

Multiphysics Phase-Field Modeling of Geological Subsurface Systems and Infrastructure

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Akash Kumar (M.Eng.)

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Referentin: Prof. Dr. rer. nat. Britta Nestler

Korreferent: Prof. Dr. rer. nat. habil.

Christoph Hilgers

Abstract

Interface-controlled processes govern both the evolution of pore space in geological porous media and the integrity of metallic installations exposed to reactive subsurface fluids. This thesis develops and applies multiphysics phase-field methodology to investigate how microscale interface motion, morphology, anisotropy, and microstructural heterogeneity control macroscopic transport and failure behavior. Three representative subsurface phenomena are considered: crystallographically controlled K-feldspar dissolution, clay-mediated quartz cementation in sandstones, and pitting corrosion with pressure-induced cracking in metallic systems.

First, an anisotropic multiphase-field model is applied to etch-pit-driven K-feldspar dissolution. The model reproduces experimentally observed faceted etch-pit morphologies, characteristic inclination angles, and direction-dependent retreat kinetics on the K-feldspar surface. A grain-wise local refinement and re-embedding workflow enables the transfer of high-resolution dissolution geometries into digital sandstone microstructures. The simulations show that dissolution does not proceed as uniform grain shrinkage, but through localized etch-pit nucleation, lateral growth, coalescence, and intra-granular channel formation. Pore-scale flow analysis demonstrates

that permeability enhancement is governed primarily by connectivity transitions rather than by porosity increase alone.

Second, a multiphase-field model for syntaxial quartz cementation is extended to clay-coated quartz grains. A digital coating-generation workflow is introduced to control coating thickness, coverage, and spatial pattern. The simulations show that clay coatings suppress quartz overgrowth by masking reactive quartz–fluid interfaces. Coating coverage is identified as the dominant control on cement volume and reservoir-quality preservation, while coating pattern and crystallographic orientation modulate the spatial localization of cement and the timing of pore-throat bridging. Comparison with natural sandstone samples supports the physical realism of the modeled coating–cement relationships.

Third, a grand-potential phase-field corrosion framework is combined with a diffuse-interface pressure boundary condition and phase-field fracture modeling to investigate the transition from localized corrosion to mechanical failure. The corrosion model is validated against established pit-growth benchmarks, and the diffuse pressure formulation is verified using analytical elasticity solutions. Corrosion-to-failure simulations show that pit depth reduces the critical pressure for crack initiation, but that failure susceptibility cannot be described by pit depth alone. Pit curvature, asymmetry, phase arrangement, and interfacial mobility mismatch also control local stress concentration and crack initiation.

Overall, this thesis demonstrates that phase-field methodology provides a unified and physically consistent framework for linking microscale interface evolution to macroscopic consequences in subsurface

systems. The results highlight that pore-space evolution, permeability change, and corrosion-induced failure are controlled not only by volume change, but by morphology, topology, anisotropy, and microstructural organization.

Kurzfassung

Grenzflächenkontrollierte Prozesse bestimmen sowohl die Entwicklung des Porenraums in geologischen porösen Medien als auch die Integrität metallischer Installationen, die reaktiven Fluiden im Untergrund ausgesetzt sind. In dieser Arbeit wird eine multiphysikalische Phasenfeldmethodik entwickelt und angewendet, um zu untersuchen, wie Grenzflächenbewegung, Morphologie, Anisotropie und mikrostrukturelle Heterogenität auf der Mikro- und Mesoskala makroskopische Transport- und Versagensprozesse beeinflussen. Drei repräsentative Prozesse werden betrachtet: kristallographisch kontrollierte K-feldspat-Auflösung, tonvermittelte Quarzzementation in Sandsteinen sowie Pitting-Korrosion mit druckinduzierter Rissinitiation in metallischen Systemen.

Zunächst wird ein anisotropes Mehrphasenfeldmodell auf die etch-pit-getriebene Auflösung von K-feldspat angewendet. Das Modell reproduziert experimentell beobachtete facettierte Ätzgrubenmorphologien, charakteristische Neigungswinkel und richtungsabhängige Rückzugsgeschwindigkeiten an der K-feldspat-Oberfläche. Mithilfe eines kornweisen lokalen Verfeinerungs- und Wiedereinbettungs-Workflows werden hochaufgelöste Auflösungsgeometrien in digitale Sandsteinmikrostrukturen übertragen. Die Simulationen zeigen, dass die Auflösung nicht als gleichmäßiges Schrumpfen der Körner abläuft,

sondern durch lokale Keimbildung, laterales Wachstum und Koaleszenz von Ätzgruben sowie durch die Bildung intragranularer Kanäle. Die anschließende Porenströmungsanalyse zeigt, dass die Permeabilitätserhöhung vor allem durch Konnektivitätsübergänge und nicht allein durch eine Zunahme der Porosität bestimmt wird.

Im zweiten Teil wird ein Mehrphasenfeldmodell für syntaxiale Quarzzementation auf tonbeschichtete Quarzkörner erweitert. Hierzu wird ein digitaler Beschichtungs-Workflow eingeführt, mit dem Schichtdicke, Bedeckungsgrad und räumliches Muster der Tonbeschichtung gezielt variiert werden können. Die Simulationen zeigen, dass Tonbeschichtungen das Quarzwachstum unterdrücken, indem sie reaktive Quarz–Fluid-Grenzflächen maskieren. Der Bedeckungsgrad wird als dominierender Einflussfaktor für Zementvolumen und Erhaltung der Reservoirqualität identifiziert, während Beschichtungsmuster und kristallographische Orientierung die räumliche Lokalisierung des Zements und den Zeitpunkt der Porenkehlenschließung zusätzlich beeinflussen. Der Vergleich mit natürlichen Sandsteinproben unterstützt die physikalische Plausibilität der modellierten Zusammenhänge zwischen Tonbeschichtung und Quarzzementation.

Im dritten Teil wird ein Grand-Potential-Phasenfeldmodell für Korrosion mit einer diffusen Druckrandbedingung und einem Phasenfeldmodell für Rissbildung kombiniert, um den Übergang von lokalisierter Korrosion zu mechanischem Versagen zu untersuchen. Das Korrosionsmodell wird anhand etablierter Benchmark-Probleme validiert, während die diffuse Druckformulierung durch analytische Elastizitätslösungen überprüft wird. Die Korrosions-Versagens-Simulationen zeigen, dass zunehmende Grubentiefe den kritischen Druck für die

Rissinitiierung reduziert. Gleichzeitig wird deutlich, dass die Versagensanfälligkeit nicht allein durch die Grubentiefe beschrieben werden kann. Auch Krümmung, Asymmetrie, Phasenordnung und Unterschiede in der Grenzflächenmobilität beeinflussen die lokale Spannungskonzentration und damit die Rissinitiierung.

Insgesamt zeigt diese Arbeit, dass die Phasenfeldmethodik einen einheitlichen und physikalisch konsistenten Rahmen bietet, um mikroskalige Grenzflächenentwicklung mit makroskopischen Auswirkungen in Untergrundsystemen zu verknüpfen. Die Ergebnisse verdeutlichen, dass Porenraumentwicklung, Permeabilitätsänderung und korrosionsinduziertes Versagen nicht allein durch Volumenänderungen bestimmt werden, sondern wesentlich durch Morphologie, Topologie, Anisotropie und mikrostrukturelle Organisation.

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List of Symbols

Symbol	Meaning
$\mathbf{x}$	Spatial coordinate vector
x, y, z	Cartesian spatial coordinates
t	Time
t_{sim}	Simulation time or simulation time step
V	Computational or physical volume/domain
dV	Differential volume element
V_s	Solid domain
V_q	Volume occupied by inert quartz grains
$V \setminus V_q$	Reactive domain excluding inert quartz grains
α, β	Phase indices
i, j	Chemical-component or chemical-potential indices
k	Vertex-vector index in anisotropy functions
N	Total number of phases
N_s	Number of solid phases
K	Number of chemical components

∇	Gradient operator
$\nabla \cdot$	Divergence operator
∇^2	Laplace operator
$\partial/\partial t$	Partial time derivative
$\delta/\delta(\cdot)$	Variational derivative
$\langle q \rangle_{\pm}$	Macaulay brackets, $\langle q \rangle_{\pm} = (q \pm q)/2$
ϕ_{α}	Phase-field variable or local volume fraction of phase α
ϕ	Collection of phase-field variables, $\phi = \{\phi_1, \phi_2, \dots, \phi_N\}$
$\nabla \phi$	Collection of phase-field gradients
ϕ_s	Solid phase-field variable or total solid indicator
ϕ_{ℓ}	Liquid/electrolyte phase-field variable
ϕ_q	Quartz phase-field variable
$\phi_q^{(j)}$	Phase-field variable of quartz grain or quartz orientation j
ϕ_{clay}	Clay-coating phase-field variable
ϕ_c	Crack phase-field variable; $\phi_c = 0$ intact, $\phi_c = 1$ fully broken
$\dot{\phi}_{\alpha}$	Time derivative of ϕ_{α}
$\dot{\phi}_c$	Time derivative of the crack phase field
Φ_{grain}	Grain phase-field value used in coating-generation figures

Φ_{clay}	Clay phase-field value used in coating-generation figures
$\mathcal{F}$	Total Helmholtz free-energy functional
$\mathcal{F}_{\text{bulk}}$	Bulk contribution to the Helmholtz free energy
$\mathcal{F}_{\text{intf.}}$	Interfacial contribution to the Helmholtz free energy
$\mathcal{F}_{\text{mech}}$	Mechanical energy functional
f	Generic free-energy density
f_{bulk}	Bulk free-energy density
$f_{\text{intf.}}$	Interfacial free-energy density
f_{α}^{bulk}	Bulk free-energy density of phase α
$f_{\text{feldspar}}^{\text{bulk}}$	Bulk free-energy density of feldspar
$f_{\text{fluid}}^{\text{bulk}}$	Bulk free-energy density of the fluid phase
f_q^{bulk}	Bulk free-energy density of quartz
f_{ℓ}^{bulk}	Bulk free-energy density of liquid
$\Delta f_{q\ell}$	Bulk free-energy driving force for quartz precipitation
f_{el}^{α}	Elastic strain-energy density of phase α
$[f_{\text{el}}^{\alpha}]^{+}$	Tensile part of the elastic strain-energy density
$[f_{\text{el}}^{\alpha}]^{-}$	Compressive part of the elastic strain-energy density
f_{el}^{-}	Effective compressive elastic energy density
$a(\phi, \nabla \phi)$	Gradient-energy density

$\omega(\phi)$	Multi-obstacle potential
$h(\phi_\alpha)$	Interpolation function for phase α
$h_\alpha(\phi_\alpha)$	Phase-specific interpolation function
$h(\phi_c)$	Crack degradation function
λ	Lagrange multiplier enforcing the phase-fraction constraint
ϵ	Diffuse-interface thickness parameter
ϵ_c	Crack regularization length scale
ϵ_d	Damage tolerance
ϵ_{ϕ_c}	Crack steady-state tolerance
ϵ_{damage}	Damage tolerance used in fracture simulations
ϕ_{th}	Residual-stiffness threshold
ϕ_c^{crit}	Critical crack phase-field value for fully cracked points
ϕ_{residual}	Residual stiffness factor
$\gamma_{\alpha\beta}$	Interfacial energy density of the α - β interface
$\mathbf{q}_{\alpha\beta}$	Anti-symmetric phase-field gradient vector, $\mathbf{q}_{\alpha\beta} = \phi_\alpha \nabla \phi_\beta - \phi_\beta \nabla \phi_\alpha$
$M(\phi)$	Phase-field mobility coefficient
$M_{\alpha\beta}$	Mobility of the α - β interface
$M_{\alpha\beta}^0$	Reference mobility of the α - β interface
$M_{s\ell}$	Solid-liquid interface mobility
$M_{s\ell}^0$	Reference solid-liquid interface mobility

M_{ql}	Quartz–liquid interface mobility
M_{ql}^0	Reference quartz–liquid interface mobility
$\mathbf{n}$	Unit normal vector
$\hat{\mathbf{n}}$	Unit interface-normal vector
$\hat{\mathbf{n}}_{\alpha\beta}$	Unit normal of the α – β interface
$\hat{\mathbf{n}}_{sl}$	Unit normal of the solid–liquid interface
$\hat{\mathbf{n}}_{ql}$	Unit normal of the quartz–liquid interface
$a_{\alpha\beta}^{\text{cap}}(\hat{\mathbf{n}})$	Capillary anisotropy function of the α – β interface
$a_{\alpha\beta}^{\text{kin}}(\hat{\mathbf{n}})$	Kinetic anisotropy function of the α – β interface
$a_{sl}^{\text{cap}}(\hat{\mathbf{n}}_{sl})$	Capillary anisotropy function for K-feldspar dissolution
$a_{sl}^{\text{kin}}(\hat{\mathbf{n}}_{sl})$	Kinetic anisotropy function for K-feldspar dissolution
$a_{ql}^{\text{cap}}(\hat{\mathbf{n}}_{ql})$	Capillary anisotropy function for quartz overgrowth
$a_{ql}^{\text{kin}}(\hat{\mathbf{n}}_{ql})$	Kinetic anisotropy function for quartz overgrowth
$\boldsymbol{\eta}_k^{\text{cap}}$	k th capillary vertex vector
$\boldsymbol{\eta}_k^{\text{kin}}$	k th kinetic vertex vector
n_{kin}	Number of kinetic vertex vectors
δ	Kinetic anisotropy strength parameter
$\mathbf{u}$	Fluid velocity field or mechanical displacement field, depending on context

p	Pressure field or applied hydrostatic pressure
μ_d	Dynamic viscosity of the fluid
Δp	Pressure difference or pressure increment, depending on context
L	Sample length or etch-pit growth length, depending on context
$\bar{v}$	Mean superficial velocity
k	Intrinsic permeability
l	Etch-pit growth trajectory or characteristic length in the x -direction
h	Etch-pit growth trajectory or characteristic depth in the z -direction
v_l	Etch-pit propagation velocity along the l direction
v_L	Etch-pit propagation velocity along the L direction
v_h	Etch-pit propagation velocity along the h direction
v_m	Mean relative etch-pit propagation velocity
v/v_h	Relative etch-pit velocity normalized by v_h
d	Clay-coating thickness or metal-wire diameter, depending on context
Ω	Total grand-potential functional
Ω_{int}	Interfacial contribution to the grand-potential functional

Ω_{bulk}	Bulk contribution to the grand-potential functional
$\psi(\phi, \boldsymbol{\mu})$	Interpolated grand-potential density
$\psi_{\alpha}(\boldsymbol{\mu})$	Phase-specific grand-potential density
$\Delta\psi_{\alpha\beta}^{\text{bulk}}$	Bulk grand-potential difference between phases α and β
$\boldsymbol{\mu}$	Collection of independent chemical-potential fields
μ_i	Chemical potential of component i
μ	Single chemical-potential field in the binary corrosion model
$c_{\alpha,i}$	Concentration of component i in phase α
c_i	Interpolated mixture concentration of component i
c'	Normalized concentration, $c' = c/c_{\text{solid}}$
c'_s	Normalized solid-phase concentration
c'_ℓ	Normalized liquid-phase concentration
$c_s'^e$	Normalized equilibrium concentration in the solid phase
$c_\ell'^e$	Normalized equilibrium concentration in the liquid phase
c_{solid}	Reference solid concentration
c_{metal}	Metal concentration
c_{sat}	Saturation concentration of dissolved metal species

A	Curvature parameter of the parabolic free-energy density
$\mathbf{j}_i$	Diffusive flux of component i
$\overline{\mathbf{M}}$	Effective chemical mobility matrix
$\overline{M}_{ij}$	Entry of the effective chemical mobility matrix
$\overline{M}(\phi_s)$	Effective chemical mobility in the binary corrosion model
M_s	Chemical mobility in the solid phase
M_ℓ	Chemical mobility in the liquid phase
D	Diffusion coefficient
D_s	Diffusion coefficient in the solid phase
D_ℓ	Diffusion coefficient in the liquid/electrolyte phase
χ	Chemical susceptibility matrix
χ_{ij}	Chemical susceptibility matrix entry, $\chi_{ij} = \partial c_i / \partial \mu_j$
$\gamma_{\text{Fe-Brine}}$	Fe-Brine interfacial energy
$\gamma_{\text{Al-Brine}}$	Al-Brine interfacial energy
$\gamma_{\text{Mn-Brine}}$	Mn-Brine interfacial energy
$\gamma_{\text{Fe-Al}}$	Fe-Al interfacial energy
$\gamma_{\text{Fe-Mn}}$	Fe-Mn interfacial energy
$\gamma_{\text{Al-Mn}}$	Al-Mn interfacial energy
$\overline{M}_R$	Interfacial mobility ratio

$\overline{M}_{\text{ferrite}}$	Ferrite–brine interfacial mobility used in the mobility-ratio analysis
$\overline{M}_{\text{non-ferrite}}$	Non-ferrite–brine interfacial mobility used in the mobility-ratio analysis
$I(\mathbf{x})$	Sharp indicator function of the solid domain
δ_S	Surface Dirac distribution
$\tilde{\delta}_S$	Diffuse approximation of the surface Dirac distribution
$\mathbf{t}_{\text{bc}}$	Boundary traction vector
$\boldsymbol{\varepsilon}$	Small-strain tensor
$\boldsymbol{\varepsilon}^\alpha$	Phase-specific strain tensor
ε_i^α	i th principal strain of phase α
$\boldsymbol{\sigma}$	Cauchy stress tensor
$\boldsymbol{\sigma}^\alpha$	Phase-specific Cauchy stress tensor
$\mathbb{C}^\alpha$	Phase-specific fourth-order stiffness tensor
E	Young’s modulus
ν	Poisson’s ratio
λ^α	First Lamé parameter of phase α
μ^α	Shear modulus of phase α
q	Distributed load in the beam benchmark
$\tilde{w}$	Normalized bending displacement
$\tilde{M}$	Normalized bending moment or torque
r	Refinement level
G_c^α	Critical energy release rate of phase α
G_0	Reference crack resistance

$w(\phi_c)$	Crack potential
M_c	Crack mobility or relaxation parameter
$\mathcal{H}$	Crack driving force
p_{crit}	Critical pressure for crack initiation
$p_{\text{crit,current}}$	Critical pressure corresponding to the current corrosion state
$p_{\text{crit,max}}$	Maximum reference critical pressure used for normalization
$\hat{p}$	Normalized critical pressure, $\hat{p} = p_{\text{crit,current}}/p_{\text{crit,max}}$
$\Delta x, \Delta y, \Delta z$	Grid spacing in the x , y , and z directions
$\mathbf{e}_x, \mathbf{e}_z$	Unit vectors in the x and z directions
S/V_R	Surface-to-volume ratio used as corrosion morphology descriptor
m	Slope of a fitted trend

List of Abbreviations

Abbreviation	Meaning
1D	One-dimensional
2D	Two-dimensional
3D	Three-dimensional
AFM	Atomic force microscopy
CCUS	Carbon capture, utilization, and storage
CFD	Computational fluid dynamics
Cl ⁻	Chloride ion
CO ₂	Carbon dioxide
H ₂	Hydrogen
HPC	High-performance computing
K-feldspar	Potassium feldspar
mD	Millidarcy
MPF	Multiphase-field
MPI	Message Passing Interface
μCT	X-ray micro-computed tomography
PACE3D	Parallel multiphysics phase-field simulation framework

PFM	Phase-field method
SEM	Scanning electron microscopy
SiO ₂	Silicon dioxide / silica
THMCB	Thermo-hydro-mechanical-chemical- biological

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Part I - Orientation & Methods

1 Introduction

The content of this chapter is based on the author’s peer-reviewed publications on etch-pit-driven K-feldspar dissolution, clay-mediated quartz cementation, and pitting corrosion with pressure-induced cracking in subsurface-related systems [1–3]. The chapter synthesizes the scientific motivation, research problems, and overall scope of these works in order to establish the common interface-centered perspective used throughout this thesis.

1.1 Motivation

Interface-controlled processes are central to the evolution of geological subsurface systems and to the long-term integrity of subsurface installations. In porous sedimentary rocks, mineral–fluid reactions continuously modify the pore structure through dissolution, precipitation, and cementation. These processes control porosity, permeability, pore connectivity, and ultimately the storage and transport capacity of reservoir rocks [4–6]. In engineered subsurface systems, such as geothermal wells, pipelines, and other metallic installations, fluid–solid interfaces are likewise critical because aggressive brines may induce localized corrosion, which can evolve into mechanically relevant damage [7–9]. Despite the different material systems involved, these

phenomena share a common characteristic: macroscopic behavior emerges from microscale interface motion, morphology development, and the coupling of chemical, transport, and mechanical processes. Recent X-ray micro-computed tomography (μ CT)-based studies have extended digital-rock and petrophysical characterization workflows beyond sedimentary rocks to metamorphic systems. In particular, calibrated μ CT segmentation combined with laboratory measurements and numerical flow simulation has been shown to quantify porosity, permeability, and permeability anisotropy in mica schists, highlighting the broader importance of microstructure-resolved approaches for understanding fluid-flow behavior in complex geological materials [10].

In sedimentary reservoirs, diagenetic reactions are among the primary controls on reservoir quality. Feldspar dissolution is an important mechanism of secondary porosity generation, particularly in siliciclastic systems where feldspar grains are common rock-forming constituents [11–13]. In K-feldspar, dissolution does not necessarily proceed by uniform surface retreat. Instead, experiments and natural observations show that dissolution may localize at defects, cleavage planes, and crystallographically favored surface sites, producing faceted etch-pits and intragranular pore structures [1, 14–16]. The coalescence of such etch-pits can generate elongated channels within grains, thereby increasing local pore connectivity and influencing permeability in a manner that cannot be described by mineral volume loss alone [1]. Consequently, morphology-resolving models are required to understand how crystallographically controlled dissolution translates into reservoir-scale transport consequences.

