.3.2 Influence of Physical Properties on the Solute Diffusion from Interface .................. 395
10.3.3 Uniformly Distributed Multi-points of Disturbance at Interface .................................. 399
10.3.4 Nonuniformly Distributed Multi-points of Disturbance at Interface ............................ 401
10.4 Random Disturbance Interfacial Model ..................................................... 402
10.5 Self-renewable Interface Model ............................................................... 412
10.6 Summary ............................................................................................... 416
References ...................................................................................................... 416
Introduction to Computational Mass Transfer
With Applications to Chemical Engineering
Yu, K.-T.; Yuan, X.
2017, XII, 417 p. 283 illus., 83 illus. in color. With online files/update., Hardcover