Contents

1 Introduction .................................................. 1
  1.1 Thermodynamic Instability ............................... 2
  1.2 Chemical Dynamic Instability ........................... 3
  1.3 Physical Surface (Including Dissolution Front) Instability .... 4
  1.4 The Contextual Arrangements of This Monograph ............ 6
References ......................................................... 8

2 Fundamental Theory for Chemical Dissolution-Front
Instability Problems in Fluid-Saturated Porous Media .......... 15
  2.1 Mathematical Theory for Simulating Chemical
Dissolution-Front Instability Problems in Fluid-Saturated
Porous Media .................................................. 17
    2.1.1 A General Case of Reactive Multi-Chemical-Species
         Transport with Consideration
         of Porosity/Permeability Feedback ................. 17
    2.1.2 A Particular Case of Reactive Single-Chemical-
         Species Transport with Consideration
         of Porosity/Permeability Feedback ................. 19
  2.2 Computational Theory for Simulating the Morphological
Evolution of a Chemical Dissolution Front .................... 30
    2.2.1 Formulation of the Segregated Algorithm
         for Simulating the Evolution of Chemical
         Dissolution Fronts .................................. 30
    2.2.2 Derivation of the Finite Element Equations
         of the Problem ..................................... 32
  2.3 Verification of the Proposed Numerical Algorithm
for Simulating the Evolution of Chemical
Dissolution Fronts ........................................... 36
  2.4 An Application Example for Simulating the Morphological
Evolution of Chemical Dissolution Fronts .................... 42
References ......................................................... 46
### Contents

#### 3 Effects of Particle Reactive Surface Areas on Chemical Dissolution-Front Instability in Fluid-Saturated Porous Media...

3.1 Theoretical Analysis of the Effect of Particle Shapes on Chemical Dissolution-Front Instability in Fluid-Saturated Porous Media ................................................................. 51

3.2 Numerical Modeling of the Chemical Dissolution-Front Evolution Within Fluid-Saturated Porous Media Consisting of Different Particle Shapes ..................................... 56

References .................................................................................................................. 70

#### 4 Effects of Mineral Dissolution Ratios on Chemical Dissolution-Front Instability in Fluid-Saturated Porous Media...

4.1 Theoretical Considerations of the Problem .......................................................... 72

4.2 Numerical Simulation of the Problem .................................................................. 77

4.3 Effects of Mineral Dissolution Ratios on the Evolution Patterns of Chemical Dissolution Fronts During Propagation in Fluid-Saturated Porous Media .......................... 80

References .................................................................................................................. 90

#### 5 Effects of Solute Dispersion on Chemical Dissolution-Front Instability in Fluid-Saturated Porous Media ...............

5.1 Mathematical Model for Chemical Dissolution-Front Instability Problems in Fluid-Saturated Porous Media Including Solute Dispersion Effects ........................................... 95

5.2 Theoretical Consideration of the Effects of Solute Dispersion on Chemical Dissolution-Front Instability in Two-Dimensional Fluid-Saturated Porous Media ................. 98

5.2.1 Derivation of Dimensionless Governing Equations for the Theoretical Problem ................................................................. 98

5.2.2 Derivation of Base Solutions for the Dimensionless Governing Equations of the Theoretical Problem in the Limit Case of the Mineral Dissolution Ratio Approaching Zero 100

5.2.3 Derivation of the Critical Condition for Unstable Chemical Dissolution-Fronts in Two-Dimensional Fluid-Saturated Porous Media Including Solute Dispersion Effects ........ 106

5.2.4 Theoretical Understanding of the Effects of Solute Dispersion on Chemical Dissolution-Front Instability in Two-Dimensional Fluid-Saturated Porous Media ......... 111

5.3 Application of the Present Theoretical Solutions ......................................................................... 112

References .................................................................................................................. 120
6 Effects of Medium Permeability Anisotropy on Chemical Dissolution-Front Instability in Fluid-Saturated Porous Media ........................................ 123