Conversely, precipitation and cementation can reduce pore space and degrade reservoir quality. Syntaxial quartz overgrowth is one of the most important cementation processes in deeply buried sandstones, progressively narrowing pore throats and reducing permeability [17–20]. However, clay mineral coatings on detrital quartz grains may inhibit or delay quartz cementation by masking reactive quartz surfaces and disrupting nucleation and attachment pathways [21–23]. The extent to which coatings preserve reservoir quality depends not only on the total coating coverage, but also on coating continuity, spatial distribution, grain orientation, and the location of coated regions relative to critical pore throats [2, 23]. Therefore, predicting cementation-driven porosity and permeability loss requires a modeling framework that can explicitly resolve evolving quartz–fluid–clay interfaces in three-dimensional pore geometries.

Beyond natural porous media, subsurface infrastructure is also governed by interface-driven degradation. Metallic components used in geothermal and hydrocarbon installations are exposed to hot, saline, and chemically aggressive fluids that can promote localized corrosion, including pitting and crevice corrosion [7, 8, 24]. Pitting corrosion is particularly dangerous because it produces localized surface defects with high curvature, which can act as stress concentrators and promote crack initiation under mechanical or pressure loading [9, 25, 26]. The transition from a microscopic corrosion pit to macroscopic failure depends on the coupling between electrochemical dissolution, alloy microstructure, evolving pit morphology, and mechanical stress [3, 26–28]. This makes corrosion-induced cracking a strongly multiphysics and multiscale problem.

The phase-field method provides a powerful framework for modeling these classes of problems because it represents moving interfaces through continuous order parameters rather than explicit sharp-interface tracking [29–33]. This diffuse-interface representation naturally handles topological changes such as coalescence, impingement, branching, and fragmentation, which are difficult to treat using explicit interface-tracking methods [31, 32]. Multiphase-field (MPF) formulations also allow systems with multiple solid phases, liquid phases, and internal interfaces to be described in a thermodynamically consistent way [34–36]. In addition, phase-field models can incorporate anisotropic interfacial energies, orientation-dependent kinetics, diffusion, fluid-flow post-processing, elasticity, and fracture within a unified computational framework [37–40].

The present thesis uses this flexibility to investigate three representative subsurface interface problems: (i) etch-pit-driven K-feldspar dissolution and the creation of secondary pore space, (ii) clay-mediated quartz cementation and the reduction or preservation of reservoir quality, and (iii) pitting corrosion and pressure-induced cracking in metallic subsurface installations. In each case, the model is adapted to the dominant physical mechanism while retaining a common phase-field foundation. The overarching objective is to connect microscale interface evolution to macroscopic consequences, including permeability evolution in sandstones and failure susceptibility in corroding metallic systems.

Although the three application areas considered in this thesis differ in material system and physical setting, they share a common mechanistic structure. In each case, microscale interface evolution

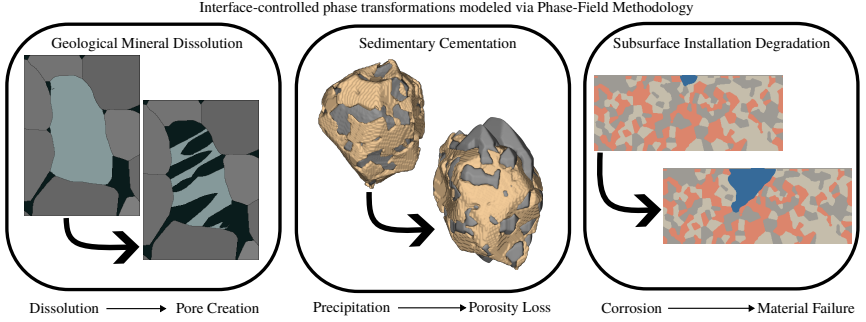


Figure 1.1: Conceptual overview of the interface-controlled processes modeled in this thesis. Faceted etch-pit dissolution in K-feldspar creates secondary pore space and enhances connectivity, clay-mediated quartz cementation controls pore-space reduction and reservoir-quality preservation, and pitting corrosion with pressure-induced cracking governs degradation of metallic subsurface installations. All three processes are treated within a unified phase-field framework that accounts for chemical, transport, interfacial, and mechanical effects.

controls morphology and topology, which in turn determine macroscopic consequences such as permeability enhancement, pore-space reduction, or failure susceptibility. For K-feldspar dissolution, the evolving feldspar–fluid interface creates secondary pore space through anisotropic etch-pit growth and coalescence. For quartz cementation, quartz–fluid–clay interfaces control the localization of overgrowth and the preservation or loss of reservoir quality. For pitting corrosion, the evolving metal–brine interface generates pit morphologies that act as stress concentrators and promote crack initiation under pressure loading. This common interface-centered viewpoint motivates the use of phase-field methodology as the unifying modeling framework throughout the thesis.

1.2 Research problems and objectives

The thesis is organized around three interrelated research problems. Each problem focuses on a specific interface-controlled subsurface process and requires a problem-specific extension of the general phase-field methodology introduced in chapter 2.

1.2.1 Etch-pit-driven K-feldspar dissolution

K-feldspar dissolution in sandstones contributes to the development of secondary porosity and may enhance reservoir permeability when newly formed intragranular pores become connected to the surrounding pore network [11, 14–16]. A key feature of this process is that dissolution may be highly localized and crystallographically controlled. Atomic force microscopy (AFM) observations show that etch-pits on the K-feldspar or orthoclase (001) surface form faceted, quasi-diamond-shaped morphologies with direction-dependent retreat rates [14]. Such morphologies cannot be captured by models that assume isotropic grain shrinkage or dissolution rates proportional only to reactive surface area.

Previous pore-scale and reactive-transport approaches have provided important insights into mineral dissolution and permeability evolution, but the explicit link between crystallographic etch-pit morphology, intragranular channel formation, and sandstone-scale flow enhancement remains difficult to quantify. The challenge is twofold: the model must reproduce the experimentally observed faceted pit geometry at the grain scale, and it must transfer this information

into larger digital sandstone geometries without globally resolving every grain at the etch-pit scale.

The first objective of this thesis is therefore to develop and apply an anisotropic multiphase-field model for K-feldspar dissolution. The model incorporates capillary and kinetic anisotropy to reproduce the characteristic etch-pit morphology and relative growth rates observed experimentally [1, 14]. A grain-wise local refinement and re-embedding workflow is then used to transfer the resulting dissolution geometries into digital sandstone structures [1]. This makes it possible to quantify how etch-pit nucleation, growth, and coalescence modify porosity, pore connectivity, and permeability. The corresponding model calibration, validation, and sandstone-scale analysis are presented in chapter 3.

1.2.2 Clay-mediated quartz cementation

Quartz cementation is a major diagenetic process that reduces porosity and permeability in deeply buried sandstones through syntaxial quartz overgrowth on detrital quartz grains [17–20]. The resulting cement can narrow or close pore throats, and because permeability is controlled disproportionately by a limited number of connected pathways, even moderate cement accumulation may cause a strong hydraulic response [19, 20]. However, clay mineral coatings on quartz grains can inhibit quartz overgrowth and thereby preserve reservoir quality [21–23].

Although the importance of clay coatings is well established, their quantitative effect remains difficult to predict because coating coverage, thickness, continuity, and spatial pattern vary strongly in natural systems [23]. A coating may suppress growth over large regions of a grain surface, but small exposed windows can still provide nucleation sites for localized overgrowth and pore-throat bridging. Therefore, reservoir-quality preservation depends not only on the total amount of coating, but also on how coated and uncoated surfaces are arranged within the pore network. Previous numerical studies of quartz cementation have demonstrated the value of pore-scale simulations, but explicit three-dimensional treatment of clay-coated quartz grains with controlled coating geometries remains limited [2, 19, 20].

The second objective of this thesis is therefore to extend the multiphase-field framework for syntaxial quartz cementation to clay-coated quartz grains. A digital coating-generation workflow is developed to impose controlled coating thickness, coverage, and spatial pattern on quartz grains of arbitrary shape [2]. The resulting coated microstructures are used as initial conditions for anisotropic quartz overgrowth simulations, followed by pore-scale flow characterization. This enables systematic investigation of how coating coverage, coating pattern, and crystallographic orientation govern cement volume, pore-throat occlusion, porosity, and permeability. The model validation and reservoir-quality analysis are presented in chapter 4.

1.2.3 Pitting corrosion and pressure-induced failure

Metallic installations in geothermal and related subsurface environments are exposed to brines containing aggressive chemical species

such as chloride ions (Cl^-), dissolved gases, and other reactive components [7, 8, 24]. Under such conditions, localized corrosion can initiate pits at the metal–electrolyte interface. These pits may grow into sharp defects that reduce the load-bearing cross-section and amplify local stresses, thereby increasing the likelihood of crack initiation [9, 25]. In multiphase alloys, pit evolution is further affected by phase arrangement, phase-dependent interfacial energies, kinetic mismatch, and microstructural connectivity [3, 27, 41].

Existing phase-field corrosion models have made significant progress in describing pit growth, diffusion-controlled dissolution, and mechano-chemical coupling [26–28, 41–43]. However, predicting the transition from corrosion morphology to pressure-induced crack initiation in heterogeneous microstructures remains challenging. Fully coupled corrosion–fracture simulations can be computationally demanding because corrosion and fracture often evolve on very different time scales. At the same time, simplified approaches that consider only pit depth may neglect important morphological features such as curvature, asymmetry, and lobe formation, which can strongly influence stress concentration.

The third objective of this thesis is therefore to formulate a corrosion-to-failure workflow that combines grand-potential phase-field corrosion, diffuse-interface pressure loading, and phase-field fracture modeling [3, 40, 44]. Corrosion morphologies are first generated in single-phase, dual-phase, and polycrystalline alloy systems. Selected pit geometries are then transferred to a mechanical model in which hydrostatic pressure is applied at the diffuse metal–brine interface and increased until crack initiation occurs [3]. This sequential strategy preserves the influence of corrosion morphology while remaining

computationally tractable. It enables analysis of how pit depth, pit curvature, phase arrangement, and interfacial mobility ratio affect the critical pressure for crack initiation and propagation. The validation and application of this framework are presented in chapter 5.

1.3 Thesis contribution and scope

The central contribution of this thesis is the development and application of a unified phase-field-based modeling strategy for interface-controlled processes in geological subsurface systems and related installations. The thesis does not aim to provide a single universal parameterization for all reservoir or installation conditions. Instead, it focuses on resolving the mechanisms by which interface morphology, anisotropy, microstructure, and coupling to transport or mechanics control macroscopic response.

For mineral dissolution, the thesis demonstrates how crystallographic anisotropy in K-feldspar dissolution can be translated into pore-scale permeability evolution through a local refinement and re-embedding workflow [1]. For quartz cementation, it introduces a digital clay-coating workflow that allows coating coverage and pattern to be varied independently, thereby enabling controlled investigation of coating-mediated reservoir-quality preservation [2]. For corrosion-induced failure, it combines a grand-potential corrosion formulation with diffuse-interface pressure loading and phase-field fracture to link evolving pit morphology to critical pressure for crack initiation [3]. Across these applications, the thesis emphasizes mechanism identification, model validation against representative experiments or

benchmarks, and interpretation of trends in a physically consistent pore-scale or microstructure-scale framework.

The scope of the thesis is therefore mesoscale and microstructure-resolving. The permeability trends obtained from sandstone simulations are interpreted as pore-scale mechanisms that require further upscaling before direct reservoir-scale prediction. Similarly, the critical pressures obtained from corrosion-to-failure simulations are interpreted as comparative microstructural failure indicators rather than direct design values for full-scale well casings or pipelines. This scope is deliberate: by resolving the controlling interface morphologies explicitly, the thesis provides mechanistic insight that can support future upscaling, uncertainty quantification, and integration into larger-scale predictive models.

1.4 Synopsis

This dissertation is organized into three parts. Part I provides the orientation and methodological foundation. The present chapter introduces the scientific motivation, research problems, and scope of the thesis. Chapter 2 then develops the theoretical and numerical framework, including phase-field fundamentals, thermodynamic formulations, anisotropic interface descriptions, pore-scale flow characterization, grand-potential corrosion modeling, diffuse-interface pressure loading, and phase-field fracture.

Part II addresses reactive porous media, with emphasis on the creation and closure of pore space in sandstone systems. Chapter 3 investigates etch-pit-driven K-feldspar dissolution. It first validates

the anisotropic phase-field model against experimentally observed etch-pit geometries and relative retreat rates, and then applies a grain-wise refinement and re-embedding workflow to quantify porosity and permeability evolution in digital sandstones [1]. Chapter 4 examines clay-mediated quartz cementation. It validates the multiphase-field model against experimental and natural sandstone observations, then uses controlled digital coating geometries to evaluate how coating coverage, coating pattern, and grain orientation affect quartz overgrowth, pore-throat bridging, and reservoir quality [2].

Part III focuses on infrastructure integrity in corrosive subsurface environments. Chapter 5 presents the grand-potential phase-field model for pitting corrosion and its coupling to pressure-induced crack initiation. The corrosion model is validated against pseudo-one-dimensional and two-dimensional benchmarks, while the diffuse-interface pressure boundary condition is validated against analytical elasticity solutions. The framework is then used to investigate how corrosion-pit morphology, alloy phase arrangement, and interfacial mobility mismatch control the critical pressure required for crack initiation [3].

Chapter 6 summarizes the main findings and scientific contributions of the thesis, while chapter 7 discusses possible extensions, including more detailed reactive-transport coupling, improved treatment of clay mineral specificity, fully coupled corrosion–fracture evolution, and upscaling toward reservoir- and component-scale prediction. Together, the chapters demonstrate how phase-field methodology can be used to link microscale interface dynamics to macroscopic consequences in geological porous media and subsurface installations.

2 Methodology

The content of this chapter is based on the methodological formulations developed and applied in the author’s peer-reviewed publications on K-feldspar dissolution, clay-mediated quartz cementation, and corrosion-induced failure [1–3]. The chapter presents the common phase-field foundation and the problem-specific extensions required for the three application areas considered in this thesis.

2.1 Phase-field fundamentals

The phase-field method (PFM) is a continuum framework for modeling microstructure evolution and moving boundaries in a diffuse manner [29–32]. Instead of explicitly tracking sharp interfaces, phase-field formulations introduce continuous field variables, commonly referred to as order parameters, to distinguish different phases or material states across an interface of finite thickness [29, 31]. The evolution of these fields is derived from thermodynamic potentials, so that interface motion follows from the minimization of an appropriate free-energy functional rather than from explicitly imposed front-tracking rules [29–31]. This variational structure provides a thermodynamically consistent basis for describing interfacial motion and morphological change [31, 32].

Figure 2.1 illustrates the basic diffuse-interface concept used throughout this chapter. Rather than treating the interface as a sharp geometrical boundary, the phase-field formulation represents the transition between phases by continuous order parameters that vary smoothly across a finite interface thickness.

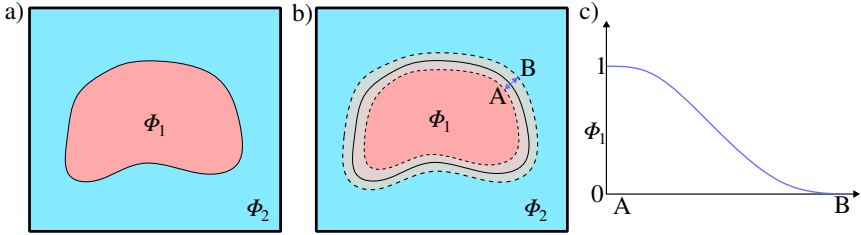


Figure 2.1: Schematic representation of the phase-field description of a diffuse interface. A sharp boundary between two phases is replaced by continuous order parameters that vary smoothly across a finite interface thickness. This representation avoids explicit front tracking and provides the basis for coupling interfacial motion to thermodynamic driving forces, anisotropy, transport, and mechanics in the models developed in this chapter.

A central advantage of the phase-field method is that it avoids repeated remeshing or explicit interface reconstruction, which makes it particularly well suited for problems involving topological change, such as interface merging, pinch-off, impingement, or the development of complex faceted morphologies [31, 32, 45]. For this reason, phase-field and multiphase-field formulations have been widely applied to microstructure evolution problems such as solidification, grain growth, and multiphase transformations [34–37, 45, 46]. In subsurface systems, these processes are typically governed by the evolution of reactive interfaces whose morphology strongly influences porosity, permeability, and material integrity. A diffuse-interface formulation

is therefore especially attractive because it provides a unified way to describe both interfacial motion and its coupling to additional physical fields [31, 36].

This is directly relevant to the processes investigated in the present thesis. In K-feldspar dissolution, evolving solid–fluid interfaces develop crystallographically controlled etch-pit morphologies that modify intragranular porosity and connectivity [1]. In quartz cementation, moving mineral–fluid and coating–fluid interfaces govern overgrowth morphology and the progressive occlusion or preservation of pore space [2]. In corrosion and mechanically induced failure, evolving metal–electrolyte interfaces interact with pressure loading and crack initiation, requiring a framework that can represent both chemical interface evolution and its coupling to mechanics [3]. Although these three problems differ in physical setting, they share a common mathematical structure: each involves interface-controlled evolution driven by thermodynamic forces, modified by kinetics, anisotropy, transport, and in some cases mechanical fields.

The phase-field method is particularly powerful in this context because it can incorporate anisotropic interfacial energy, orientation-dependent kinetics, and spatially varying material properties within a single continuum description [34–37, 46]. It is likewise well suited for coupling with complementary field equations, including diffusion, fluid flow, and elasticity, thereby enabling multiphysics descriptions of evolving geological and engineering systems [31, 32, 36]. In the present work, this flexibility is used to formulate a unified modeling framework for three classes of subsurface phenomena: faceted mineral dissolution, clay-mediated cementation, and corrosion-driven

failure [1–3]. The following sections therefore introduce the thermodynamic basis of the phase-field approach and then present its problem-specific adaptations for each of these processes.

2.1.1 Thermodynamic formulations

In the phase-field method, diffuse order parameters $\phi_\alpha(\mathbf{x}, t) \in [0, 1]$ are used to represent the local volume fraction of each phase α in a system comprising N phases [29–32]. A thermodynamic potential, typically formulated as a Helmholtz free-energy functional, is defined in terms of these phase fields and their spatial gradients [29, 31, 33]. The total free energy $\mathcal{F}$ of the system is written as the sum of bulk and interfacial contributions,

$$\begin{aligned}\mathcal{F}(\phi, \nabla \phi) &= \mathcal{F}_{\text{bulk}} + \mathcal{F}_{\text{intf.}} \\ &= \int_V \left[f_{\text{bulk}}(\phi) + \epsilon a(\phi, \nabla \phi) + \frac{1}{\epsilon} \omega(\phi) \right] dV, \quad (2.1)\end{aligned}$$

where f_{bulk} denotes the bulk free-energy density and the remaining terms represent the interfacial contribution [34–36, 46]. The bulk term is commonly constructed by interpolating phase-specific free-energy densities f_α^{bulk} using suitable interpolation functions, often chosen in the simplest form as $h(\phi_\alpha) = \phi_\alpha$ for multiphase systems [34, 35, 47]. Accordingly,

$$f_{\text{bulk}}(\phi) = \sum_{\alpha=1}^N f_\alpha^{\text{bulk}} h(\phi_\alpha). \quad (2.2)$$

Differences in the bulk free-energy densities of the phases provide the thermodynamic driving force for phase transformation. In dissolution or growth problems, assigning different bulk free-energy levels to solid and fluid phases induces interface motion in the thermodynamically preferred direction [29, 31, 33]. In the present work, the liquid phase is taken as the reference state, whereas the solid-phase free energy is shifted depending on whether dissolution or precipitation is to be modeled. In this way, a higher solid free energy promotes dissolution, whereas a lower solid free energy promotes growth or precipitation.

The interfacial free-energy density consists of a gradient term, which penalizes sharp spatial variations of the phase field, and a potential term, which stabilizes the pure-phase states. For multiphase systems, a multi-obstacle potential $\omega(\phi)$ is employed, as it enforces the constraint $\sum_{\alpha=1}^N \phi_{\alpha} = 1$ and suppresses non-physical third-phase contributions at binary interfaces [34, 35, 46, 48]. The gradient energy density can be written as

$$a(\phi, \nabla \phi) = \sum_{\substack{\alpha, \beta=1 \\ \alpha < \beta}}^{N, N} \gamma_{\alpha\beta} |\mathbf{q}_{\alpha\beta}|^2, \quad \text{with} \quad \mathbf{q}_{\alpha\beta} = \phi_{\alpha} \nabla \phi_{\beta} - \phi_{\beta} \nabla \phi_{\alpha}, \quad (2.3)$$

where $\gamma_{\alpha\beta}$ is the interfacial energy density of the α - β interface [34, 35, 46]. The parameter ϵ controls the diffuse-interface thickness through the balance between the gradient and potential terms [29, 31, 32]. In the absence of a bulk driving force, the potential $\omega(\phi)$ has equal minima for the pure phases, while the gradient term ensures a finite energetic penalty for spatial transitions between them [29, 31].

Minimization of the free-energy functional in Eq. (2.1) leads to Allen–Cahn-type evolution equations for the phase fields [30–32]. In variational form, and including a Lagrange multiplier λ to enforce the summation constraint, the evolution equation is written as

$$\epsilon \frac{\partial \phi_\alpha}{\partial t} = -M(\phi) \left(\frac{\delta \mathcal{F}}{\delta \phi_\alpha} - \lambda \right), \quad \alpha = 1, \dots, N. \quad (2.4)$$

Here, $M(\phi)$ denotes a mobility coefficient, which may in general depend on phase and interface orientation, and $\delta \mathcal{F} / \delta \phi_\alpha$ is the functional derivative of the free energy with respect to ϕ_α [30, 35, 36]. This formulation ensures that the total free energy decreases monotonically in time and that the phase fields satisfy the constraint $\sum_\alpha \phi_\alpha = 1$ at every point. The Lagrange multiplier λ is obtained from the condition $\sum_{\alpha=1}^N \dot{\phi}_\alpha = 0$, thereby preserving the local phase-fraction constraint [48, 49]. As the system evolves, interfaces move in response to free-energy gradients: a positive difference $f_\alpha^{\text{bulk}} - f_\beta^{\text{bulk}}$, for example, drives phase α to shrink and phase β to grow, corresponding to dissolution of α into β or, conversely, growth of β at the expense of α . The mobility M is directly related to interface kinetics, such that larger values produce faster interface motion for a given thermodynamic driving force [30, 31, 37].

