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Chongbin Zhao

Physical and Chemical Dissolution Front Instability in Porous Media

Theoretical Analyses and Computational
Simulations

 Springer

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Preface

Physical and chemical dissolution-front instability problems exist ubiquitously in many scientific and engineering fields. In geoenvironmental engineering, remediation of contaminated sites using fresh water to flush the contaminated soils involves the propagation of dissolved contaminant fronts in water-saturated porous media. In mineral mining engineering, the extraction of minerals in the deep Earth using the in-situ leaching technique may result in the propagation of dissolved mineral fronts in fluid-saturated porous media. In petroleum industry, the secondary recovery of oil by acidifying the oil field to uniformly increase porosity and hence the yield of oil is associated with the propagation of acid-dissolved material fronts in porous rocks. The common feature of physical and chemical dissolution-front propagation is that it can be mathematically treated as an instability problem involving a highly nonlinear system. When the nonlinear system is in a stable state, any small perturbation applied to the system does not cause any change in the basic characteristic of the dynamic response of the nonlinear system. However, when the nonlinear system is in an unstable state, any small perturbation applied to the system can cause a qualitative change in the basic characteristic of the dynamic response of the system. For this reason, the study of nonlinear system instability has become an important topic in many scientific and engineering fields over the past few decades.

Although dynamic mechanisms of physical and chemical dissolution-front instability phenomena in porous media have been studied and discussed for many years, there is a lack of a systematic and theoretical treatment of these phenomena in the world. Such a treatment is beneficial not only for understanding ore forming mechanisms, which are imperative to develop advanced techniques for exploring new ore deposits in the deep Earth, but also for understanding dissolved contaminant transport, which is important to develop innovative techniques for rehabilitating contaminated soils. By keeping this consideration in mind, this monograph aims to provide state-of-the-art theoretical and computational results in this particular research field, based on the author's own work during the last decade.

For this purpose, although some numerical results are provided to complement theoretical ones, the main focus of this monograph is on theoretical aspects of the topic. This means that the theoretical treatment contained in this monograph is also applicable to a wide range of scientific and engineering problems involving instability phenomena of highly nonlinear dynamic systems. To broaden the readership of this monograph, common mathematical notations are used to derive the theoretical solutions. This enables this monograph to be used either as a useful textbook for postgraduate students or as a valuable reference book for mathematicians, engineers and geoscientists. In addition, each chapter is written independently of the remainder of the monograph so that readers may read the chapter of interest separately.

In this monograph, a series of fundamental theories have been presented for dealing with physical and chemical dissolution-front instability in fluid-saturated porous media. The key of developing these theories is to mathematically establish some theoretical criteria that are used to assess whether or not physical and chemical dissolution fronts can become unstable in the dissolution systems. On the other hand, these fundamental theories can provide some benchmark solutions, which are used to verify numerical methods and algorithms that can be used to simulate complicated physical and chemical dissolution systems in the fluid-saturated porous media. Although theoretical analyses can be conducted for some physical and chemical dissolution problems with simple geometry, it is very difficult, if not impossible, to predict analytically the complicated morphological evolution of either physical or chemical dissolution front in the case of the dissolution system becoming supercritical. As an alternative, numerical methods are developed to overcome this difficulty. Specifically, the overall arrangements of this monograph are as follows: (1) a fundamental theory is presented, in Chap. 2, to deal with chemical dissolution-front instability problems in fluid-saturated porous media. The mathematical analysis is used to establish a theoretical criterion, which is employed to judge the instability of chemical dissolution fronts in a chemical dissolution system, while the computational method is used to simulate the morphological evolution of chemical dissolution fronts when the chemical dissolution system is in a supercritical state. (2) To understand the fundamental behaviors of a chemical dissolution-front instability problem, several key factors, such as the particle reactive surface area, mineral dissolution ratio, solute dispersion, medium permeability anisotropy, and medium/pore-fluid compressibility, have been deliberately considered to investigate their effects on chemical dissolution front instability in Chaps. 3–7, respectively. (3) Three-dimensional computational simulations are conducted, in Chap. 8, to investigate the three-dimensional morphological evolution of chemical dissolution fronts when the chemical dissolution system is in a supercritical state. (4) In Chap. 9, a fundamental theory is presented to deal with physical dissolution-front (known as NAPL dissolution-front) instability problems in fluid-saturated porous media. (5) Based on this theory, domain shapes and mesh discretization errors are considered, in Chap. 10, to investigate their effects on the

morphological evolution of NAPL dissolution fronts in fluid-saturated porous media. In particular, the propagation theory of mesh discretization errors associated with a NAPL dissolution system is presented for both rectangular and trapezoidal domains. This further leads to the establishment of the finger-amplitude growing theory, which can be used to make the approximate error estimation of the corresponding computational simulation results. (6) A fundamental theory is presented, in Chap. 11, for dealing with acidization dissolution-front instability problems in fluid-saturated carbonate rocks. (7) Some conclusions and future research directions in this field are summarized at the end of the monograph.

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Chongbin Zhao

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Nomenclature

The following symbols are commonly used with the attached definitions, unless otherwise specified in the monograph.

A	Area of a finite element
C	Species concentration
C_{eq}	Equilibrium concentration of the chemical species
C_1	Nonzero constant
C_2	Arbitrary constant
c_p	Specific heat of pore-fluid
D	Mass diffusivity
g	Acceleration due to gravity
H	Reference length
k	Medium permeability
$k_{chemical}$	Conventional rate constant of the chemical reaction
K_{eq}	Equilibrium constant of the chemical reaction
$k_{Echemical}$	Comprehensive rate constant of the chemical reaction
K_h	Reference medium permeability in the horizontal direction
L	Length of a problem domain
Le	Lewis number
p	Pressure
p_0	Hydrostatic pressure
q_C	Mass flux on the boundary of a finite element
q_T	Heat flux on the boundary of a finite element
Ra	Rayleigh number
$Ra_{critical}$	Critical Rayleigh number
S	Boundary length of a finite element
T	Temperature
t	Temporal variable
u	Darcy velocity in the x direction

U	Darcy velocity vector
v	Darcy velocity in the y direction
w	Darcy velocity in the z direction
x, y, z	Spatial coordinates
Zh	Zhao number
$Zh_{critical}$	Critical Zhao number
λ	Thermal conductivity
λ_{e0}	Reference thermal conductivity in the horizontal direction
ϕ	Porosity
ρ_0	Reference density of pore-fluid
μ	Dynamic viscosity of pore-fluid
β	Permeability ratio
σ	Stress on the boundary of a finite element
Φ	Shape function vector for the temperature, species concentration and Darcy velocity of a finite element
ζ	Thermal conductivity ratio of the underlying medium to its overlying folded layer
ε	Mineral dissolution ratio

Subscripts

- f Pertaining to pore-fluid
 0 Pertaining to reference quantities

Superscripts

- e Pertaining to equivalent quantities of a porous medium
 e Pertaining to quantities in a finite element level
 $*$ Pertaining to dimensionless quantities
 s Pertaining to solid matrix