6.1 Mathematical Governing Equations for Chemical Dissolution-Front Instability Problems in Fluid-Saturated Porous Media Including Medium Anisotropy Effects ........ 125

6.2 Theoretical Analyses of Medium Permeability Anisotropy Effects .......................................................... 128

6.2.1 Derivation of Dimensionless Governing Equations . . . . . . 129

6.2.2 Derivation of Base Solutions for the Dimensionless Governing Equations of the Theoretical Problem Including the Consideration of Medium Orthotropic Effects (in the Case of $\varepsilon \to 0$) .......... 130

6.2.3 Derivation of the Critical Condition for Unstable Chemical Dissolution-Fronts in Two-Dimensional Fluid-Saturated Porous Media Including Medium Orthotropic Effects (in the Case of $\varepsilon \to 0$) .......... 133

6.3 Application of the Present Theoretical Solutions .................. 140

6.3.1 Theoretical Understanding of the Effects of Medium Permeability Anisotropy on Chemical Dissolution-Front Instability in Two-Dimensional Fluid-Saturated Porous Media ............... 140

6.3.2 Effects of Medium Permeability Anisotropy on the Morphological Evolution of the Chemical Dissolution Front in Two-Dimensional Fluid-Saturated Porous Media ............... 142

References .......................................................... 149

7 Effects of Medium and Pore-Fluid Compressibility on Chemical Dissolution-Front Instability in Fluid-Saturated Porous Media . . . 151

7.1 Theoretical Considerations of the Chemical Dissolution-Front Instability Problem in Deformable Fluid-Saturated Porous Media ......................... 152

7.1.1 Dimensional and Dimensionless Governing Equations of the Problem ......................... 152

7.1.2 Analytical Solutions Derived from Using a Fully-Compressible Pore-Fluid Model ............... 157

7.1.3 Analytical Solutions When the Pore-Fluid in the Upstream Region Is Incompressible ............... 158
7.2 Effects of Pore-Fluid Compressibility on the Evolution of a Chemical Dissolution Front in Subcritical Chemical Dissolution Systems............................................................... 162

7.2.1 Derivation of Analytical Solutions for the Benchmark Problem in the Subcritical Chemical Dissolution System of a Finite Domain ................................................................. 162

7.2.2 Evaluation of the Dimensionless Propagating Speed of the Chemical Dissolution Front Associated with the Derived Analytical Solutions for the Benchmark Problem .................. 166

7.2.3 Effects of Pore-Fluid Compressibility on the Evolution of a Chemical Dissolution Front in Subcritical Chemical Dissolution Systems ..................................................... 168

7.3 Computational Theory for Simulating the Morphological Evolution of a Chemical Dissolution Front with the Consideration of Pore-Fluid and Medium Compressibility ...................................................................................... 172

7.3.1 Derivation of the Finite Difference Equations of the Problem ................................................................................................................................. 174

7.3.2 Derivation of the Proposed Porosity-Gradient Replacement Approach .................................................................................................................. 175

7.3.3 Derivation of the Finite Element Equations of the Problem .................................................................................................................. 178

7.3.4 Verification of the Proposed Numerical Procedure ................................................................................................................................. 183

7.4 Effect of Pore-Fluid Compressibility on the Morphological Evolution of a Chemical Dissolution Front in the Supercritical Chemical Dissolution System ................................................................. 188

7.5 Effect of Medium Compressibility on the Morphological Evolution of a Chemical Dissolution Front in the Supercritical Chemical Dissolution System ................................................................. 190

References ................................................................................................................................................. 196

8 Computational Simulation of Three-Dimensional Behaviour of Chemical Dissolution-Front Instability in Fluid-Saturated Porous Media ................................................................................................................. 199

8.1 Governing Equations of the Problem and the Proposed Numerical Procedure ................................................................................................................................. 202

8.1.1 Governing Equations of the Problem ................................................................................................................................. 202

8.1.2 The Proposed Numerical Procedure ................................................................................................................................. 204

8.2 Verification of the Proposed Numerical Procedure ................................................................................................................................. 206