2.1.1.1 Interfacial properties

The formulation in section 2.1.1 can be extended to anisotropic interfacial energies and orientation-dependent kinetics, both of which are essential for modeling faceted crystal growth and dissolution.

In crystalline materials, the equilibrium or near-equilibrium interface morphology is governed by the orientation dependence of the interfacial free energy, commonly interpreted through the Wulff construction [50, 51]. In a phase-field setting, this effect is introduced by allowing the interfacial energy coefficient $\gamma_{\alpha\beta}$ to depend on the local interface normal $\hat{\mathbf{n}}$, or equivalently by scaling the gradient-energy term using an anisotropy function $a_{\alpha\beta}^{\text{cap}}(\hat{\mathbf{n}})$ [34, 35, 37, 38].

In practice, the isotropic coefficient $\gamma_{\alpha\beta}$ in Eq. (2.3) is replaced by the orientation-dependent contribution

$$\gamma_{\alpha\beta} \left[a_{\alpha\beta}^{\text{cap}}(\hat{\mathbf{n}}) \right]^2,$$

where $a_{\alpha\beta}^{\text{cap}}(\hat{\mathbf{n}})$ prescribes the capillary anisotropy of the corresponding interface. For strongly faceted systems, this function can be constructed from a prescribed equilibrium or target Wulff shape, such that selected interface orientations are energetically favored and stable facets emerge naturally during the simulation [38, 39, 52]. This capillary contribution controls the thermodynamic preference for specific interface orientations, whereas kinetic anisotropy controls the rate at which these orientations advance or retreat.

Accordingly, the mobility coefficient in the phase-field evolution equation can also be made orientation dependent. The effective mobility of the α - β interface is written as

$$M_{\alpha\beta} = M_{\alpha\beta}^0 a_{\alpha\beta}^{\text{kin}}(\hat{\mathbf{n}}),$$

where $M_{\alpha\beta}^0$ denotes the base mobility and $a_{\alpha\beta}^{\text{kin}}(\hat{\mathbf{n}})$ modulates the interface kinetics as a function of direction [37–39]. This distinction between capillary and kinetic anisotropy is important because equilibrium shape and growth or dissolution trajectory need not be controlled by the same crystallographic dependence. In the present thesis, this framework is used to represent facet-specific dissolution rates in K-feldspar etch-pitting [1] and crystallographically controlled quartz overgrowth during cementation [2]. The problem-specific anisotropy functions used for these two applications are introduced in sections 2.2.2 and 2.3.3, respectively.

2.1.2 Computational fluid dynamics (CFD) analysis for the determination of permeability

To connect the microstructure evolution simulations with macroscopic transport properties, fluid-flow calculations are performed on the evolving pore geometries at selected simulation stages. This post-processing step converts the phase-field-resolved solid–fluid morphology into a hydraulic response by solving the creeping-flow problem in the connected pore space. Because the characteristic pore-scale velocities considered here correspond to low Reynolds number conditions, the flow is described by the steady incompressible Stokes equations [4–6]. This approach is commonly used in digital-rock and pore-scale modeling to estimate permeability from resolved pore geometries [1, 2, 19, 20].

The pore space is treated as the fluid domain, while regions occupied by solid phases are considered impermeable. The governing equations are the Stokes momentum balance and continuity equation,

$$\mu_d \nabla^2 \mathbf{u} - \nabla p = \mathbf{0}, \quad \nabla \cdot \mathbf{u} = 0, \quad (2.5)$$

where $\mathbf{u}(\mathbf{x})$ is the fluid velocity field, $p(\mathbf{x})$ is the pressure field, and μ_d is the dynamic viscosity of the fluid. A prescribed pressure difference Δp is imposed between two opposite faces of the sample to drive flow in the selected direction. The remaining outer boundaries are treated as no-flow or symmetry boundaries, depending on the chosen flow direction, and a no-slip condition is imposed at the solid–fluid interface,

$$\mathbf{u} = \mathbf{0} \quad \text{on solid–fluid interfaces.} \quad (2.6)$$

Such boundary conditions are consistent with standard pore-scale Stokes-flow calculations in resolved porous media [4, 20, 53].

After solving Eq. (2.5), the intrinsic permeability k is obtained from Darcy’s law. For a sample of length L in the imposed flow direction and mean superficial velocity $\bar{v}$, the permeability is calculated as

$$k = \frac{\mu_d \bar{v} L}{\Delta p}. \quad (2.7)$$

Equivalently, the relation may be written as $\bar{v} = (k/\mu_d)(\Delta p/L)$, which expresses the proportionality between pressure gradient and average flow velocity in the Darcy regime [4, 5, 54]. In this thesis, Eq. (2.7) is used to quantify how dissolution and precipitation modify permeability through changes in pore geometry, pore connectivity, and tortuosity. This procedure is applied in chapter 3 to evaluate

permeability enhancement during K-feldspar dissolution and in chapter 4 to quantify permeability reduction during clay-mediated quartz cementation [1, 2].

2.2 Framework for etch-pit dissolution in K-feldspar

2.2.1 Phase-field model for K-feldspar dissolution

K-feldspar dissolution is modeled as a two-phase solid–fluid transformation, in which the solid phase represents the K-feldspar grain and the liquid phase represents the surrounding undersaturated aqueous solution [1]. The formulation is obtained as a special case of the general multiphase-field framework introduced in section 2.1.1, with $N = 2$ phases: ϕ_s for the solid feldspar phase and $\phi_\ell = 1 - \phi_s$ for the liquid phase. The free-energy functional retains the form of Eq. (2.1), while the corresponding phase-field evolution equation follows the Allen–Cahn-type formulation introduced in Eq. (2.4).

Dissolution is driven by prescribing a bulk free-energy difference between the feldspar and liquid phases. The liquid phase is taken as the reference state, while the feldspar bulk free-energy density is shifted relative to this reference to generate a thermodynamic driving force for motion of the solid–liquid interface into the feldspar grain [1]. This treatment represents a sustained undersaturated fluid environment in which feldspar dissolution can proceed continuously. In the present framework, the aqueous solution chemistry is not explicitly resolved; that is, ionic concentrations, advective solute

transport, and diffusive mass transport in the liquid are not directly modeled. Instead, the effect of undersaturation is represented through a fixed chemical driving force, corresponding to a reaction-controlled or locally renewed fluid condition.

This simplification is appropriate for the objective of this chapter, which is to resolve the morphology of crystallographically controlled etch-pit formation rather than to quantify concentration-dependent dissolution rates. The relevant model parameters, particularly the solid–liquid interfacial energy, kinetic mobility, and anisotropy functions, are calibrated against experimentally observed etch-pit morphologies and relative growth rates on the K-feldspar (001) surface [1, 14]. The calibration and validation of these parameters are discussed in chapter 3, where the model is shown to reproduce the characteristic faceted pit geometry and anisotropic retreat behavior reported in laboratory studies.

2.2.2 Capillary and kinetic anisotropy for faceted dissolution

A defining feature of K-feldspar dissolution is the formation of faceted etch-pits on crystallographically controlled surfaces. Experimental observations on the (001) surface show that these pits commonly develop quasi-diamond-shaped plan-view geometries, with pit walls aligned along preferred crystallographic directions and with strongly direction-dependent retreat rates [1, 14]. To reproduce this behavior, the phase-field formulation introduces anisotropy in both the interfacial-energy contribution and the interface mobility of the solid–liquid interface. These two contributions represent different physical

effects: capillary anisotropy controls the thermodynamic preference for selected interface orientations, whereas kinetic anisotropy controls the direction-dependent rate of interface motion [37–39].

The capillary anisotropy is introduced through an orientation-dependent function $a_{sl}^{\text{cap}}(\hat{\mathbf{n}}_{sl})$, where $\hat{\mathbf{n}}_{sl}$ denotes the unit normal of the solid–liquid interface. Following the vertex-vector construction used for faceted phase-field simulations, the anisotropy function is defined as

$$a_{sl}^{\text{cap}}(\hat{\mathbf{n}}_{sl}) = \max_k (\hat{\mathbf{n}}_{sl} \cdot \boldsymbol{\eta}_k^{\text{cap}}), \quad (2.8)$$

where $\boldsymbol{\eta}_k^{\text{cap}}$ denotes the k th vertex vector of the prescribed capillary shape. The set of capillary vertex vectors is chosen such that the resulting anisotropic surface-energy landscape reproduces the target etch-pit morphology observed for K-feldspar dissolution [1, 39]. Through this construction, selected interface orientations are stabilized during evolution, allowing planar facets to emerge without prescribing the pit walls geometrically.

In addition to capillarity, kinetic anisotropy is required because different crystallographic directions retreat at different rates during K-feldspar dissolution. Experimental observations indicate that etch-pits grow substantially faster parallel to the cleavage plane than perpendicular to it; Kumar et al. [1], following the experimental basis of Pollet-Villard et al. [14], use this behavior to calibrate the relative kinetic response. The effective mobility of the solid–liquid interface is therefore written as

$$M_{sl}(\hat{\mathbf{n}}_{sl}) = M_{sl}^0 a_{sl}^{\text{kin}}(\hat{\mathbf{n}}_{sl}), \quad (2.9)$$

where $M_{s\ell}^0$ is the reference mobility and $a_{s\ell}^{\text{kin}}$ is the kinetic anisotropy function. Analogous to the capillary term, the kinetic anisotropy can be represented using a vertex-vector construction,

$$a_{s\ell}^{\text{kin}}(\hat{\mathbf{n}}_{s\ell}) = \max_k (\hat{\mathbf{n}}_{s\ell} \cdot \boldsymbol{\eta}_k^{\text{kin}}), \quad (2.10)$$

where $\boldsymbol{\eta}_k^{\text{kin}}$ denotes the k th vector of the kinetic anisotropy shape. These vectors are calibrated such that the simulated etch-pit evolution reproduces the relative shift velocities of the relevant facets [1, 39].

The combined use of capillary and kinetic anisotropy is essential because the final morphology and its temporal evolution are not controlled by a single mechanism. Capillary anisotropy stabilizes the faceted geometry, while kinetic anisotropy determines the relative rates at which different pit walls advance or retreat. Together, these ingredients allow the model to reproduce the characteristic faceted etch-pit shapes and anisotropic growth trajectories observed in K-feldspar dissolution experiments [1, 14]. The calibration of these anisotropy functions and their influence on single- and multiple-pit growth are discussed in chapter 3.

2.2.3 Embedding quartz grains as inert phases

Natural sandstones are mineralogically heterogeneous, and K-feldspar grains commonly coexist with quartz grains within the same pore-scale microstructure. For the dissolution conditions considered here, quartz is assumed to be effectively inert relative to K-feldspar because reported feldspar dissolution rates are orders of magnitude higher than those of quartz under comparable conditions [1, 11–13]. This

assumption allows the model to focus on the etch-pit-driven alteration of K-feldspar while preserving quartz grains as non-reactive obstacles within the digital sandstone geometry.

To incorporate quartz in the multiphase-field representation, an additional phase field ϕ_q is introduced for the quartz phase. The quartz domain is not allowed to participate in the feldspar–liquid transformation, and the free-energy functional is evaluated only over the reactive part of the domain. Following Kumar et al. [1], this is written as

$$\mathcal{F}(\phi, \nabla \phi) = \int_{V \setminus V_q} [f_{\text{bulk}}(\phi) + f_{\text{intf.}}(\phi, \nabla \phi)] dV, \quad (2.11)$$

where V_q denotes the volume occupied by quartz grains. Within this region, $\phi_q \approx 1$, whereas the feldspar and liquid phase fields vanish. The exclusion of V_q from the reactive free-energy contribution ensures that the thermodynamic driving force acts only on K-feldspar–liquid interfaces and not on quartz–liquid interfaces.

Numerically, quartz grains are therefore treated as rigid, non-reactive inclusions. Their phase field is kept fixed during the dissolution simulation, and the mobilities associated with quartz–liquid and quartz–feldspar transformations are set to zero. As a result, K-feldspar can dissolve up to quartz boundaries, but the quartz grains themselves retain their original geometry. This treatment is analogous to previous inert-phase strategies used in multiphase-field simulations of microstructure evolution [1, 55]. It enables realistic mixed-mineral sandstone geometries to be considered while restricting dissolution to the K-feldspar phase, which is the reactive mineral of interest in this chapter.

2.3 Framework for cementation with clay-coated quartz grains in sandstone

2.3.1 Multiphase-field model for syntaxial quartz cementation

Quartz cementation in sandstones is modeled using a multiphase-field framework capable of representing multiple quartz grains, a pore-fluid phase, and, where required, an additional clay-coating phase. Syntaxial cementation refers to the precipitation of quartz overgrowth on detrital quartz grains while preserving crystallographic continuity between the substrate and the newly formed cement [2, 18–20]. In the phase-field representation, each quartz grain, or each group of grains sharing the same crystallographic orientation, is assigned an individual solid phase field $\phi_q^{(j)}$. Interfaces between grains of different orientations are therefore represented as diffuse solid–solid interfaces, while quartz–fluid interfaces represent surfaces on which syntaxial overgrowth may occur. The formulation follows the general multiphase-field framework introduced in section 2.1.1, which is suitable for systems containing multiple solid phases and a fluid phase [2, 34–36].

The thermodynamic driving force for quartz cementation is introduced through a bulk free-energy difference between the quartz and fluid phases. Under supersaturated conditions with respect to silica (SiO_2), the quartz phase is energetically favored relative to the pore

fluid, so that the quartz–fluid interface advances into the pore space. This can be expressed by prescribing a driving force $\Delta f_{q\ell}$ such that

$$f_q^{\text{bulk}} - f_\ell^{\text{bulk}} = -\Delta f_{q\ell}, \quad \Delta f_{q\ell} > 0, \quad (2.12)$$

where f_q^{bulk} and f_ℓ^{bulk} denote the bulk free-energy densities of quartz and liquid, respectively. The negative sign indicates that precipitation of quartz from the supersaturated fluid is thermodynamically favored. In the present formulation, the pore fluid is treated as well mixed and maintained at prescribed supersaturation, so that explicit silica transport and concentration evolution are not resolved. Consequently, the cementation process is represented as interface-controlled, with the rate of overgrowth governed by the chosen driving force, interface mobility, and crystallographic anisotropy [2, 19, 20].

The interfacial and kinetic contributions follow the multiphase-field formulation described in section 2.1.1, with anisotropic modifications introduced to reproduce faceted quartz overgrowth. In particular, the orientation dependence of quartz growth is incorporated through capillary and kinetic anisotropy functions, which are defined in section 2.3.3. This enables the model to capture crystallographically controlled overgrowth morphologies and the development of faceted cement textures, as previously demonstrated for syntaxial quartz cementation in three-dimensional digital sandstones [2, 19, 20].

To represent clay-coated quartz grains, an additional phase field ϕ_{clay} is introduced. The clay phase is treated as non-growing and non-reactive during quartz cementation, but it occupies part of the quartz surface and thereby prevents direct quartz–fluid contact at coated locations. Thus, quartz overgrowth can proceed only where

exposed quartz surfaces remain in contact with the supersaturated fluid. This treatment reflects the role of clay coatings as nucleation discontinuities that inhibit or delay syntaxial quartz overgrowth, as observed in natural samples and previous experimental and numerical studies [2, 18, 21–23]. The digital construction of such coating geometries, including their coverage, thickness, and spatial pattern, is described in section 2.3.2.

2.3.2 Digital coating generation on quartz surfaces

To investigate the role of clay coatings systematically, a digital pre-processing workflow is used to generate clay-coated quartz grains with controlled coating thickness, coverage, and spatial pattern [2]. This workflow provides reproducible initial microstructures for the multiphase-field cementation simulations and allows the coating geometry to be varied independently from the underlying quartz-grain geometry. Such control is essential because coating attributes such as coverage and pattern are generally difficult to isolate in natural samples and laboratory experiments [2].

Starting from a digital quartz-grain geometry embedded in a liquid phase, the first step generates a complete clay coating of prescribed thickness along the quartz–fluid interface. This is performed using the diffuse phase-field representation of the quartz grain: grid points within the interfacial region are assigned to the clay phase according to the local value of the quartz phase field and the chosen coating thickness [2]. The result is a fully coated quartz grain, which is then modified in a second step to impose the desired coverage and spatial arrangement.

Two principal classes of coating patterns are considered. For continuous or layered coatings, selected regions of the initially complete clay layer are replaced by liquid according to user-defined spatial planes, producing one-sided or layered coating geometries. For discontinuous random coatings, an iterative removal algorithm is applied: random points are selected within the clay phase, spherical regions of prescribed radius are replaced by liquid, and the remaining clay volume fraction is recalculated until the target coating coverage is reached [2]. This procedure enables coatings of prescribed thickness, percentage coverage, and morphology to be generated on grains of arbitrary shape.

The resulting coated grains are used as initial conditions for anisotropic quartz overgrowth simulations. During cementation, the clay phase is treated as inert by immobilizing the clay–liquid interface, such that

$$\frac{\partial \phi_{\text{clay}}}{\partial t} = 0. \quad (2.13)$$

Consequently, quartz overgrowth proceeds only on exposed quartz–fluid interfaces, while clay-coated regions remain non-reactive. This digital workflow makes it possible to compare, in a controlled manner, the effects of coating coverage, coating pattern, and grain orientation on cement volume, pore-throat occlusion, porosity, and permeability, as analyzed in chapter 4 [2].

2.3.3 Capillary and kinetic anisotropy for quartz overgrowth

Quartz overgrowth commonly develops crystallographically controlled facets, including prismatic and pyramidal faces, during syntaxial cementation. To reproduce these morphologies, the quartz–fluid interface is assigned anisotropic interfacial energy and orientation-dependent kinetic mobility. The capillary anisotropy controls the relative stability of interface orientations and therefore the faceted equilibrium tendency, whereas kinetic anisotropy controls the direction-dependent rate at which the quartz–fluid interface advances during precipitation [2, 20, 37, 38].

For the quartz–fluid interface, the capillary anisotropy function $a_{q\ell}^{\text{cap}}(\hat{\mathbf{n}}_{q\ell})$ is defined using a prescribed set of vertex vectors corresponding to the target quartz growth morphology. Following the vertex-vector construction used in previous multiphase-field studies of quartz cementation, the anisotropy function can be expressed as

$$a_{q\ell}^{\text{cap}}(\hat{\mathbf{n}}_{q\ell}) = \max_k (\hat{\mathbf{n}}_{q\ell} \cdot \boldsymbol{\eta}_k^{\text{cap}}), \quad (2.14)$$

where $\hat{\mathbf{n}}_{q\ell}$ is the unit normal of the quartz–liquid interface and $\boldsymbol{\eta}_k^{\text{cap}}$ denotes the k th vertex vector of the capillary anisotropy shape. This construction stabilizes selected crystallographic orientations and allows faceted quartz overgrowth morphologies to emerge naturally during simulation, without prescribing the final cement shape geometrically [2, 20, 39]. The specific vertex-vector set used for quartz

growth follows the established quartz-cementation phase-field framework and is adopted in the present work for coated and uncoated quartz grains [2, 20, 56].

Kinetic anisotropy is introduced because different quartz faces may grow at different rates under the same supersaturation. The effective mobility of the quartz–liquid interface is therefore written as

$$M_{q\ell}(\hat{\mathbf{n}}_{q\ell}) = M_{q\ell}^0 a_{q\ell}^{\text{kin}}(\hat{\mathbf{n}}_{q\ell}), \quad (2.15)$$

where $M_{q\ell}^0$ is the reference quartz–liquid mobility and $a_{q\ell}^{\text{kin}}$ modulates the growth kinetics as a function of interface orientation. Following Wendler et al. [56] and the subsequent quartz-cementation implementation of Prajapati et al. [20], the kinetic anisotropy function is defined as

$$a_{q\ell}^{\text{kin}}(\hat{\mathbf{n}}_{q\ell}) = \left\{ 1 + \delta \left[\max_k (\hat{\mathbf{n}}_{q\ell} \cdot \boldsymbol{\eta}_k^{\text{kin}}) - \max_{k=1} (\hat{\mathbf{n}}_{q\ell} \cdot \boldsymbol{\eta}_k^{\text{kin}}) \right] \right\} \\ \times \max_k (\hat{\mathbf{n}}_{q\ell} \cdot \boldsymbol{\eta}_k^{\text{kin}}), \quad k = 1, \dots, n_{\text{kin}}, \quad (2.16)$$

where δ is the kinetic anisotropy strength and $\boldsymbol{\eta}_k^{\text{kin}}$ denotes the k th vertex vector of the kinetic anisotropy shape. This function accounts for faster pre-faceting quartz growth tendencies through δ and for relative growth velocities of different facets through the prescribed set of kinetic vertex vectors [2, 56]. The same formulation is used in the clay-coated quartz-cementation model, with clay coatings locally suppressing growth by preventing direct quartz–fluid contact rather than by altering the intrinsic anisotropy of the exposed quartz–fluid interface [2].

Together, the capillary and kinetic anisotropy functions enable the model to reproduce crystallographically controlled quartz overgrowth on exposed grain surfaces. In the present thesis, these anisotropy functions are used to study how quartz growth interacts with clay coating coverage, coating pattern, and grain orientation to control cement volume, pore-throat occlusion, porosity, and permeability evolution, as discussed in chapter 4.

2.4 Framework for corrosion and failure in installations

2.4.1 Multiphase-field grand-potential model of corrosion

Localized corrosion in metallic subsurface installations is modeled using a multiphase-field formulation based on the grand-potential approach. This formulation is particularly suitable for multiphase and multicomponent systems because the chemical state is described in terms of chemical potentials rather than phase-specific concentrations, which facilitates the treatment of large concentration differences across phases and avoids the need to solve separate equilibrium constraints for each phase independently [3, 44]. In the present thesis, this framework is adapted to simulate metal–electrolyte interface motion during pitting corrosion and is subsequently combined with a mechanical failure model to evaluate pressure-induced crack initiation from corrosion pits [3]. The corrosion framework used in this thesis adopts the grand-potential formulation because it enables

independent control of interfacial energy and interface width and is naturally suited to multiphase, multicomponent corrosion scenarios.

For a system consisting of N phases and K chemical components, the phase state is described by the phase-field vector $\boldsymbol{\phi} = \{\phi_1, \phi_2, \dots, \phi_N\}$, while the chemical state is described by the set of independent chemical potentials $\boldsymbol{\mu} = \{\mu_1, \mu_2, \dots, \mu_{K-1}\}$. Only $K - 1$ independent chemical potentials are required because one component is taken as dependent through the compositional constraint. The grand-potential functional is written as

$$\begin{aligned}\Omega(\boldsymbol{\phi}, \nabla \boldsymbol{\phi}, \boldsymbol{\mu}) &= \Omega_{\text{int}} + \Omega_{\text{bulk}} \\ &= \int_V \left[\frac{1}{\epsilon} \omega(\boldsymbol{\phi}) + \epsilon a(\boldsymbol{\phi}, \nabla \boldsymbol{\phi}) + \psi(\boldsymbol{\phi}, \boldsymbol{\mu}) \right] dV. \quad (2.17)\end{aligned}$$

Here, $\omega(\boldsymbol{\phi})$ is the multi-obstacle potential and $a(\boldsymbol{\phi}, \nabla \boldsymbol{\phi})$ is the gradient-energy density; together, these terms define the interfacial contribution. The parameter ϵ controls the diffuse-interface thickness. The bulk contribution is represented by the grand-potential density $\psi(\boldsymbol{\phi}, \boldsymbol{\mu})$, which depends on the phase fractions and chemical potentials [3, 44]. In the present corrosion formulation, the corresponding functional is written in this form, with the multi-obstacle and gradient terms forming the interfacial part and ψ forming the bulk grand-potential contribution.

The interpolated grand-potential density is given by

$$\psi(\boldsymbol{\phi}, \boldsymbol{\mu}) = \sum_{\alpha=1}^N h_{\alpha}(\phi_{\alpha}) \psi_{\alpha}(\boldsymbol{\mu}), \quad (2.18)$$

where $h_\alpha(\phi_\alpha)$ denotes the interpolation function of phase α , and ψ_α is the phase-specific grand-potential density. The latter is related to the Helmholtz free-energy density f_α by a Legendre transformation,

$$\psi_\alpha(\boldsymbol{\mu}) = f_\alpha(c_{\alpha,1}, c_{\alpha,2}, \dots, c_{\alpha,K}) - \sum_{i=1}^{K-1} \mu_i c_{\alpha,i}, \quad (2.19)$$

where $c_{\alpha,i}$ denotes the concentration of component i in phase α . Using chemical potentials as independent variables enforces local chemical equilibrium across coexisting phases through a common value of μ_i at diffuse interfaces [44]. This is advantageous for corrosion modeling because the metal and electrolyte phases may exhibit strongly different equilibrium compositions while sharing common diffusion potentials at the interface.

The phase-field evolution equations are obtained by variational differentiation of the grand-potential functional with respect to the phase fields. For an interface between phases α and β , the evolution equation can be written in pairwise form as

$$\frac{\partial \phi_\alpha}{\partial t} = -\frac{M_{\alpha\beta}}{2\epsilon} \left[\frac{\delta \Omega_{\text{int}}}{\delta \phi_\alpha} - \frac{\delta \Omega_{\text{int}}}{\delta \phi_\beta} + \frac{8}{\pi} \sqrt{\phi_\alpha \phi_\beta} \Delta \psi_{\alpha\beta}^{\text{bulk}} \right], \quad (2.20)$$

where $M_{\alpha\beta}$ is the interface mobility and $\Delta \psi_{\alpha\beta}^{\text{bulk}} = \psi_\alpha - \psi_\beta$ is the bulk grand-potential difference between the two phases. The first two terms in Eq. (2.20) arise from the interfacial contribution and control the diffuse-interface regularization, while the final term represents the chemical driving force for transformation between phases α and β [3, 44]. In the corrosion problem, this driving force governs the

motion of the metal–electrolyte interface and therefore controls the local dissolution of the metallic phase.

In this thesis, the grand-potential model is used to simulate pitting corrosion in single-phase, dual-phase, and polycrystalline metallic systems. The formulation enables the corrosion front to evolve naturally without explicit tracking of the metal–electrolyte boundary, while allowing phase-dependent interfacial energies and mobilities to represent microstructural heterogeneity. This is important for studying multiphase alloys, where phase arrangement and kinetic mismatch influence pit depth, pit curvature, and subsequent mechanical vulnerability [3]. The resulting corrosion morphologies are then used as inputs to the pressure-induced cracking framework introduced in sections 2.4.4 and 2.4.5.

2.4.2 General multiphase and multicomponent formulation

The grand-potential framework introduced in section 2.4.1 can be formulated for systems containing multiple phases and multiple chemical components. This generality is important for corrosion in heterogeneous alloys, where different metallic phases, precipitates, oxide films, or electrolyte regions may coexist and interact through a moving metal–electrolyte interface. In the most general case, the phase state is represented by N phase fields,

$$\boldsymbol{\phi} = \{\phi_1, \phi_2, \dots, \phi_N\},$$

and the chemical state is represented by $K - 1$ independent chemical potentials,

$$\boldsymbol{\mu} = \{\mu_1, \mu_2, \dots, \mu_{K-1}\}.$$

The use of $K - 1$ independent chemical potentials follows from the compositional constraint in a K -component system, where one component is dependent on the remaining components [3, 44].

Within the grand-potential formulation, phase-specific concentrations are expressed as functions of the chemical potentials, i.e., $c_{\alpha,i} = c_{\alpha,i}(\boldsymbol{\mu})$, where $c_{\alpha,i}$ denotes the concentration of component i in phase α . The mixture concentration of component i is then obtained by interpolation over all phases,

$$c_i(\boldsymbol{\phi}, \boldsymbol{\mu}) = \sum_{\alpha=1}^N h_{\alpha}(\phi_{\alpha}) c_{\alpha,i}(\boldsymbol{\mu}), \quad i = 1, \dots, K - 1. \quad (2.21)$$

Here, $h_{\alpha}(\phi_{\alpha})$ is the interpolation function associated with phase α . This formulation allows composition discontinuities between phases while maintaining continuous chemical potentials across diffuse interfaces, which is one of the main advantages of the grand-potential approach for systems with large concentration contrasts [3, 44].

Mass conservation for each independent component is expressed as

$$\frac{\partial c_i}{\partial t} = -\nabla \cdot \mathbf{j}_i, \quad (2.22)$$

where $\mathbf{j}_i$ is the flux of component i . Assuming diffusion driven by gradients of chemical potential, the flux can be written in the form

$$\mathbf{j}_i = - \sum_{j=1}^{K-1} \overline{M}_{ij}(\phi, \boldsymbol{\mu}) \nabla \mu_j, \quad (2.23)$$

where $\overline{M}_{ij}$ denotes the effective mobility matrix. Combining Eqs. (2.22) and (2.23) gives

$$\frac{\partial c_i}{\partial t} = \nabla \cdot \left(\sum_{j=1}^{K-1} \overline{M}_{ij}(\phi, \boldsymbol{\mu}) \nabla \mu_j \right). \quad (2.24)$$

Thus, diffusion is expressed in terms of chemical-potential gradients rather than concentration gradients, which is particularly useful when concentration jumps occur across phase boundaries but the diffusion potentials remain continuous [44].

For numerical solution, Eq. (2.24) can be rewritten in terms of the chemical potentials as the primary variables. Differentiating Eq. (2.21) with respect to time gives

$$\frac{\partial c_i}{\partial t} = \sum_{j=1}^{K-1} \chi_{ij} \frac{\partial \mu_j}{\partial t} + \sum_{\alpha=1}^N c_{\alpha,i}(\boldsymbol{\mu}) \frac{\partial h_{\alpha}}{\partial t}, \quad (2.25)$$

where

$$\chi_{ij} = \frac{\partial c_i}{\partial \mu_j} = \sum_{\alpha=1}^N h_{\alpha}(\phi_{\alpha}) \frac{\partial c_{\alpha,i}}{\partial \mu_j} \quad (2.26)$$

is the chemical susceptibility matrix. Substitution into Eq. (2.24) yields the chemical-potential evolution equation

$$\sum_{j=1}^{K-1} \chi_{ij} \frac{\partial \mu_j}{\partial t} = \nabla \cdot \left(\sum_{j=1}^{K-1} \overline{M}_{ij}(\phi, \boldsymbol{\mu}) \nabla \mu_j \right) - \sum_{\alpha=1}^N c_{\alpha,i}(\boldsymbol{\mu}) \frac{\partial h_{\alpha}}{\partial t}. \quad (2.27)$$

The last term accounts for changes in local composition caused by phase transformation, for example when metal is converted into electrolyte during dissolution. In the corrosion simulations considered in this thesis, this general formulation is reduced to a two-phase, two-component model, which is presented in section 2.4.3. That reduction is sufficient for the benchmark corrosion studies while retaining the essential advantages of the grand-potential formulation for evolving metal–electrolyte interfaces [3].

2.4.3 Binary reduction for two-phase, two-component corrosion

For the benchmark corrosion simulations considered in this thesis, the general grand-potential formulation is reduced to a binary solid–liquid system. The two phases represent the metallic solid and the electrolyte, described by the phase-field vector

$$\boldsymbol{\phi} = \{\phi_s, \phi_\ell\}, \quad \phi_s + \phi_\ell = 1.$$

The two chemical components are the metal species and the solvent/electrolyte background; because only one concentration is independent, the chemical state is described by a single chemical potential field $\mu(\mathbf{x}, t)$ [3, 44]. This reduction isolates the essential mechanisms

of corrosion at a moving metal–electrolyte interface while providing an efficient basis for validation and for later extension to multiphase alloy microstructures [3].

In the binary solid–liquid case, the grand-potential density is interpolated between the solid and liquid phase contributions as

$$\psi(\phi_s, \mu) = h(\phi_s) \psi_s(\mu) + [1 - h(\phi_s)] \psi_\ell(\mu), \quad (2.28)$$

where $h(\phi_s)$ is the interpolation function. In the present implementation, the simple choice $h(\phi_s) = \phi_s$ is used unless otherwise stated. The phase-specific grand-potential densities are obtained from the corresponding Helmholtz free-energy densities by

$$\psi_s(\mu) = f_s(c'_s(\mu)) - \mu c'_s(\mu), \quad \psi_\ell(\mu) = f_\ell(c'_\ell(\mu)) - \mu c'_\ell(\mu), \quad (2.29)$$

where c'_s and c'_ℓ denote normalized concentrations in the solid and liquid phases, respectively. The normalization is defined with respect to the solid concentration, $c' = c/c_{\text{solid}}$ [3].

Following the corrosion formulation used in this thesis, the phase-specific Helmholtz free-energy densities are approximated by parabolic functions around their equilibrium concentrations,

$$f_\ell(c'_\ell) = A (c'_\ell - c_\ell^e)^2, \quad f_s(c'_s) = A (c'_s - c_s^e)^2, \quad (2.30)$$

where A is the free-energy curvature parameter, and c_s^e and c_ℓ^e are the normalized equilibrium concentrations in the solid and liquid phases. For an almost pure metallic solid,

$$c_s^e = 1, \quad c_\ell^e = \frac{c_{\text{sat}}}{c_{\text{solid}}}, \quad (2.31)$$

where c_{sat} is the saturation concentration of the metal species in the liquid. The common chemical potential follows from the local equilibrium condition,

$$\mu = \frac{\partial f_s}{\partial c'_s} = \frac{\partial f_\ell}{\partial c'_\ell}. \quad (2.32)$$

Using Eq. (2.30), the phase concentrations can be expressed explicitly as functions of μ ,

$$c'_\ell(\mu) = \frac{\mu}{2A} + c_\ell^e, \quad c'_s(\mu) = \frac{\mu}{2A} + c_s^e. \quad (2.33)$$

Thus, at equilibrium, $\mu = 0$ recovers $c'_\ell = c_\ell^e$ and $c'_s = c_s^e$.

The interpolated normalized concentration is then given by

$$c'(\mu, \phi_s) = h(\phi_s)c'_s(\mu) + [1 - h(\phi_s)]c'_\ell(\mu). \quad (2.34)$$

Mass transport is governed by conservation of the interpolated concentration,

$$\frac{\partial c'}{\partial t} = \nabla \cdot [\overline{M}(\phi_s) \nabla \mu], \quad (2.35)$$

where $\overline{M}(\phi_s)$ is the effective chemical mobility. It is interpolated from the phase-specific mobilities as

$$\overline{M}(\phi_s) = h(\phi_s)\overline{M}_s + [1 - h(\phi_s)]\overline{M}_\ell, \quad (2.36)$$

with

$$\overline{M}_\alpha = D_\alpha \frac{\partial c'_\alpha}{\partial \mu}, \quad \alpha \in \{s, \ell\}. \quad (2.37)$$

Here, D_s and D_ℓ denote the diffusion coefficients in the solid and liquid phases. In the corrosion simulations, diffusion of dissolved metal species in the solid is neglected relative to diffusion in the electrolyte, such that $D_s = 0$ and $D_\ell = D$ [3, 27].

For numerical integration, the transport equation is rewritten in terms of the chemical potential as the primary variable. Differentiating Eq. (2.34) with respect to time and combining it with Eq. (2.35) yields

$$\begin{aligned} \frac{\partial \mu}{\partial t} = & \left[h(\phi_s) \frac{\partial c'_s(\mu)}{\partial \mu} + (1 - h(\phi_s)) \frac{\partial c'_\ell(\mu)}{\partial \mu} \right]^{-1} \\ & \times \left[\nabla \cdot (\overline{M}(\phi_s) \nabla \mu) - (c'_s(\mu) - c'_\ell(\mu)) \frac{\partial h(\phi_s)}{\partial t} \right]. \end{aligned} \quad (2.38)$$

The second term on the right-hand side accounts for the change in local composition caused by phase transformation at the moving metal–electrolyte interface. In other words, when solid metal transforms into electrolyte, the concentration field must be updated consistently with the difference between the phase-specific concentrations c'_s and c'_ℓ .

Solving Eq. (2.38) rather than directly evolving the interpolated concentration is advantageous because the chemical potential remains continuous across diffuse interfaces even when phase concentrations differ. This improves numerical robustness and avoids artificial concentration oscillations at the interface [3, 44]. The binary reduction is used for the pseudo-one-dimensional and two-dimensional corrosion validation problems in chapter 5. It also provides the basis for the later multiphase corrosion simulations, where additional metallic phase

fields are introduced while retaining the same chemical-potential-based transport structure [3].

2.4.4 Diffuse-interface pressure boundary condition

A central requirement of the corrosion-to-failure framework is the ability to apply pressure on an evolving internal corrosion surface without explicitly tracking or remeshing the pit geometry. In a sharp-interface description, a hydrostatic pressure acting on the solid–fluid boundary enters the mechanical problem as a Neumann traction condition. However, because the pit surface evolves implicitly through the corrosion phase field, the corresponding pressure load must also be applied in a diffuse-interface form. This is achieved by reformulating the sharp-interface traction condition as an equivalent volumetric contribution localized at the diffuse solid–fluid interface [3, 57].

The derivation starts from the quasi-static momentum balance in the solid domain V_s , neglecting inertia and body forces. Let $I(\mathbf{x})$ denote the sharp indicator function of the solid region, with $I = 1$ in the solid and $I = 0$ in the void or fluid region. The surface Dirac distribution associated with the solid boundary is denoted by δ_S , and satisfies

$$\nabla I = -\delta_S \mathbf{n}, \quad (2.39)$$

where $\mathbf{n}$ is the outward unit normal to the solid boundary. Using this identity, the sharp-interface momentum balance with a prescribed boundary traction can be written in whole-domain form as

$$\nabla \cdot (I\boldsymbol{\sigma}) + \mathbf{t}_{bc} \delta_S = \mathbf{0}, \quad (2.40)$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor and $\mathbf{t}_{bc}$ is the traction vector applied at the internal boundary [3, 57]. For a purely hydrostatic pressure p acting normal to the interface,

$$\mathbf{t}_{bc} = -p \mathbf{n}. \quad (2.41)$$

In the phase-field setting, the sharp indicator function I is replaced by the solid phase field ϕ_s , which varies smoothly from $\phi_s = 1$ in the solid to $\phi_s = 0$ in the fluid or void region. The surface Dirac distribution is then replaced by a smooth approximation $\tilde{\delta}_S$ localized within the diffuse interface. Following the diffuse-interface pressure formulation used in this thesis, the mechanical equilibrium equation becomes

$$\nabla \cdot (\phi_s \boldsymbol{\sigma}) + \mathbf{t}_{bc} \tilde{\delta}_S = \mathbf{0}. \quad (2.42)$$

Among several possible diffuse approximations of the surface Dirac distribution, the present thesis uses

$$\tilde{\delta}_S = 6\phi_s(1 - \phi_s) |\nabla \phi_s|. \quad (2.43)$$

Together with Eq. (2.41) and the relation between the phase-field gradient and the interface normal, this gives the diffuse pressure contribution

$$\mathbf{t}_{bc} \tilde{\delta}_S = 6\phi_s(1 - \phi_s) p \nabla \phi_s. \quad (2.44)$$

Consequently, the pressure-loaded whole-domain momentum balance is written as

$$\nabla \cdot (\phi_s \boldsymbol{\sigma}) + 6\phi_s(1 - \phi_s) p \nabla \phi_s = \mathbf{0}. \quad (2.45)$$

The factor $6\phi_s(1 - \phi_s)$ localizes the pressure contribution to the diffuse solid–fluid interface, so that the pressure load vanishes in the bulk solid and in the bulk fluid. As the corrosion pit evolves, the transition region of ϕ_s moves with the metal–electrolyte interface, and the applied pressure therefore follows the evolving pit surface automatically. This avoids explicit interface reconstruction and enables pressure loading of complex, evolving corrosion morphologies [3]. In the sharp-interface limit, the diffuse formulation recovers the standard momentum balance in the solid together with the traction condition $\boldsymbol{\sigma}\mathbf{n} = -p\mathbf{n}$ on the internal boundary.

For multiphase metallic systems, the solid indicator is obtained from the sum of all solid phase fields,

$$\phi_s = \sum_{\alpha=1}^{N_s} \phi_\alpha, \quad (2.46)$$

and the corresponding stress contribution can be written as

$$\phi_s \boldsymbol{\sigma} = \sum_{\alpha=1}^{N_s} \phi_\alpha \boldsymbol{\sigma}^\alpha, \quad (2.47)$$

where N_s is the number of solid phases and $\boldsymbol{\sigma}^\alpha$ is the phase-specific stress. This whole-domain interpolation assigns mechanical stiffness only to the solid region while treating the fluid or void phase as mechanically inactive, consistent with diffuse-domain mechanical formulations used for complex microstructures [3, 58]. In the corrosion simulations presented in chapter 5, all metallic phases are assigned identical elastic properties, so the analysis isolates the effect of corrosion-pit morphology on pressure-induced crack initiation

rather than the influence of phase-specific elastic contrast [3]. The validation of this diffuse pressure boundary condition against analytical elasticity solutions is discussed in section 5.1.2.

2.4.5 Phase-field based crack modeling

To simulate crack initiation and propagation from corrosion-induced stress concentrations, a phase-field fracture model is introduced for the solid phases. The crack is represented by a scalar phase field $\phi_c(\mathbf{x}, t)$, where $\phi_c = 0$ denotes intact material and $\phi_c = 1$ denotes fully broken material. This diffuse representation regularizes sharp crack surfaces over a finite length scale and avoids explicit tracking of the crack geometry. The formulation follows the variational phase-field approach to brittle fracture, in which the total mechanical energy consists of an elastic strain-energy contribution and a regularized crack-surface energy contribution [40, 59–61]. In the present thesis, the crack model is adapted to multiphase metallic systems and coupled to the diffuse-interface pressure loading introduced in section 2.4.4 [3, 62].

Under the small-strain assumption, the strain tensor is defined as

$$\boldsymbol{\varepsilon} = \frac{1}{2} (\nabla \mathbf{u} + \nabla^T \mathbf{u}), \quad (2.48)$$

where $\mathbf{u}$ is the displacement field. For a heterogeneous material containing N_s solid phases, the mechanical free-energy functional is written as

$$\begin{aligned}\mathcal{F}_{\text{mech}}[\boldsymbol{\varepsilon}, \phi_c, \nabla \phi_c] &= \int_V f \, dV \\ &= \int_V \left[\sum_{\alpha=1}^{N_s} \phi_\alpha f_{\text{el}}^\alpha(\boldsymbol{\varepsilon}^\alpha, \phi_c) \right. \\ &\quad \left. + \frac{1}{2} \sum_{\alpha=1}^{N_s} \phi_\alpha G_c^\alpha \left(\epsilon_c |\nabla \phi_c|^2 + \frac{1}{\epsilon_c} w(\phi_c) \right) \right] dV.\end{aligned}\tag{2.49}$$

Here, f_{el}^α is the elastic strain-energy density of phase α , G_c^α is the phase-specific critical energy release rate, and ϵ_c controls the width of the diffuse crack interface. The second term in Eq. (2.49) is the regularized crack-surface energy. In the present implementation, an obstacle-type crack potential is used,

$$w(\phi_c) = \frac{9}{16} \phi_c, \tag{2.50}$$

consistent with the phase-field crack formulation adopted in the corrosion-to-failure model [3]. The phase-wise interpolation in Eq. (2.49) allows elastic stiffness and crack resistance to vary across multiphase microstructures.