8.3 Morphological Evolution of Three-Dimensional Chemical-Dissolution Fronts in Fluid-Saturated Porous Media ................................................................................................................................. 215

References ................................................................................................................................................. 219
9 Fundamental Theory for Nonaqueous-Phase-Liquid Dissolution-Front Instability Problems in Fluid-Saturated Porous Media

9.1 Mathematical Modeling of NAPL Dissolution Problems in Two-Dimensional Fluid-Saturated Porous Media ........................................ 224

9.2 Theoretical Analysis of NAPL Dissolution Induced Instability Problems in Two-Dimensional Fluid-Saturated Porous Media ........................................ 227

9.2.1 Previous Approach .................................................. 227

9.2.2 Current Approach .................................................. 234

9.2.3 Theoretical Understanding of the Effects of Solute Dispersion on NAPL Dissolution-Front Instability in Two-Dimensional Fluid-Saturated Porous Media ........................................ 244

9.3 Computational Simulation of NAPL Dissolution-Front Instability Problems in Two-Dimensional Fluid-Saturated Porous Media ........................................ 245

9.3.1 Formulation of the Proposed Numerical Procedure for Simulating the Evolution of NAPL Dissolution Fronts ........................................ 246

9.3.2 Verification of the Proposed Numerical Procedure for Simulating the Evolution of NAPL Dissolution Fronts ........................................ 249

9.4 Three Different Kinds of Modes Associated with Morphological Evolution of NAPL Dissolution Fronts in Supercritical Systems ........................................ 257

9.4.1 The Fundamental Mode ............................................ 259

9.4.2 The Fingering Mode ............................................ 259

9.4.3 The Fractal Mode ............................................ 261

References ................................................................. 263

10 Effects of Domain Shapes and Mesh Discretization Error on the Morphological Evolution of Nonaqueous-Phase-Liquid Dissolution Fronts in Fluid-Saturated Porous Media ................. 267

10.1 Governing Equations of NAPL Dissolution Problems in Two-Dimensional Fluid-Saturated Porous Media ........................................ 270

10.2 Effects of Domain Shapes on the Morphological Evolution of NAPL Dissolution Fronts in Supercritical Systems ........................................ 277

10.3 Effects of Mesh Discretization Error on the Morphological Evolution of NAPL Dissolution Fronts in Supercritical Systems ........................................ 289
10.3.1 The Theoretical Basis of Mesh Discretization Error Estimation for NAPL Dissolution Problems . . . 290
10.3.2 Corner and Mesh Discretization Effects on the Morphological Evolution of NAPL Dissolution Fronts in Supercritical Systems of Trapezoidal Domains .......................... 299

References .................................................. 311

11 Fundamental Theory for Acidization Dissolution-Front Instability in Fluid-Saturated Carbonate Rocks ............... 315
11.1 Mathematical Analysis of the Acidization Dissolution Problem ............................................. 317
11.1.1 Determination of the Propagation Speed of the Acidization Dissolution Front in a Fluid-Saturated Carbonate Rock .................. 319
11.1.2 Instability Analysis of the Acidization Dissolution Front in a Fluid-Saturated Carbonate Rock .... 322

11.2 Theoretical Understanding of Some Fundamental Characteristics of Acidization Dissolution-Front Instability Problems .................................................. 331
11.2.1 The Intrinsic Time and Length Scales of an Acidization Dissolution System ........... 331
11.2.2 The Asymptotic Behavior of an Acidization Dissolution System under Two Limit Conditions . . . 332
11.2.3 Effects of Several Factors on the Critical Zhao Number of an Acidization Dissolution System . . . 333
11.2.4 Effects of Several Factors on the Propagation Speed of an Acidization Dissolution Front ........ 335

11.3 Application of the Proposed Theory .................. 336

References .................................................. 342

Summary Statements ........................................ 345

Index .................................................. 351
Physical and Chemical Dissolution Front Instability in Porous Media
Theoretical Analyses and Computational Simulations
Zhao, C.
2014, XVIII, 354 p. 93 illus., 68 illus. in color., Hardcover
ISBN: 978-3-319-08460-2