To avoid non-physical crack growth under compression, the elastic energy is decomposed into tensile and compressive contributions

following the isotropic tension–compression split of Miehe et al. [40]. The degraded phase-specific elastic energy is written as

$$f_{\text{el}}^{\alpha}(\boldsymbol{\varepsilon}^{\alpha}, \phi_c) = h(\phi_c) [f_{\text{el}}^{\alpha}(\boldsymbol{\varepsilon}^{\alpha})]^+ + [f_{\text{el}}^{\alpha}(\boldsymbol{\varepsilon}^{\alpha})]^- , \quad (2.51)$$

where $[\cdot]^+$ and $[\cdot]^-$ denote the positive and negative parts of the elastic energy density. The degradation function is defined as

$$h(\phi_c) = \begin{cases} (1 - \phi_c)^2, & \text{if } 1 - \phi_c > \phi_{\text{th}}, \\ \phi_{\text{th}}^2, & \text{otherwise,} \end{cases} \quad (2.52)$$

where ϕ_{th} is a residual-stiffness threshold. This function smoothly reduces the tensile stiffness in damaged regions while retaining a small residual stiffness to avoid numerical singularities [3, 40]. The tensile and compressive energy densities are expressed in terms of the phase-specific Lamé parameters λ^{α} and μ^{α} and the principal strains ε_i^{α} as

$$[f_{\text{el}}^{\alpha}(\boldsymbol{\varepsilon}^{\alpha})]^{\pm} = \frac{1}{2} \lambda^{\alpha} \langle \varepsilon_1^{\alpha} + \varepsilon_2^{\alpha} + \varepsilon_3^{\alpha} \rangle_{\pm}^2 + \mu^{\alpha} \sum_{i=1}^3 \langle \varepsilon_i^{\alpha} \rangle_{\pm}^2 , \quad (2.53)$$

with the Macaulay brackets defined as

$$\langle q \rangle_{\pm} = \frac{q \pm |q|}{2} . \quad (2.54)$$

The crack phase field evolves according to an Allen–Cahn-type relaxation equation obtained from the variational derivative of the mechanical free energy,

$$\epsilon_c \frac{\partial \phi_c}{\partial t} = -M_c \frac{\delta \mathcal{F}_{\text{mech}}}{\delta \phi_c}, \quad (2.55)$$

where $M_c \geq 0$ is a crack mobility or relaxation parameter. Substitution of Eq. (2.49) gives

$$\begin{aligned} \epsilon_c \frac{\partial \phi_c}{\partial t} = M_c \left[- \sum_{\alpha=1}^{N_s} \phi_\alpha \frac{\partial f_{\text{el}}^\alpha(\boldsymbol{\epsilon}^\alpha, \phi_c)}{\partial \phi_c} - \frac{1}{\epsilon_c} \frac{\partial w(\phi_c)}{\partial \phi_c} \right. \\ \left. + \nabla \cdot \left(\sum_{\alpha=1}^{N_s} \phi_\alpha G_c^\alpha \epsilon_c \nabla \phi_c \right) \right]. \end{aligned} \quad (2.56)$$

The first term on the right-hand side represents the crack driving force arising from tensile elastic energy, while the remaining terms regularize the crack surface through the crack potential and gradient energy [3, 40, 62]. With the degradation function in Eq. (2.52), the crack driving force can be expressed as

$$\mathcal{H} = 2(1 - \phi_c) \sum_{\alpha=1}^{N_s} \phi_\alpha [f_{\text{el}}^\alpha(\boldsymbol{\epsilon}^\alpha)]^+. \quad (2.57)$$

The effective compressive energy density is

$$f_{\text{el}}^- = \sum_{\alpha=1}^{N_s} \phi_\alpha [f_{\text{el}}^\alpha(\boldsymbol{\epsilon}^\alpha)]^-. \quad (2.58)$$

The mechanical equilibrium equation is solved together with the crack evolution equation. Including the crack degradation, the interpolated phase-specific stresses, and the diffuse-interface pressure loading, the momentum balance is written as

$$\nabla \cdot \left[h(\phi_c) \sum_{\alpha=1}^{N_s} \phi_\alpha \boldsymbol{\sigma}^\alpha \right] = -p \tilde{\delta}_S \mathbf{n}, \quad (2.59)$$

where $\boldsymbol{\sigma}^\alpha = \mathbb{C}^\alpha : \boldsymbol{\varepsilon}^\alpha$ is the phase-specific stress, $\mathbb{C}^\alpha$ is the stiffness tensor of phase α , p is the applied pressure, $\tilde{\delta}_S$ localizes the pressure load at the diffuse solid–fluid interface, and $\mathbf{n}$ is the local outward normal. The stress interpolation corresponds to a Voigt–Taylor homogenization assumption in which the phase-specific strains are taken to be identical at a material point [3]. In the simulations presented in chapter 5, the metallic phases are assigned identical elastic stiffness, so that the analysis focuses on the effect of corrosion morphology and pressure loading rather than elastic contrast.

The crack evolution and mechanical equilibrium equations are solved in a staggered manner. At each pressure increment, the displacement field is first obtained from the mechanical equilibrium problem, followed by relaxation of the crack phase field according to Eq. (2.56). The irreversibility condition

$$\dot{\phi}_c \geq 0 \quad (2.60)$$

is enforced to prevent crack healing. For computational efficiency, points exceeding a critical damage threshold are treated as fully cracked,

$$\phi_c \geq \phi_c^{\text{crit}} = 1 - \epsilon_d \quad \Rightarrow \quad \phi_c = 1, \quad (2.61)$$

where ϵ_d is the damage tolerance [3]. This quasi-static treatment allows the crack field to relax to equilibrium under a prescribed corrosion morphology and pressure load.

In the overall corrosion-to-failure workflow, the grand-potential corrosion model first generates the evolving pit morphology. Selected corrosion states are then transferred to the mechanical model, where pressure is applied at the diffuse metal–electrolyte interface and increased until crack initiation occurs. This sequential strategy reflects the distinct time scales of corrosion and crack propagation while keeping the simulations computationally tractable [3]. The resulting framework enables evaluation of how pit depth, pit curvature, alloy phase arrangement, and interfacial mobility influence the critical pressure for crack initiation and propagation in chapter 5.

2.5 Model implementation

All phase-field simulations presented in this thesis were performed using the PACE3D simulation framework [63]. PACE3D is a parallel multiphysics phase-field environment designed for large-scale microstructure simulations on structured grids. The framework supports distributed-memory computations using the Message Passing Interface (MPI), together with domain decomposition and workload balancing strategies for efficient execution on high-performance computing (HPC) systems [63]. These capabilities are essential for the present thesis because the investigated problems involve evolving three-dimensional geometries, multiple phase fields, anisotropic

interface kinetics, and, in the corrosion case, coupled mechanical fields [1–3].

The models developed in this chapter were implemented in a modular manner within this computational environment. The K-feldspar dissolution model resolves anisotropic etch-pit formation and intragranular channel development within digital sandstone geometries. The quartz cementation model extends the multiphase-field framework to clay-coated grains and enables controlled simulation of coating-dependent overgrowth, porosity loss, and permeability evolution. The corrosion framework combines grand-potential-based interface motion, diffuse-interface pressure loading, and phase-field crack evolution to examine the transition from localized pitting to pressure-induced cracking. Although these applications differ in physical setting, they share a common numerical structure based on phase-field evolution equations, interfacial anisotropy, and post-processing or coupling to transport and mechanical solvers.

The numerical framework established in this chapter therefore provides the methodological basis for the simulation studies presented in the remainder of the thesis. In Part II, it is used to investigate how mineral–fluid interface motion creates and destroys pore space through K-feldspar dissolution and clay-mediated quartz cementation. In Part III, the framework is extended to metallic installations, where corrosion morphology is coupled to pressure loading and fracture initiation. Together, these applications demonstrate how a unified phase-field methodology can connect microscale interface evolution to macroscopic transport properties and structural integrity in geological subsurface systems and related installations.

Part II - Reactive Porous Media: Creating and Closing Pore Space

3 Etch-Pit Driven K-feldspar Dissolution

This chapter is based primarily on the peer-reviewed publication by Kumar et al. [1], published in *Journal of Geophysical Research: Solid Earth*. It investigates how crystallographically controlled etch-pit dissolution of K-feldspar modifies pore-space structure and permeability evolution in siliciclastic sandstones. Feldspar dissolution is a major mechanism of secondary porosity generation in sedimentary reservoirs; however, in K-feldspar this process does not proceed through uniform surface retreat. Instead, dissolution localizes through the nucleation and growth of faceted etch-pits, which originate preferentially at defects, cleavage steps, and other crystallographically favored surface sites [1, 14]. Experimental and petrographic observations show that etch-pits on the (001) surface develop diamond-shaped morphologies with characteristic facet angles and strongly anisotropic growth kinetics, indicating that both capillary and kinetic anisotropy govern the dissolution process. Representative natural examples of cleavage-plane-controlled dissolution and intragranular pore development are shown in figure 3.1 [1, 14–16].

These geometric and kinetic characteristics exert a fundamental control on pore-space evolution. As etch-pits nucleate, deepen, and

laterally expand, neighboring dissolution sites may interact and coalesce into elongated intragranular channels, thereby enhancing pore connectivity and permeability disproportionately relative to the dissolved mineral volume [1]. Such behavior is not captured by conventional isotropic surface-recession models or reactive-surface-area formulations. To address this limitation, the present chapter applies the thermodynamically consistent multiphase-field framework introduced in chapter 2, specifically in section 2.2. This framework enables explicit resolution of evolving solid–fluid interfaces while naturally incorporating anisotropic surface energy and orientation-dependent interface kinetics. A central methodological contribution is the grain-wise local refinement and re-embedding workflow introduced in [1], in which individual K-feldspar grains are locally refined to resolve etch-pit formation at high spatial resolution and subsequently mapped back into digital sandstone geometries. On this basis, the chapter first establishes model validity at the grain scale through calibration and validation, and then applies the workflow to quantify porosity evolution, connectivity development, and permeability enhancement in digital sandstone microstructures.

3.1 Model calibration and validation

The predictive capability of the multiphase-field framework for K-feldspar dissolution must be established at the scale at which crystallographically controlled etch-pits nucleate and evolve. As introduced in section 2.2, the governing formulation incorporates anisotropic interfacial energy and orientation-dependent kinetic mobility to represent faceted dissolution. The corresponding capillary and kinetic

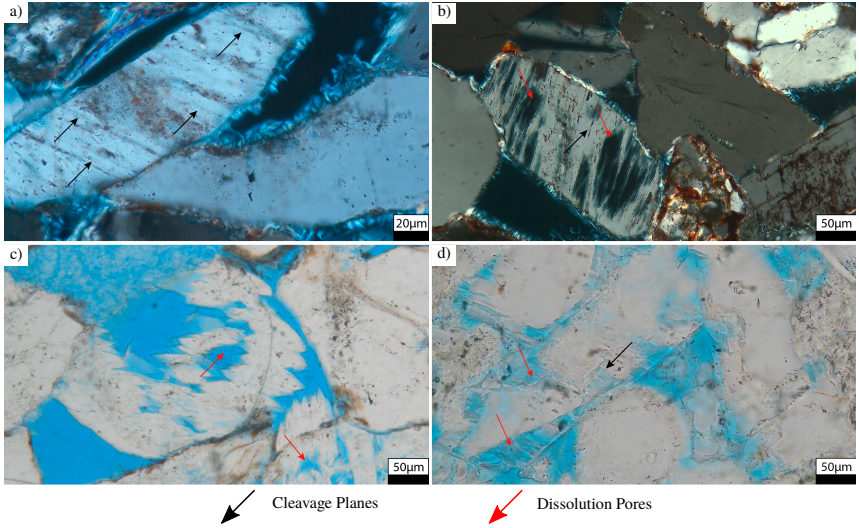


Figure 3.1: Thin section images highlighting cleavage planes (black arrows in a, b, d) and intragranular dissolution pores in detrital K-feldspar grains (red arrows in b, c, d). All samples are retrieved from the Triassic Buntsandstein in southern Germany (see also [15, 16]). a, b) under crossed polarizers; c, d) under plane polarizers. Reproduced from figure 1 in [1].

shapes used in the simulations are shown in figure 3.2. However, the presence of anisotropy alone is not sufficient to guarantee realistic pit morphologies. Rather, the relative magnitude and interplay of capillary and kinetic contributions must be calibrated such that the model reproduces the experimentally observed pit geometry, facet inclination, and relative retreat behavior before being applied to more complex grain and sandstone geometries.

Following the calibration strategy of Kumar et al. [1], the validation is carried out in two stages. First, the growth of an isolated etch-pit on a planar (001) K-feldspar surface is simulated to assess

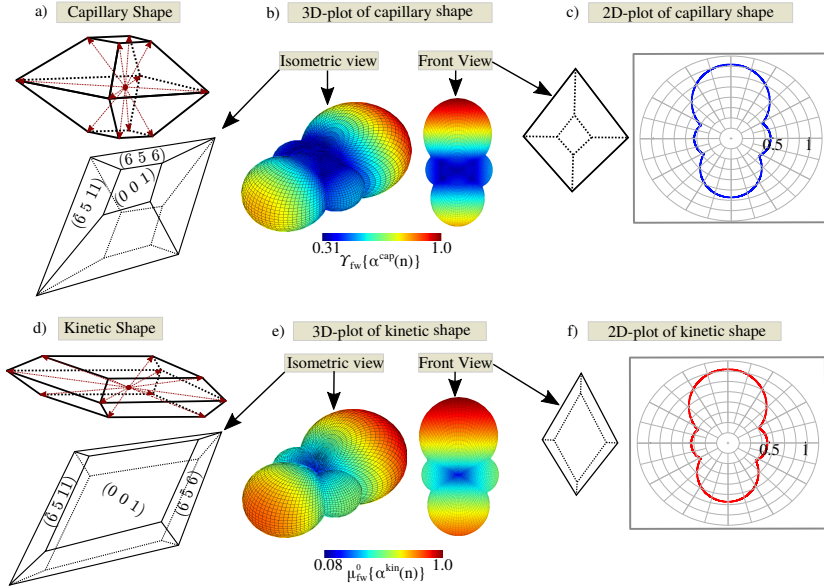


Figure 3.2: Crystallographic shapes of etch-pits formed during dissolution and used in the phase-field simulations. (a) Resulting capillary shape of the etch-pit after numerical modeling. (b) Surface-energy plot of the resulting shape (isometric and front view). (c) Two-dimensional projection of the surface-energy plot. (d) Resulting kinetic shape of the etch-pit after numerical modeling. (e) Kinetic plot of the resulting shape (isometric and front view). (f) Two-dimensional projection of the kinetic plot. Reproduced from figure 2 in [1].

facet stabilization and the reproduction of anisotropic dissolution kinetics (see figure 3.3). Second, multiple interacting pits are simulated in a two-dimensional section to examine whether the model captures pit coalescence and channel formation without further parameter adjustment (see figure 3.4). All simulations in this section use the governing equations and anisotropy formulations introduced in sections 2.1 and 2.2, without further modification.

Consistent with the assumptions adopted in [1], dissolution is simulated under sustained undersaturation. The chemical driving force for dissolution, defined in sections 2.1.1 and 2.2.1, is taken to be spatially uniform and temporally constant. This simplification isolates the effect of anisotropic interface physics from mass-transport limitations and enables direct comparison with atomic force microscopy observations of etch-pit morphology [14]. Accordingly, the aim of this section is not to reproduce absolute dissolution rates, but to validate the morphology and relative kinetic behavior generated by the anisotropic formulation.

3.1.1 Single etch-pit growth

The formation of a single etch-pit on the (001) surface of K-feldspar represents the most fundamental expression of crystallographically controlled dissolution. Atomic force microscopy observations show that etch-pits nucleate at surface defects and evolve into diamond-shaped cavities bounded by well-defined crystallographic facets [14]. In plan view, the characteristic geometry is defined by facet angles of approximately 63° and 121° , while the inclination of the pit walls relative to the (001) surface is approximately 27° [1, 14]. In addition,

lateral propagation along the surface plane proceeds significantly faster than vertical retreat into the crystal interior.

To reproduce these characteristics, the anisotropic interfacial-energy formulation described in section 2.2.2 is employed. Capillary anisotropy stabilizes selected interface orientations by penalizing deviations from crystallographically preferred normals. During the initial stage of dissolution, a localized surface perturbation evolves into a faceted cavity as the interface minimizes its total free energy under the imposed anisotropic surface-energy density. The emergence of planar facets therefore constitutes the first validation criterion of the model, as illustrated in figure 3.3.

The simulations show that the initially smooth perturbation rapidly reorganizes into a faceted geometry consistent with the crystallographic symmetry of K-feldspar. The stabilized facet orientations correspond closely to those observed experimentally, and the simulated inclination of the pit walls relative to the (001) plane agrees well with reported values [14]. This confirms that the capillary anisotropy parameters introduced in section 2.2.2 are appropriate for reproducing the faceted etch-pit geometry.

Facet stabilization alone, however, is not sufficient to describe realistic pit evolution. Experimental observations indicate a pronounced kinetic anisotropy, with in-plane propagation exceeding vertical retreat by approximately one order of magnitude [1]. This behavior is reproduced by incorporating orientation-dependent interface mobility, also described in section 2.2.2. The kinetic anisotropy selectively enhances dissolution rates along specific crystallographic directions while maintaining slower retreat in others. As a result, the simulated

pit deepens and widens anisotropically while preserving its faceted morphology, thereby reproducing the experimentally observed relative growth behavior (see, figure 3.3).

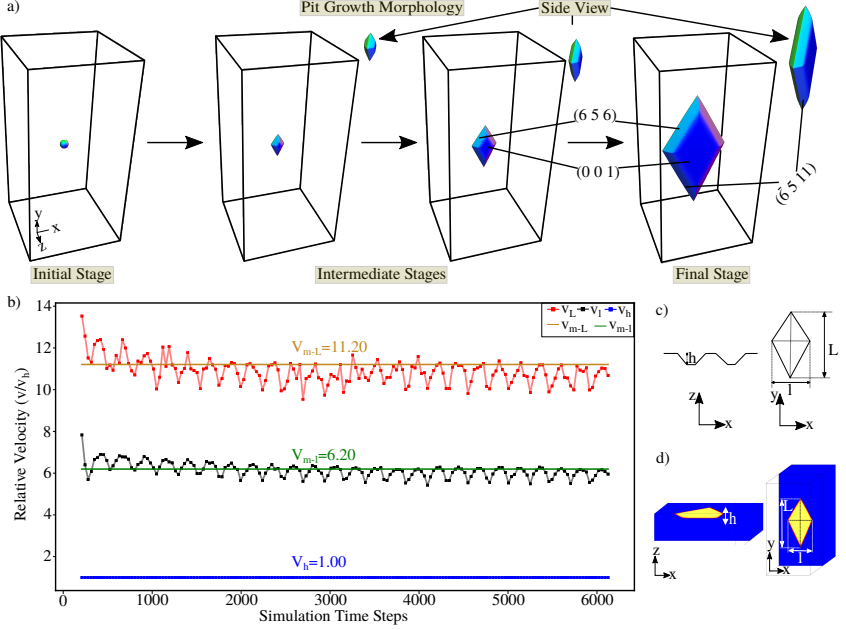


Figure 3.3: (a) Evolution of a single etch-pit, showing the development of distinct facets at successive simulation stages. (b) Relative velocity (v/v_h) and mean relative velocity (v_m) of a single etch-pit facet along the x- (l), y- (L), and z- (h) directions, normalized with respect to the h -direction. (c) Schematic illustration of the distinct facet growth trajectories (l, L, h) in two dimensions. (d) Three-dimensional cross-sectional view of the final simulation stage shown in (a), highlighting the corresponding growth trajectories. Reproduced from figure 3 in [1].

The simulated retreat velocities confirm that the ratio of lateral to vertical propagation is consistent with experimental estimates. Quantitatively, the mean relative velocities shown in figure 3.3 are $v_{m,L}/v_h = 11.20$ and $v_{m,l}/v_h = 6.20$, confirming that lateral widening is several times faster than vertical retreat. The model therefore reproduces both the geometric and kinetic characteristics of single etch-pit evolution. Importantly, no geometric constraints or prescribed facet orientations are imposed; instead, the faceted morphology emerges naturally from the anisotropic thermodynamic and kinetic formulation introduced in chapter 2. This demonstrates that the phase-field implementation captures the essential physics governing isolated etch-pit growth.

3.1.2 Multiple etch-pit growth in a 2D section

In natural systems, K-feldspar dissolution is characterized by the simultaneous nucleation and evolution of numerous etch-pits. The predictive capability of the anisotropic multiphase-field framework must therefore be assessed not only for isolated pit growth, but also for interacting dissolution sites. The aim of this subsection is to determine whether pit-pit interaction, coalescence, and channel formation emerge intrinsically from the anisotropic formulation introduced in section 2.2, without further parameter adjustment.

To this end, a two-dimensional computational section parallel to the (001) surface is considered, consistent with the configuration presented in [1]. Multiple localized perturbations are introduced along an initially planar K-feldspar interface to represent distributed defect-controlled nucleation sites. All capillary and kinetic anisotropy

parameters are kept identical to those calibrated in section 3.1.1, such that the collective behavior observed in the simulations arises solely from the governing equations and calibrated anisotropic description.

During the initial stages of dissolution, individual pits evolve independently while preserving the faceted morphology established in the single-pit calibration. Because lateral propagation dominates over vertical retreat, adjacent cavities progressively widen and begin to interact. As dissolution proceeds, the expanding fronts overlap, modifying the local curvature distribution and accelerating retreat in the intervening regions. This interaction ultimately produces pit coalescence and the formation of elongated channel-like voids aligned with crystallographically preferred directions.

The full evolution sequence of interacting etch-pits is shown in figure 3.4, reproduced from [1]. The comparison illustrates the transition from initially isolated pits to interconnected channel structures without any imposed geometric constraints. The preservation of faceted boundaries during interaction confirms the robustness of the capillary anisotropy implementation described in section 2.2.2. At the same time, the dominance of lateral propagation over vertical retreat, governed by orientation-dependent mobility, drives preferential merging parallel to the surface plane. The resulting channelization emerges at comparatively small overall mineral volume loss, underscoring the nonlinear relationship between dissolution morphology and pore-space evolution.

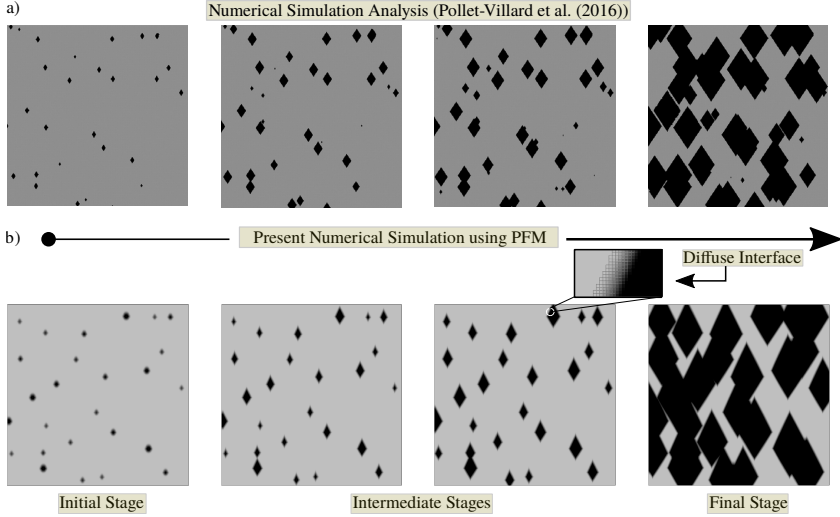


Figure 3.4: Etch-pit growth in a numerical two-dimensional section representing the (001) plane of K-feldspar. Comparison of (a) the numerical study of [14] and (b) the corresponding results obtained with the present phase-field approach. Reproduced from figure 4 in [1].

These simulations demonstrate that the anisotropic multiphase-field framework captures not only the geometric characteristics of individual etch-pits but also the collective dynamics governing pit coalescence. The emergence of elongated intragranular channels therefore provides the mechanistic basis for enhanced pore connectivity at the grain scale and establishes the foundation for the subsequent application to digital sandstone geometries.

3.2 Findings and discussion

The calibration and validation results presented in section 3.1 show that the anisotropic multiphase-field framework captures the essential geometric and kinetic characteristics of etch-pit growth at the grain scale. Building on this validated basis, the analysis is now extended to digitally reconstructed sandstone geometries in order to examine how crystallographically controlled K-feldspar dissolution modifies pore-space structure and transport behavior at the rock scale. The central question addressed in this section is how localized, anisotropic etch-pit growth within individual feldspar grains translates into changes in pore connectivity and permeability when embedded in a heterogeneous porous medium [1].

3.2.1 Dissolution of K-feldspar grains in digital sandstone

To transfer grain-scale etch-pit dynamics to the sandstone scale without globally refining the computational domain, the grain-wise local refinement and re-embedding workflow introduced by Kumar et al. [1] is employed. This workflow enables high-resolution simulation of dissolution within individual K-feldspar grains while preserving the surrounding sandstone geometry and avoiding the prohibitive computational cost that would arise from resolving sub-micrometer etch-pit features throughout the full sample.

The procedure begins with a digitally reconstructed sandstone sample containing quartz and K-feldspar grains. Quartz grains are treated as inert phases, consistent with the formulation described in section 2.2.3,

whereas selected K-feldspar grains are extracted individually for localized refinement. Each extracted grain is discretized on a finer grid in order to resolve etch-pit nucleation, facet development, and pit coalescence with sufficient spatial fidelity. Dissolution is then simulated to representative stages using the calibrated anisotropic formulation established in section 3.1. In a subsequent post-processing step, the dissolved grain geometries are mapped back onto the original sandstone grid, thereby re-embedding the evolving intragranular pore structure into the larger digital rock volume [1].

The complete workflow is summarized in figure 3.5. It provides the key methodological link between sub-grain-scale dissolution physics and sandstone-scale pore-space evolution by combining local geometric refinement with a consistent re-embedding strategy.

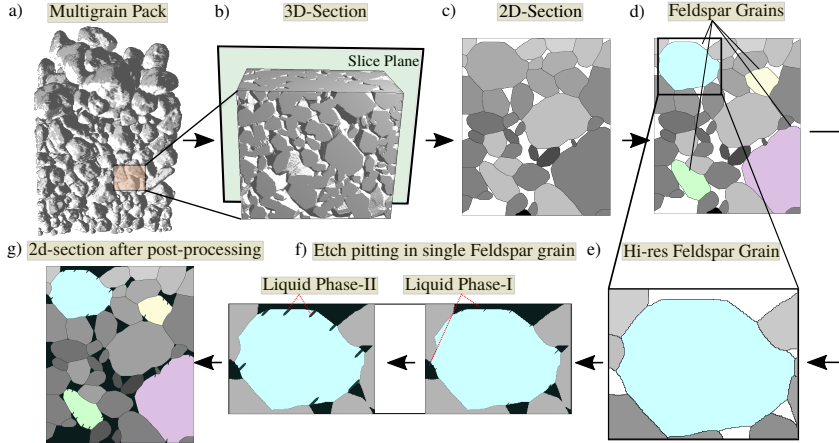


Figure 3.5: Grain-wise local refinement and re-embedding workflow for etch-pit-driven dissolution of K-feldspar in digital sandstone. Reproduced from figure 5 in [1].

This strategy ensures that crystallographically controlled dissolution features are explicitly resolved within individual grains while the broader sandstone framework remains geometrically consistent. Importantly, the workflow does not introduce any additional governing equations. All dissolution simulations continue to rely exclusively on the multiphase-field formulation presented in chapter 2, specifically in sections 2.1.1 and 2.2.2. Its contribution is therefore methodological rather than constitutive: it enables the validated anisotropic model to be applied across scales without altering the underlying physics [1].

Application of this workflow to three-dimensional digital sandstone geometries shows that etch-pits nucleate preferentially at fluid-accessible surfaces of K-feldspar grains and evolve into intragranular voids that progressively interact with the surrounding pore network. Because dissolution is anisotropic, the evolving void space does not expand uniformly. Instead, lateral growth along crystallographically favored directions promotes the development of elongated internal channels, which in turn facilitate earlier topological connection with adjacent pores [1]. The resulting pore-space evolution is therefore governed not simply by mineral removal, but by the geometry and orientation of the dissolution features that emerge within the grains.

The three-dimensional evolution of etch-pits within K-feldspar grains embedded in the sandstone matrix is illustrated in figure 3.6. The figure shows that dissolution remains strongly localized within the feldspar phase and progressively transforms isolated intragranular pits into connected void structures.

The simulations demonstrate that K-feldspar dissolution does not proceed as uniform grain shrinkage. Instead, dissolution remains highly

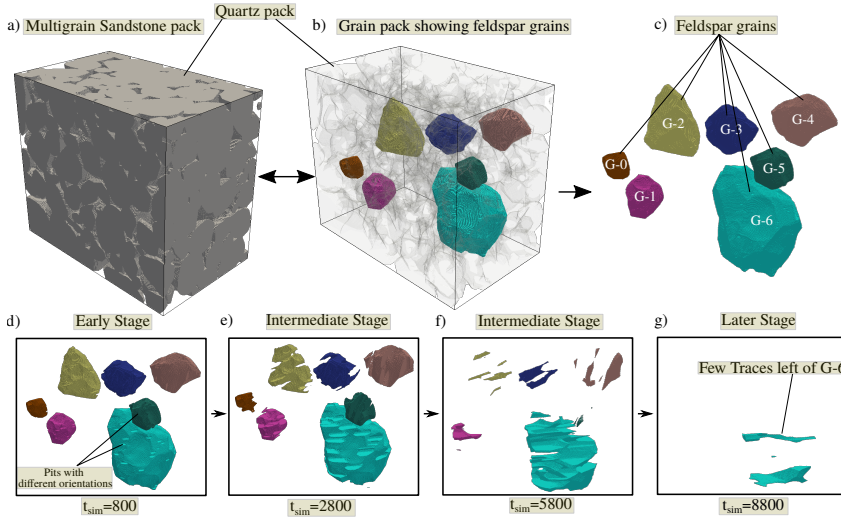


Figure 3.6: Three-dimensional application of etch-pit-driven dissolution within a digital sandstone sample. Intragranular voids develop and progressively connect to the surrounding pore network. Reproduced from figure 7 in [1].

localized, producing internal voids that grow, merge, and alter grain topology before substantial reduction in bulk grain volume occurs. This distinction is important because the hydraulic consequences of dissolution are controlled less by total mineral loss than by the emergence and interconnection of new pore pathways. In this sense, etch-pit-driven dissolution acts as a topology-modifying mechanism that can enhance pore connectivity at comparatively small overall mineral loss, thereby providing the physical basis for the permeability evolution analyzed in the following subsection [1].

3.2.2 Implication on porosity and permeability evolution

While section 3.2.1 showed that etch-pit-driven dissolution produces intragranular channels within individual K-feldspar grains, the hydraulic significance of this morphology is best understood through analysis of the evolving flow field and the corresponding permeability response. In contrast to uniform grain shrinkage, anisotropic etch-pit growth modifies pore connectivity in a spatially localized and topologically nontrivial manner. The following analysis therefore examines how fluid pathways reorganize during dissolution and how permeability responds to variations in feldspar fraction and crystallographic orientation [1].

3.2.2.1 Evolution of flow connectivity during dissolution

The progressive reorganization of fluid pathways within the sandstone matrix is illustrated in figure 3.7, reproduced from [1]. The streamline evolution provides direct evidence of how localized intragranular dissolution modifies the connectivity structure of the pore network rather than merely increasing pore volume.

At the initial stage, fluid flow is largely confined to the pre-existing intergranular pore network. As etch-pits nucleate, grow, and coalesce within K-feldspar grains, new void space develops inside the dissolving grains. Once these intragranular channels intersect the surrounding pore system, local connectivity increases markedly and the streamline pattern reorganizes accordingly. The figure shows that dissolution does not simply widen existing flow conduits; instead, it creates new hydraulic pathways that alter the topology of the flow field [1].

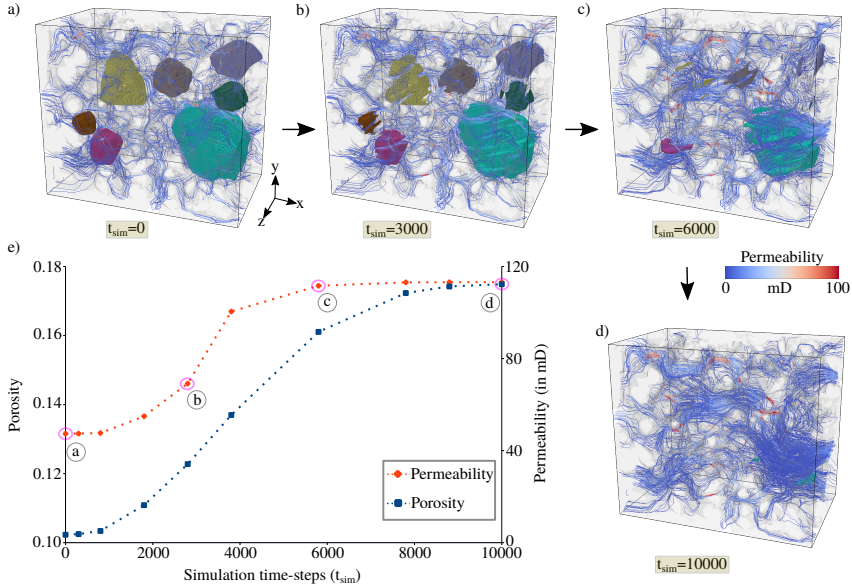


Figure 3.7: Evolution of fluid streamlines during progressive K-feldspar dissolution in digital sandstone. Fluid initially flows through pre-existing pore channels; as dissolution proceeds, new intragranular voids form and connect, locally enhancing flow connectivity. Reproduced from figure 9 in [1].

This effect is especially important because the resulting permeability enhancement depends on when and where such connectivity transitions occur. In some configurations, complete dissolution of a feldspar grain produces an additional increase in connectivity, whereas in others the hydraulic impact is more limited and depends on the spatial relationship between grain orientation, pit-growth direction, and the original pore network. The flow-field evolution therefore confirms that permeability enhancement is governed primarily by the creation and interconnection of new pathways, rather than by gradual

pore enlargement alone. This provides the mechanistic basis for the quantitative porosity-permeability trends discussed in the following subsections.

3.2.2.2 Influence of K-feldspar grain volume fraction

The quantitative influence of dissolving mineral abundance on permeability evolution is shown in figure 3.8(a), reproduced from [1]. The results compare permeability evolution for sandstone packs containing different volume fractions of dissolving K-feldspar grains.

For lower feldspar fractions, permeability increases only gradually, reflecting the limited hydraulic interaction between dissolving grains and the surrounding pore network. As the feldspar fraction increases, however, the intragranular channels generated by etch-pit growth are more likely to intersect neighboring pores and adjacent dissolving grains. This leads to a markedly stronger permeability response. The results therefore indicate the presence of a connectivity threshold, beyond which permeability increases disproportionately relative to porosity. Importantly, this behavior does not arise from uniform mineral removal, but from the spatial overlap and progressive integration of newly formed intragranular flow pathways [1].

3.2.2.3 Influence of crystallographic orientation

Figure 3.8(b) shows the sensitivity of permeability evolution to crystallographic orientation. Because etch-pit growth is anisotropic, lateral channel expansion occurs preferentially along specific crystallographic directions. When these directions are favorably aligned with

the macroscopic hydraulic gradient, connected pathways form earlier and permeability increases more rapidly. By contrast, less favorable orientations delay pathway integration and produce a weaker hydraulic response, even when the overall degree of dissolution remains comparable [1].

This orientation dependence highlights a fundamental difference between anisotropic etch-pit-driven dissolution and isotropic grain-shrinkage models. In isotropic descriptions, dissolution proceeds uniformly and permeability evolution depends primarily on the total amount of mineral removed. In the present anisotropic framework, by contrast, permeability is governed by directionally controlled connectivity transitions that alter the topology of the pore network. The hydraulic response is therefore controlled not only by how much material dissolves, but also by how the resulting void space is oriented relative to the prevailing flow direction.

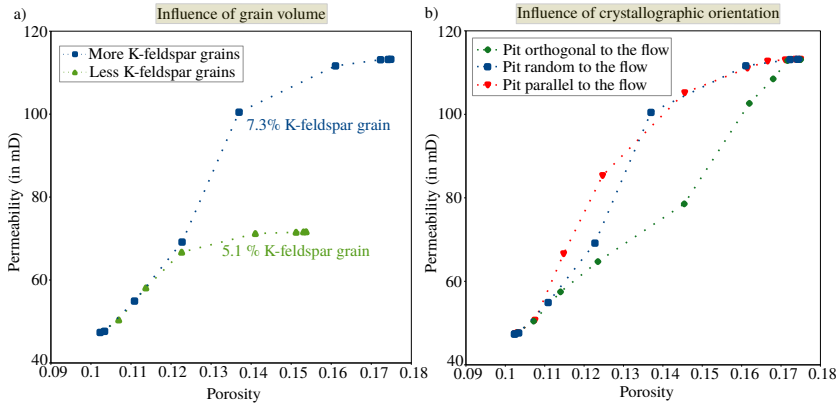


Figure 3.8: (a) Influence of K-feldspar grain volume fraction on permeability evolution. (b) Influence of crystallographic orientation on permeability response. Reproduced from figure 10 in [1].

3.2.2.4 Consistency with natural permeability ranges

To assess the physical plausibility of the simulated hydraulic response, the predicted permeability evolution is compared with reported permeability ranges for feldspar-bearing sandstones in figure 3.9, reproduced from [1].

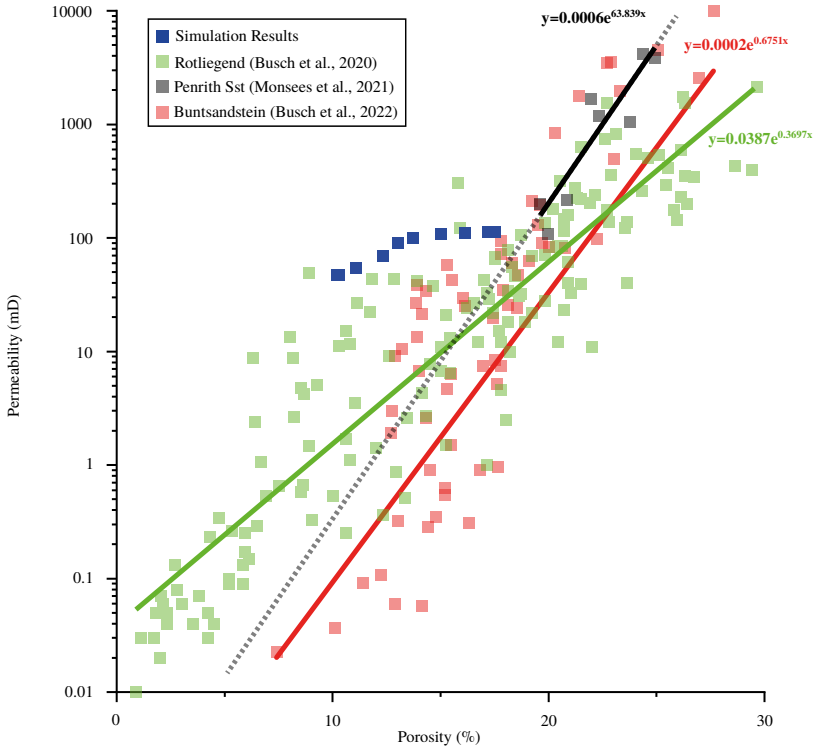


Figure 3.9: Comparison between simulated permeability evolution and reported permeability ranges from feldspar-bearing sandstones. Reproduced from figure 11 in [1].

The simulated permeability values lie within the variability observed in natural systems, indicating that the magnitude of hydraulic enhancement predicted by the anisotropic etch-pit model is physically plausible. This agreement supports the interpretation that localized, crystallographically controlled feldspar dissolution contributes significantly to secondary porosity development and to the observed variability of permeability in feldspar-bearing sandstones [1].

Taken together, these results show that permeability evolution in reactive porous media is governed by the combined effects of dissolving mineral fraction, crystallographic orientation, and the connectivity transitions induced by anisotropic etch-pit growth. Uniform isotropic dissolution models cannot capture these topology-driven effects and therefore tend to underestimate the hydraulic consequences of feldspar alteration.

3.3 Concluding remarks

This chapter investigated crystallographically controlled etch-pit-driven dissolution of K-feldspar and its implications for pore-scale structural evolution and macroscopic transport behavior in siliciclastic sandstones. Using the thermodynamically consistent multiphase-field framework introduced in chapter 2, the model was first calibrated and validated at the grain scale. The simulations reproduced the experimentally observed facet geometries, inclination angles, and anisotropic retreat kinetics of etch-pits, confirming that the implemented capillary and kinetic anisotropy provide an adequate representation of dissolution on the (001) surface.

Extension of the calibrated formulation to digital sandstone geometries through the grain-wise local refinement and re-embedding workflow enabled explicit resolution of intragranular channel formation within dissolving K-feldspar grains. The results showed that dissolution does not proceed through uniform grain shrinkage, but rather through localized etch-pit nucleation, lateral expansion, and pit coalescence. This morphology-driven evolution alters grain topology well before substantial bulk mineral loss occurs.

Analysis of the evolving flow field further demonstrated that permeability enhancement is governed primarily by connectivity transitions within the pore network. At early stages, fluid flow remains restricted to the pre-existing intergranular pore space. As dissolution progresses, however, intragranular channels intersect the surrounding pore system and create new hydraulic pathways that reorganize the flow field and locally reduce flow resistance. The sensitivity analyses further showed that permeability evolution depends strongly on both the volumetric fraction of dissolving K-feldspar grains and their crystallographic orientation relative to the hydraulic gradient. Favorably oriented grains promote earlier channel integration and more rapid hydraulic enhancement, whereas less favorable orientations delay connectivity development despite comparable overall dissolution. It should be noted that the analyzed digital sandstone volumes are representative of pore-scale mechanisms rather than full reservoir-scale heterogeneity; therefore, the permeability trends are interpreted mechanistically and require further upscaling for direct reservoir-scale prediction.

Comparison of the simulated permeability ranges with reported values from feldspar-bearing sandstones showed that the anisotropic etch-pit model yields physically realistic magnitudes of permeability increase.

This agreement supports the interpretation that crystallographically controlled dissolution provides a mechanistic explanation for permeability variability associated with secondary porosity development in natural reservoir systems.

Overall, this chapter demonstrates that anisotropic etch-pit growth acts as a topology-modifying mechanism that governs pore connectivity and hydraulic response in reactive porous media. The results highlight the limitations of isotropic surface-recession models and underscore the importance of morphology-resolving approaches for linking mesoscale dissolution processes to macroscopic transport properties. In this sense, the framework developed here provides the conceptual and computational basis for the complementary analysis in chapter 4, where pore space is reduced rather than created through precipitation and cementation processes.

4 Clay-Mediated Quartz Cementation in Sandstones

This chapter is based primarily on the peer-reviewed publication by Kumar et al. [2], published in *Petroleum Exploration and Development*. It investigates how clay coatings on quartz grains influence syntaxial quartz overgrowth, pore-throat evolution, and the resulting porosity-permeability response in sandstones. Quartz cementation is one of the principal diagenetic processes responsible for reservoir-quality degradation in deeply buried sandstones, whereas clay grain coatings may inhibit or delay cement precipitation by masking reactive quartz surfaces and disrupting nucleation and attachment pathways [2, 21–23]. Experimental observations, natural samples, and numerical studies consistently indicate that coating coverage, coating pattern, and crystallographic orientation strongly influence both the amount and spatial localization of quartz cement, and thereby govern how rapidly critical pore throats are constricted or preserved [2, 18, 23].

To address these coupled controls, the present chapter applies the thermodynamically consistent multiphase-field framework introduced in chapter 2, specifically in sections 2.1 and 2.3, with emphasis on crystallographically controlled quartz overgrowth and digitally generated clay-coating geometries. A central contribution is the

coating-generation workflow, which enables systematic variation of coating thickness, coverage, and spatial pattern on digital quartz grains and grain packs, thereby allowing their individual influence on cement growth and reservoir-quality evolution to be examined in a controlled pore-scale setting [2]. On this basis, the chapter first validates the model against experimental observations and natural sandstone textures, and then applies the framework to quantify how coating attributes govern cement volume, pore-throat bridging, porosity, permeability, and their comparison with geological samples.

4.1 Model validation

Quartz cementation in sandstones proceeds predominantly through syntaxial quartz overgrowth on detrital quartz grains during burial diagenesis, progressively reducing porosity and constricting pore throats [17, 18, 23]. It is likewise well established that clay grain coatings can substantially inhibit or delay quartz cementation by masking reactive quartz surfaces and disrupting nucleation and attachment pathways [21–23]. Because permeability is controlled disproportionately by a limited number of critical pore throats, even partial suppression of cementation at strategically important locations can preserve flow capacity far more effectively than porosity trends alone would suggest [19, 20].

The validation strategy adopted in this chapter follows two complementary routes. First, the model is assessed against controlled experimental observations of quartz overgrowth morphologies and coating-mediated growth inhibition. Second, the predicted cement

textures are compared with natural sandstone samples, with particular attention to the spatial distribution of cement, coating-controlled exclusion zones, and signatures of pore-throat occlusion. All simulations employ the governing equations introduced in chapter 2, specifically in sections 2.1 and 2.3, and these equations are therefore not re-derived here. The validation workflow and the associated comparisons follow the framework established in Kumar et al. [2].

4.1.1 Validation with experiments

Laboratory studies of quartz overgrowth provide a controlled basis for validating crystallographically governed cement morphologies, including facet development and epitaxial continuity [18, 23]. In coated systems, experiments and microstructural observations indicate that cement growth is suppressed on coated grain surfaces and preferentially develops on exposed quartz windows [2, 18, 21, 22]. These experimental trends motivate two validation requirements: (i) the model must reproduce faceted quartz overgrowth on uncoated surfaces under supersaturation, and (ii) it must reproduce growth inhibition when a coating phase masks the quartz–fluid interface [2].

In the simulations, quartz overgrowth develops epitaxially on exposed quartz surfaces, while coated regions remain largely inactive, consistent with experimental and petrographic interpretations of coatings as nucleation discontinuities or kinetic barriers [2, 21–23]. The ability to reproduce these qualitative signatures validates the anisotropic growth formulation and coating representation introduced in chapter 2, specifically in sections 2.3.1 and 2.3.3 (see figure 4.1). Since the reference experiments involve multi-component fluids and

supplementary minerals that are not explicitly represented in the present simulations, the comparison is interpreted as a morphological validation rather than a direct calibration of absolute growth rates.

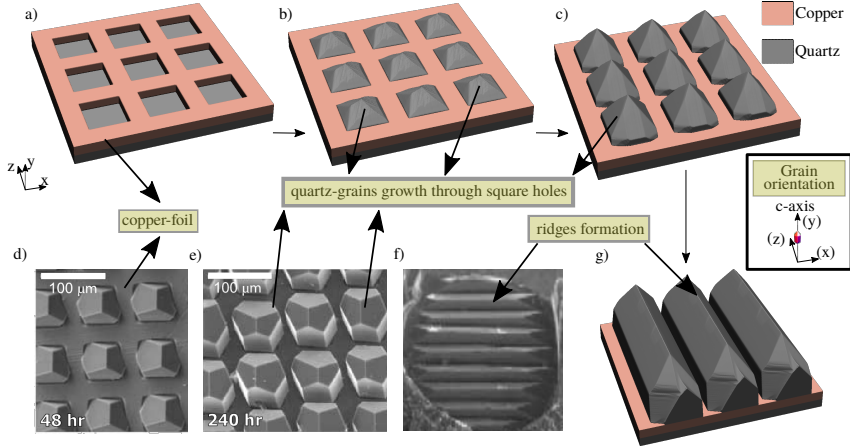


Figure 4.1: Validation of simulated quartz overgrowth morphologies against the quartz plate/copper-grid experiment of Lander et al. [18], showing faceted cement growth through exposed windows and inhibited growth beneath coated or masked regions. Reproduced from figure 4 in [2].

4.1.2 Validation with natural samples

Natural sandstones provide additional validation constraints beyond laboratory settings, including spatially heterogeneous coating coverage, mixed coating patterns, and pore-network-scale consequences of cementation [17, 23]. Petrographic and SEM studies commonly show

that coated grain contacts preserve intergranular volume, whereas uncoated regions exhibit quartz overgrowth thickening and progressive pore-throat constriction [21, 22].

The model is validated by comparing simulated cement-distribution patterns and pore-throat occlusion textures with representative natural samples presented in [2] (see figure 4.2). The comparison focuses on three key features: (i) localization of cement on exposed quartz surfaces, (ii) preservation of pore space at coated grain contacts, and (iii) the emergence of connectivity loss through cement bridging across narrow pore throats. Overall, the observed agreement supports the

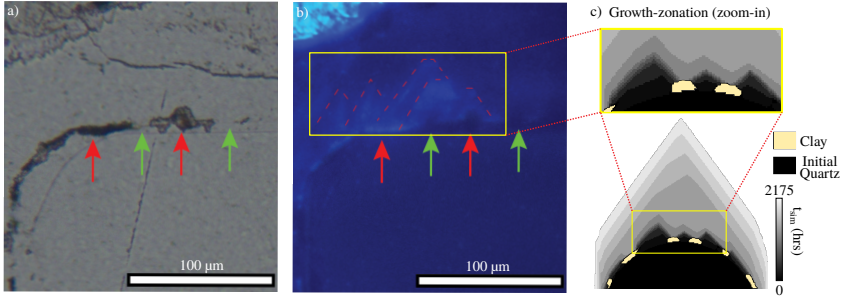


Figure 4.2: Validation against natural sandstone samples: clay-mediated inhibition of quartz overgrowth and preservation of pore space at coated contacts. Reproduced from figure 5 in [2].

use of the model for systematic pore-scale investigation of how coating characteristics govern quartz cementation and reservoir-quality evolution [2].

4.2 Findings and discussion

This section examines how coating attributes control both (i) quartz overgrowth morphology and (ii) the evolution of transport properties. The analysis is organized around three coating descriptors that can be varied independently within the digital workflow: coating coverage fraction, coating pattern, and the crystallographic orientation of the coated grains [2]. The guiding hypothesis is that coatings alter cementation primarily by controlling where quartz–fluid interfaces remain reactive and how rapidly cement bridges critical pore throats [19, 20, 23].

4.2.1 Overgrowth dynamics

4.2.1.1 Digital workflow for coating generation and simulation setup

A central contribution of this thesis is a digital tool-chain for generating clay coatings on quartz grain surfaces with controlled thickness, coverage, and spatial pattern, thereby enabling a systematic parametric investigation. Starting from a digital quartz-grain pack, a coating generator assigns a clay phase to selected surface regions according to prescribed rules, allowing the reproducible construction of (i) continuous layered coatings and (ii) discontinuous patchy coatings while preserving the same underlying grain geometry [2]. The resulting coated microstructures serve as initial conditions for multiphase-field simulations of quartz cementation and subsequent pore-scale flow analysis. Figure 4.3 illustrates the schematic workflow for a single arbitrarily shaped quartz grain, which is subsequently extended to

larger digital sandstone structures. Under supersaturated conditions,

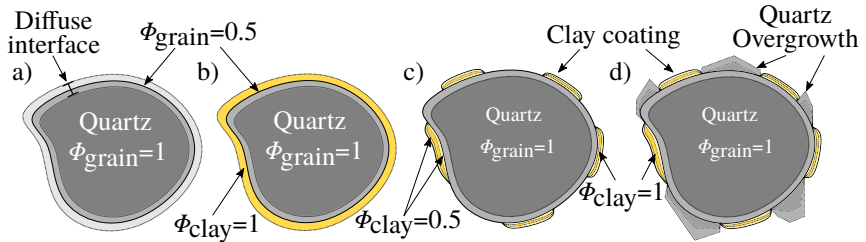


Figure 4.3: Digital workflow for coating generation and pore-scale simulation: coating assignment (thickness, coverage, pattern) on quartz grain surfaces, followed by multiphase-field cementation and pore-scale flow characterization. Reproduced from figure 3 in [2].

quartz overgrowth proceeds epitaxially on exposed quartz surfaces and forms faceted growth morphologies governed by crystallographic anisotropy (see figure 4.4). Clay coatings suppress growth locally by masking reactive quartz–fluid contact and thereby altering the locations at which growth can nucleate and advance. As a result, cementation becomes spatially heterogeneous even under uniform thermodynamic driving conditions, overgrowth thickens on exposed regions, whereas coated patches remain largely unchanged [2]. This spatial heterogeneity provides the basis for analyzing how crystallographic orientation, coating coverage, and coating pattern influence the resulting overgrowth dynamics.

4.2.1.2 Effect of crystallographic orientation

Quartz growth anisotropy implies that the crystallographic orientation of grains influences both facet stabilization and the effective

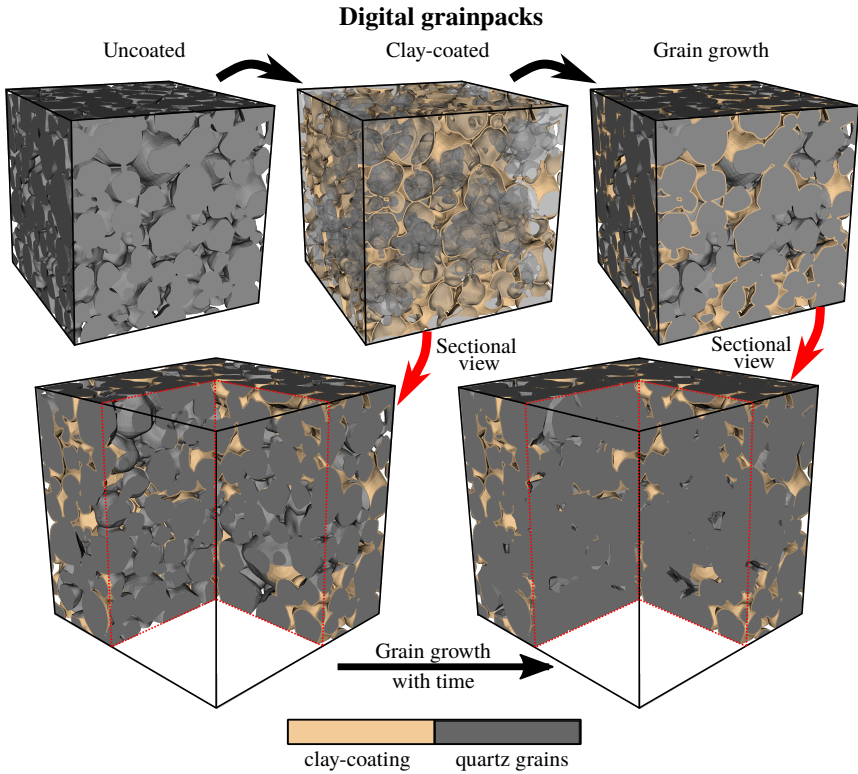


Figure 4.4: Representative evolution of quartz overgrowth in a coated-grain pack, illustrating spatially heterogeneous growth localized to exposed quartz surfaces and pore-throat narrowing through cement accumulation.

growth rate of cement in different directions [2, 20]. In coated systems, crystallographic orientation additionally interacts with coating placement, if exposed windows coincide with directions of faster growth, cement bridging and pore-throat occlusion may be accelerated, whereas less favorable orientations may delay bridging and preserve connectivity for longer. As reported by Kumar et al. [2], growth is slowest for vertically oriented crystal faces, while diagonal orientations may catch up at later stages as growth reorganizes around accessible surfaces (see figure 4.5).

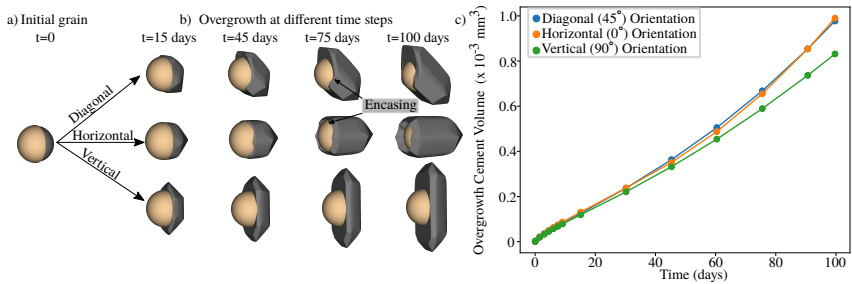


Figure 4.5: Effect of crystallographic orientation on quartz overgrowth morphology and growth evolution. Reproduced from figure 6 in [2].

4.2.1.3 Effect of coating coverage

Coating coverage fraction is expected to be the dominant control on cementation because it directly limits the reactive quartz–fluid interface area. Consistent with petrographic interpretations, increasing coating coverage suppresses the total cement volume and thereby promotes the preservation of porosity and permeability [2, 21–23].

At the pore scale, this effect is strongly nonlinear, once coating coverage becomes sufficiently high to inhibit cement bridging across critical pore throats, permeability loss is delayed markedly even if cement continues to accumulate locally on the remaining exposed surfaces [2, 19, 20]. This trend is illustrated in figure 4.6, which shows the temporal evolution of overgrowth cement volume for different coating coverages on a single coated quartz grain.

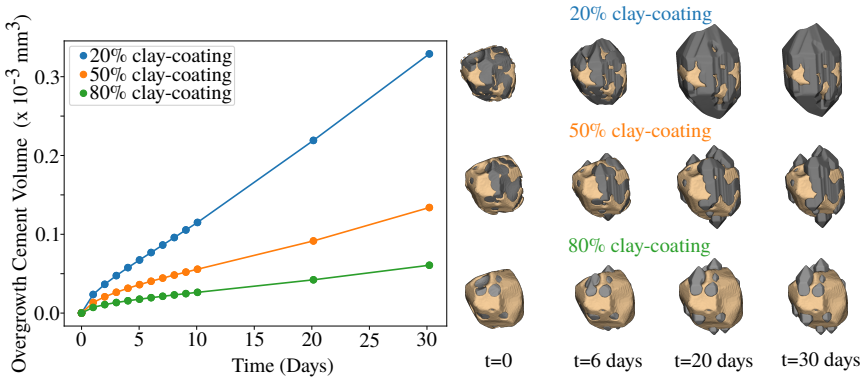


Figure 4.6: Effect of coating coverage fraction on a single arbitrarily shaped quartz grain, showing the temporal evolution of overgrowth cement volume for different coating coverages. Reproduced from figure 7 in [2].

4.2.1.4 Effect of coating pattern

Beyond the overall coating coverage, the spatial pattern of the coating controls whether cement can bypass coated regions and bridge pore throats. Discontinuous or patchy coatings may permit localized growth windows that act as preferential nucleation sites for bridging, whereas continuous layered coatings suppress growth over extended

regions and redirect cementation to a smaller number of exposed surfaces [2]. The simulations reported in [2] show that coating pattern therefore modulates the localization of overgrowth and the emergence of preferential pore-throat occlusion, thereby influencing permeability evolution beyond what would be predicted from coating coverage alone. This effect is illustrated in figure 4.7, which compares the temporal evolution of overgrowth for different coating morphologies at fixed coverage.

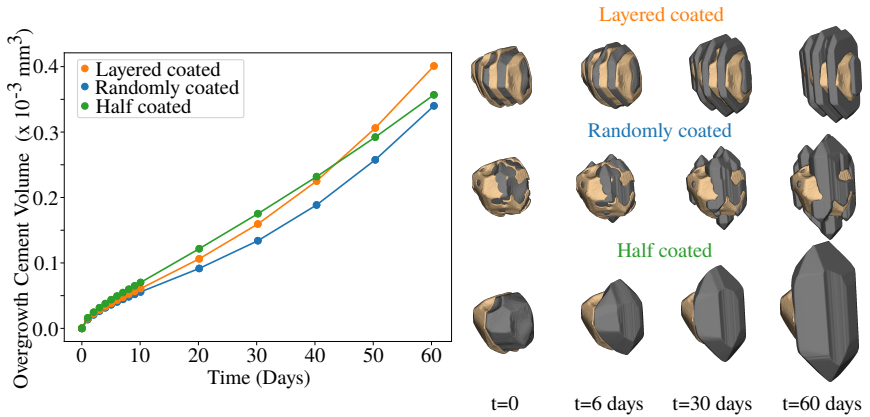


Figure 4.7: Influence of coating morphology (layered, random, and half-coated configurations) on a single quartz grain at a fixed coating coverage of 50%. Reproduced from figure 7 in [2].

4.2.2 Influence of coating on reservoir quality

To quantify the evolution of reservoir quality, porosity and permeability are evaluated at successive stages of cementation using the flow-characterization methodology introduced in chapter 2 [2, 19, 20]. Because permeability is highly sensitive to a limited number of

connected pore throats, coating-controlled suppression of cement bridging can preserve permeability disproportionately relative to porosity [19, 20].

A central quantitative result of Kumar et al. [2] is that increasing coating coverage correlates positively with retained porosity and permeability, while correlating negatively with the net overgrowth cement volume. This coupled trend is illustrated in figure 4.8, which summarizes the temporal evolution of permeability, porosity, and net cement volume for different coating coverages.

These results confirm that coating coverage is the primary determinant of reservoir-quality preservation, consistent with field-based interpretations of coated sandstones exhibiting reduced cement volumes and better retained porosity under burial conditions [2, 21–23]. The simulations further show that crystallographic orientation and coating pattern introduce a secondary modulation of permeability decline by controlling when and where cement bridges critical pore throats [2].

4.2.3 Comparison with geological samples

A key requirement for predictive pore-scale cementation modeling is that simulated cement volumes and coating–cement relationships fall within realistic geological ranges. Kumar et al. [2] compare simulation outputs with field-sample measurements of quartz cement content as a function of coating coverage, demonstrating that the model reproduces the observed correlation structure and yields physically plausible cement volumes. In addition, comparisons at different

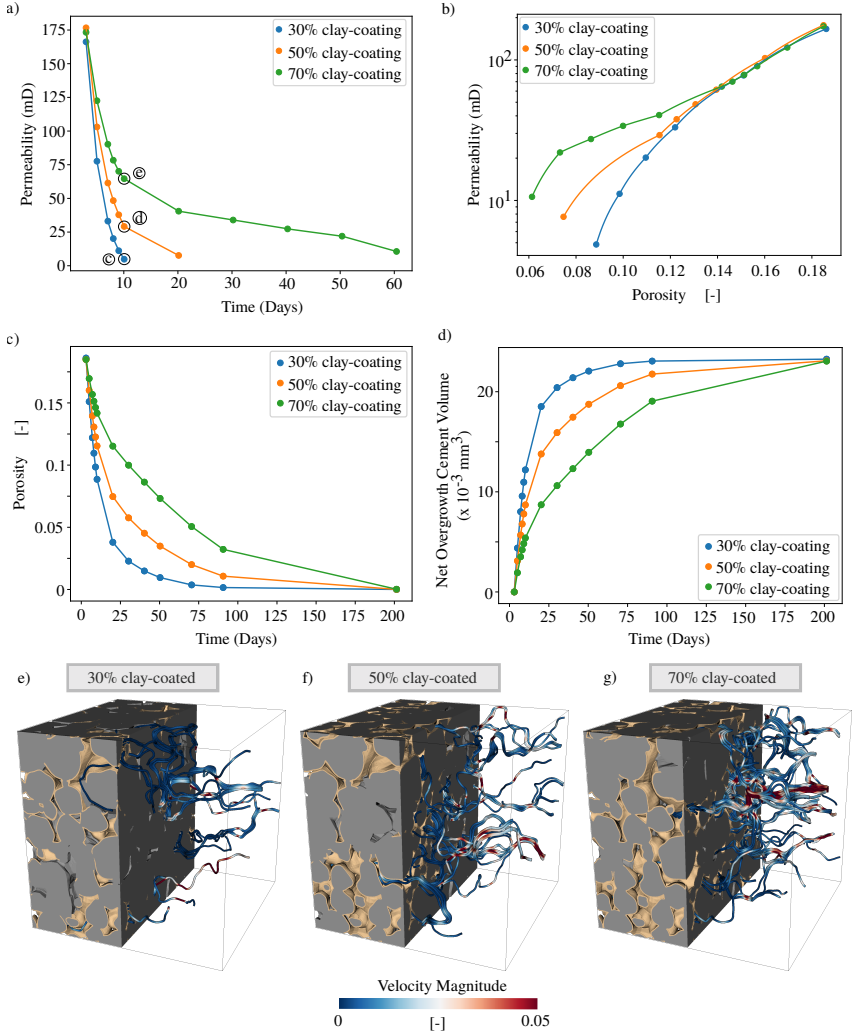


Figure 4.8: Temporal evolution of permeability, porosity, and net overgrowth cement volume in digital grain packs for different clay-coating coverages (30%, 50%, and 70%), illustrating the progressive reduction in porosity and permeability due to quartz cement overgrowth and the corresponding increase in cement volume. Reproduced from figure 10 in [2].

thermal exposures capture the expected increase in cementation with increasing diagenetic time and temperature. This comparison is summarized in figure 4.9.

The overall agreement supports the interpretation that clay coatings act as effective nucleation and growth inhibitors, and that coating attributes exert a mechanistic control on reservoir-quality evolution that can be captured within a microstructure-resolving simulation framework [2, 21–23].

4.3 Concluding remarks

This chapter investigated clay-mediated quartz cementation in sandstones using a multiphase-field framework that explicitly resolves evolving pore geometry and crystallographically controlled cement growth. Validation against experimental benchmarks and natural sandstone textures demonstrated that the model reproduces key microstructural signatures of syntaxial quartz overgrowth and coating-mediated growth inhibition [2, 18, 21, 22].

The results show that coating coverage exerts the dominant control on cement volume and reservoir-quality preservation, while coating pattern and crystallographic orientation modulate the spatial localization of cement and the timing of pore-throat bridging [2]. Pore-scale flow analysis further indicates that permeability loss is governed by connectivity disruption at a limited number of critical pore throats, which explains why coatings can preserve permeability disproportionately relative to porosity [19, 20]. Comparison with geological samples

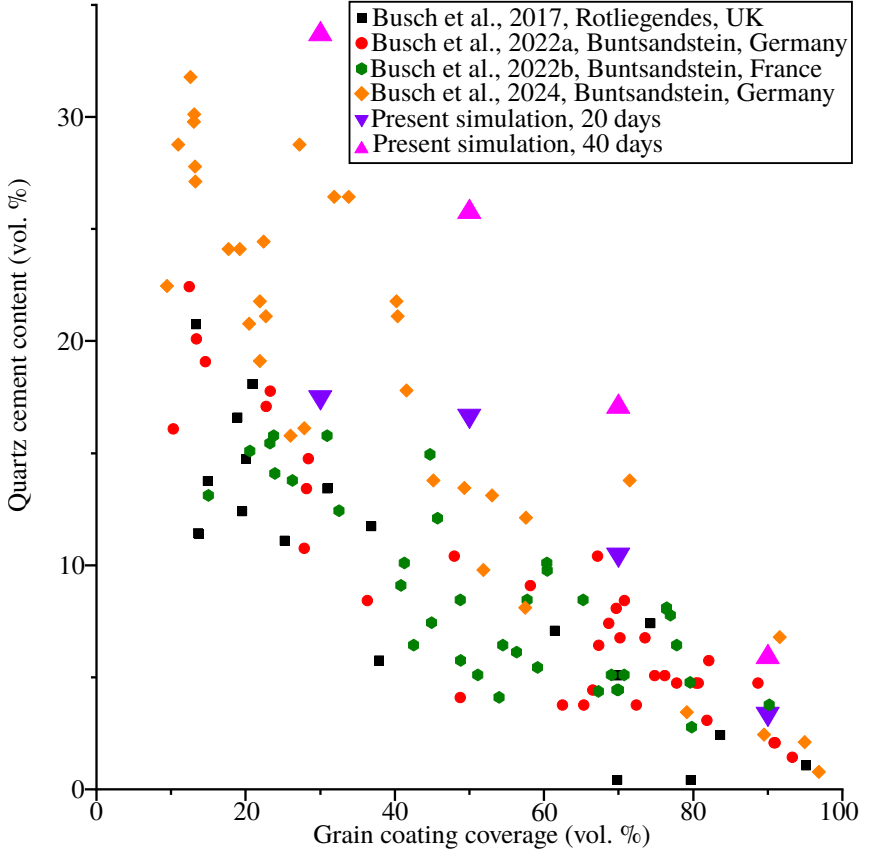


Figure 4.9: Correlation of quartz cement content with coating coverage for field samples and simulation results at different thermal exposures. Reproduced from figure 11 in [2].

shows that the simulated cement volumes and coating–cement relationships are consistent with field observations, thereby supporting the physical realism of the modeling approach [2, 23].

Together with Chapter 3, this chapter completes the pore-space evolution narrative of Part II: while etch-pit dissolution creates pore space and enhances connectivity through topology-modifying dissolution, clay-mediated quartz cementation reduces pore space through anisotropic precipitation and pore-throat bridging. The combined framework therefore provides a microstructure-informed basis for linking mineral-scale reaction mechanisms to the macroscopic evolution of transport properties in reactive porous media.

**Part III - Infrastructure
Integrity: When Corrosion
Morphology Becomes
Failure**

5 Pitting Corrosion in Geological Installations & Related Failure

This chapter is based primarily on the peer-reviewed publication by Kumar et al. [3], published in *Journal of Materials Research and Technology*. It investigates how corrosion-pit morphology in metallic systems evolves under reactive brine exposure and how that morphology subsequently governs pressure-induced crack initiation and failure. In geothermal and related subsurface installations, localized corrosion is a major integrity concern because metals are exposed to hot, saline, and chemically aggressive fluids that can promote severe pitting and associated degradation [7, 8, 24]. In particular, pitting corrosion generates sharp surface defects that may act as stress concentrators and accelerate mechanical failure through perforation or crack nucleation, making the interplay between corrosion morphology and stress especially important for infrastructure integrity [3, 9, 25]. In multiphase alloys, these effects are further influenced by phase arrangement, interfacial energy, and kinetic mismatch, all of which affect the localization, depth, and curvature of the evolving corrosion front [3].

To examine these coupled degradation mechanisms, the present chapter applies the corrosion and fracture formulations introduced in

chapter 2, particularly the grand-potential phase-field framework for corrosion, the diffuse-interface pressure boundary condition, and the phase-field crack model developed in sections 2.4.1–2.4.5. A central contribution of the chapter is the sequential corrosion-to-failure workflow, in which evolving pit morphologies are first generated in single-phase, dual-phase, and polycrystalline systems and then transferred to mechanical simulations to determine the critical pressure required for crack initiation [3]. On this basis, the chapter first validates both the corrosion model and the diffuse pressure-loading formulation, and then examines how pit morphology, microstructural configuration, and interfacial mobility collectively govern the transition from localized corrosion to mechanically critical failure.

5.1 Model validation

5.1.1 Validation of corrosion model

The corrosion model introduced in chapter 2, specifically in sections 2.4.1–2.4.3, is validated using pseudo-1D and 2D benchmark configurations following the validation framework presented in Kumar et al. [3]. Unless stated otherwise, all validation cases employ the baseline parameter set listed in table 5.1.

5.1.1.1 Pseudo-1D benchmark (pencil electrode analogue)

The pseudo-1D configuration follows the benchmark setup introduced by Mai et al. [27] and subsequently adopted in the corrosion study underlying this chapter. A metal wire of diameter $d = 25 \mu\text{m}$

Table 5.1: Simulation parameter set for corrosion validation (reported in [3]).

Parameter	Symbol	Value	Nondim. value
Interfacial energy	γ	$1.0 \times 10^1 \text{ J m}^{-2}$	1
Diffusion coefficient	D	$8.5 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$	4.25×10^{-5}
Interface mobility coefficient	M	$2 \text{ m}^3 \text{ J}^{-1} \text{ s}^{-1}$	1
Curvature of free energy density	A	$5.35 \times 10^7 \text{ J mol}^{-1}$	5.35
Metal concentration	c_{metal}	$1.43 \times 10^2 \text{ mol L}^{-1}$	143
Saturation concentration	c_{sat}	5.1 mol L^{-1}	5.1
Interface thickness parameter	ϵ	$5 \mu\text{m}$	5

is embedded in epoxy, with only one circular face exposed to the electrolyte, while the lateral boundaries act as no-flux surfaces due to epoxy insulation (see figure 5.1a). The principal comparison metric is the pit depth as a function of $\sqrt{t}$, which serves to verify the diffusion-controlled scaling of pit growth and the agreement with the reference datasets used for validation. These include the analytical one-dimensional solution of Scheiner and Hellmich et al. [64] and the experimental datasets of Ernst and Newman et al. [65, 66], as compiled in Zhi et al. [67] (see figure 5.1c) [3].

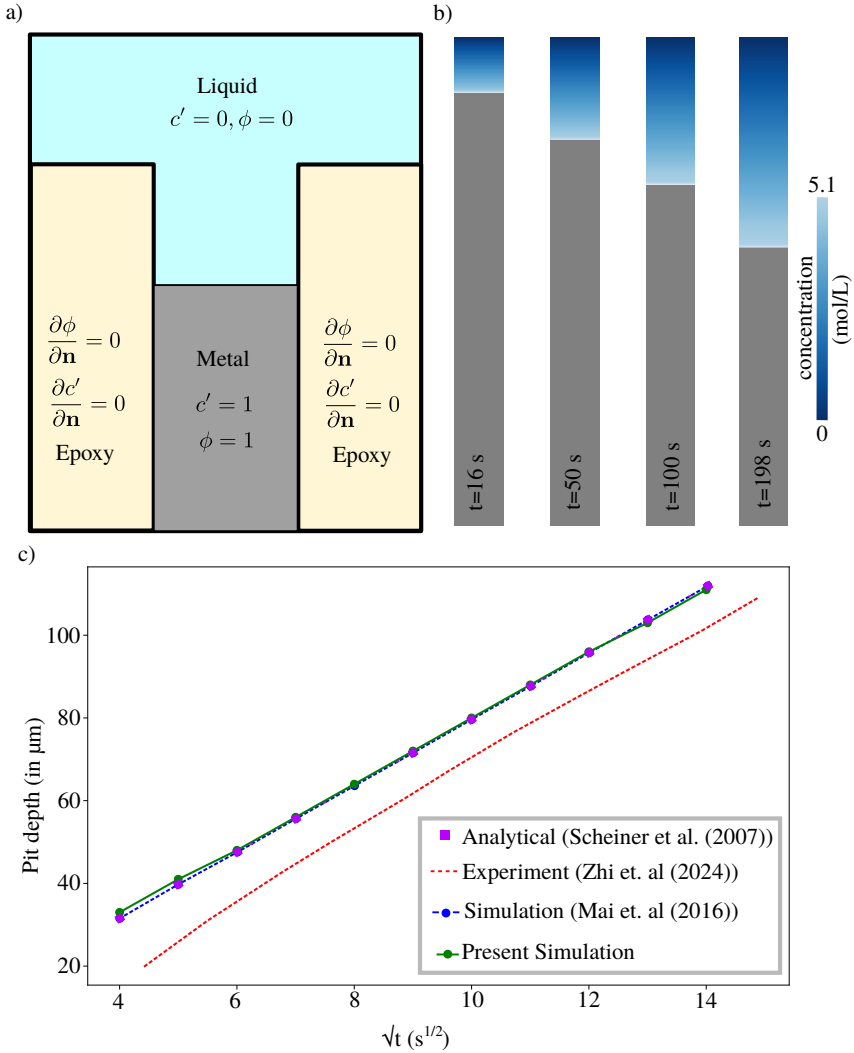


Figure 5.1: Validation of the 1D phase-field corrosion model. (a) Pseudo-1D simulation setup. (b) Concentration profiles at different time steps. (c) Pit depth versus $\sqrt{t}$ compared with experiments, the analytical 1D solution, published benchmark results, and the present study. Reproduced from figure 1 in [3].

5.1.1.2 2D benchmark

A two-dimensional pitting benchmark is further considered in accordance with the results reported by Zhi et al. [67]. The comparison includes pit morphologies and concentration fields at representative times, $t = \{20, 35, 50, 90\}$ s, and demonstrates that the evolution of pit depth with time follows the near-parabolic trend characteristic of diffusion-controlled pitting. The simulated results show close agreement with the benchmark data of Zhi et al. [67], thereby providing additional validation of the present corrosion model in two dimensions (see figure 5.2) [3].

5.1.1.3 Parameter anchoring for validation

Table 5.1 summarizes the dimensional and nondimensional parameter values adopted for the validation studies, as reported in [3]. These parameters are rooted in the established benchmark lineage, including the phase-field corrosion study of Mai et al. [27] and the parameter compilation employed by Zhi et al. [67]. They are used here as the default validation baseline and serve as the reference framework against which the later qualitative multiphase parameterization is interpreted.

5.1.2 Validation of diffuse-interface pressure boundary conditions

The diffuse-interface pressure boundary condition introduced in chapter 2, specifically in section 2.4.4, is validated against analytical

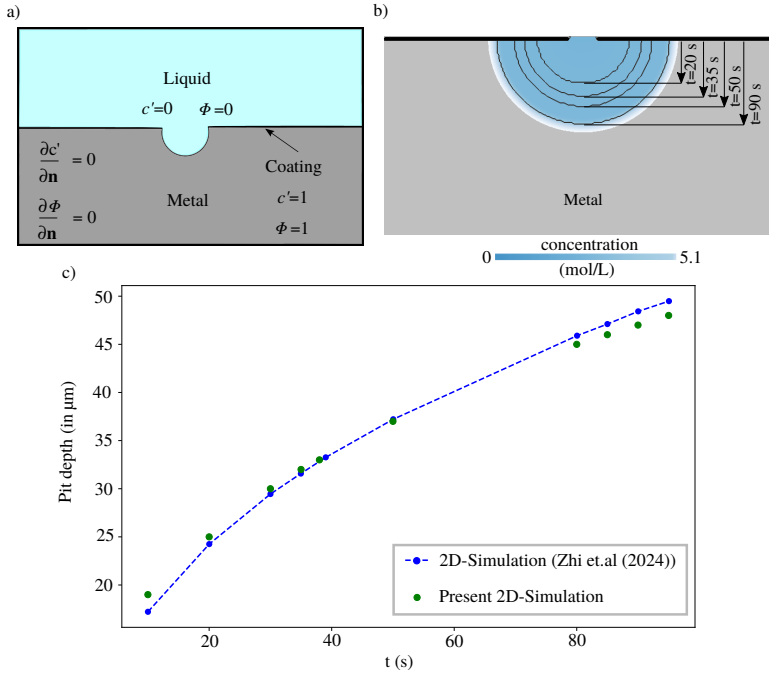


Figure 5.2: Validation of the 2D phase-field corrosion model. (a) 2D simulation setup. (b) Concentration profiles at different time steps. (c) Pit depth versus time compared with Zhi et al. [67] and the present study. Reproduced from figure 2 in [3].

elasticity solutions, following the framework presented in [3]. The purpose of this validation is to verify that pressure applied to a diffuse internal interface reproduces the correct mechanical response as the interface thickness is progressively reduced. This step is essential because the subsequent simulations apply hydrostatic pressure to evolving pit surfaces without explicit tracking of the solid–fluid interface.

5.1.2.1 Euler–Bernoulli bending beam benchmark

An Euler–Bernoulli bending beam subjected to pressure loading is simulated using both sharp-interface and diffuse-interface representations. Figure 5.3 shows the corresponding geometry and boundary conditions for the two setups. Figure 5.4 compares the normalized

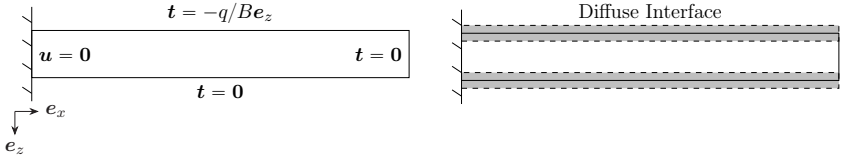


Figure 5.3: Euler–Bernoulli bending beam used for validation. Left: sharp-interface model with boundary conditions. Right: diffuse-interface model with diffusively applied stress boundary conditions. Reproduced from figure 3 in [3].

bending displacement ($\tilde{w}$) and normalized bending torque ($\tilde{M}$) obtained from simulations at multiple refinement levels, r , with the analytical solutions, including Richardson extrapolation. The results show systematic convergence with increasing refinement, confirming that the diffuse-interface formulation approaches the sharp-interface reference solution. In particular, the torque generally exhibits a smaller relative error than the displacement, which is attributed to the diffuse-interface overestimation of the geometrical moment of inertia. As discussed in [3], this discrepancy diminishes in the sharp-interface limit.

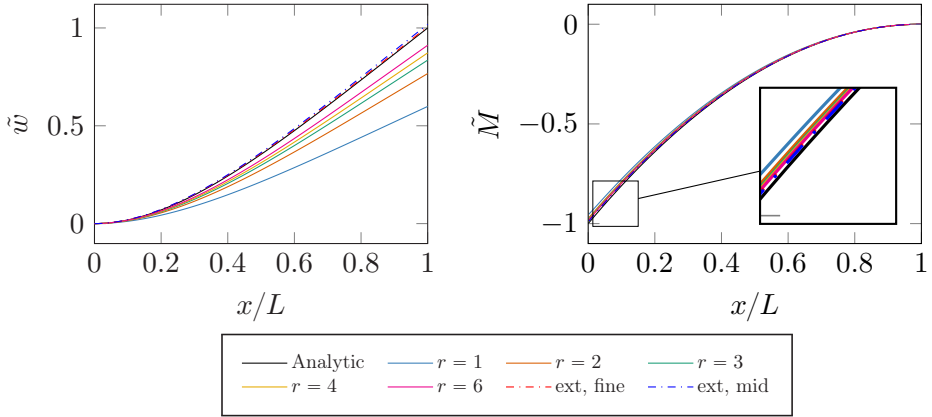


Figure 5.4: Comparison of the analytical and numerical results for the normalized bending displacement $\tilde{w}$ and torque $\tilde{M}$ at different refinement levels r . Dash-dotted lines show Richardson extrapolation based on $r = \{3, 4, 6\}$ (ext, fine) and $r = \{2, 3, 4\}$ (ext, mid). Reproduced from figure 4 in [3].

5.1.2.2 Spherical hydrostatic stress state benchmark

As an additional verification case, a solid sphere subjected to uniform external pressure is simulated with the load applied through the diffuse interface. For this configuration, the analytical solution corresponds to a homogeneous hydrostatic stress and strain state, thereby providing a direct benchmark for assessing the accuracy of the diffuse pressure implementation [3].

5.2 Findings and discussion

5.2.1 Pit morphology evolution in multiphase alloys

The evolution of pit morphology is examined for (i) two-phase Fe–Al layered systems with different phase orientations and (ii) a three-phase Fe–Al–Mn polycrystalline system. In the corrosion figures and parameter tables, Fe, Al, and Mn denote iron, aluminum, and manganese phases, respectively, while Brine denotes the electrolyte phase. The computational domain used for these corrosion-only morphology studies has dimensions of $400\Delta x \times 160\Delta y$, with $\Delta x = \Delta y = 1 \mu\text{m}$. Since the focus of this part of the analysis is on microstructure-controlled morphological evolution rather than on an absolute calibration of physical time, the diffusion coefficients are increased by six orders of magnitude in order to accelerate the simulations. Accordingly, the resulting trends are interpreted in a qualitative sense, with emphasis on the underlying morphology evolution rather than on exact temporal scales [3].

The non-dimensional parameter set used for these multiphase morphology studies is listed in table 5.2. In the initial part of the analysis presented in this section, the interfacial kinetics are kept identical for all metal–brine interfaces, while the interfacial energies are assigned according to table 5.2. As a result, pit evolution is governed primarily by differences in interfacial energy and by the underlying microstructural geometry, including phase arrangement, triple-junction angles, and phase connectivity [3].

Table 5.2: Non-dimensional parameter set for corrosion in the multiphase alloy system (reported in [3]).

Parameter	Symbol	Non-dim. value
Interfacial energy (Fe–Brine)	$\gamma_{\text{Fe–Brine}}$	1
Interfacial energy (Al–Brine)	$\gamma_{\text{Al–Brine}}$	0.8
Interfacial energy (Mn–Brine)	$\gamma_{\text{Mn–Brine}}$	0.6
Interfacial energy (Fe–Al)	$\gamma_{\text{Fe–Al}}$	0.28
Interfacial energy (Fe–Mn)	$\gamma_{\text{Fe–Mn}}$	0.32
Interfacial energy (Al–Mn)	$\gamma_{\text{Al–Mn}}$	0.32
Diffusion coefficient	D	10
Interface mobility coefficient	M	0.001
Curvature of free energy density	A	5.35
Metal concentration	c_{metal}	143
Saturation concentration	c_{sat}	5.1
Interface thickness parameter	ϵ	4

5.2.1.1 Morphological trends in multiphase pit evolution

The key morphology trends observed in figure 5.5 can be summarized as follows [3]:

- In the horizontally layered two-phase system, pit growth remains comparatively symmetric with respect to the vertical axis when corrosion is localized primarily within the Fe phase.
- In contrast, inclined and vertical phase arrangements break this symmetry and give rise to persistent high-curvature regions along the evolving pit front.
- In the three-phase polycrystalline system, the presence of an additional phase increases interfacial complexity and leads to more irregular pit morphologies. In addition, variations in interfacial energy among the distinct metal–brine interfaces become more pronounced in their effect, thereby exerting a stronger influence on the overall corrosion evolution.

5.2.2 Corrosion-driven failure via pressure-induced cracking

The simulations of pressure-induced cracking follow the sequential workflow described in chapter 2, specifically in sections 2.4.4–2.4.5. In this approach, the corrosion morphologies obtained from the preceding simulations are used as inputs for the mechanical analysis, in which hydrostatic pressure is applied at the diffuse metal–brine interface and increased incrementally until crack initiation and subsequent propagation are observed [3].

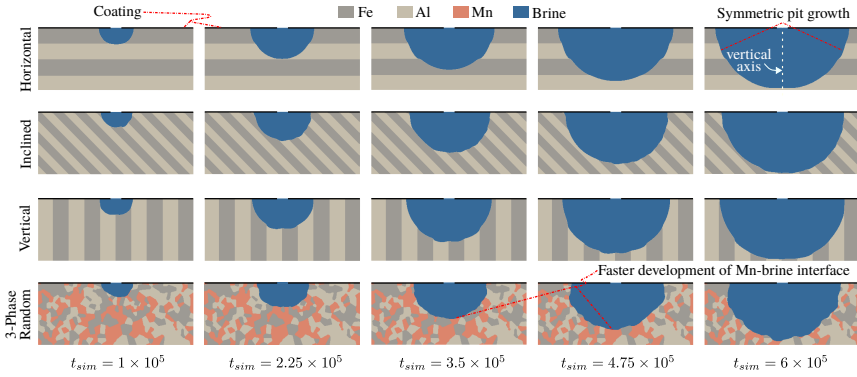


Figure 5.5: Evolution of pit morphology in two-phase and three-phase polycrystalline alloys. Inclined, vertical, and polycrystalline configurations show asymmetric pit growth due to phase arrangement, while the horizontal case remains symmetric. In the polycrystalline system, surface energy effects are strongest at the Mn–Brine interface compared to Fe–Brine and Al–Brine. Reproduced from figure 5 in [3].

The pressure values reported in this section are interpreted as comparative mesoscale indicators for the specified geometry, material parameters, pressure increment, and phase-field regularization length scale. They are used to compare the relative failure susceptibility of different corrosion morphologies and microstructural configurations. They should not be interpreted as direct design pressures for full-scale well casings, pipelines, or geothermal installations.

5.2.2.1 Mechanical domain and loading setup

All failure simulations presented in this section are performed on the same computational domain, with dimensions of $400 \mu\text{m} \times 180 \mu\text{m}$ and a uniform grid spacing of $\Delta x = \Delta y = 1 \mu\text{m}$. A thin brine layer is introduced above the metal phase to enable the uniform

application of pressure along the diffuse metal–brine interface. The applied pressure is then increased linearly in order to determine the critical value at which crack initiation occurs [3].

For simplicity, all material phases are assumed to possess identical elastic stiffness. Nevertheless, the underlying framework is sufficiently general to incorporate stiffness contrasts through mechanical jump conditions [68]. The boundary-condition schematic, the diffuse pressure distribution, and the applied pressure ramp are shown in figure 5.6, while the mechanical parameters used in the simulations, including E , ν , G_0 , Δp , and the damage tolerance, are listed in table 5.3 [3].

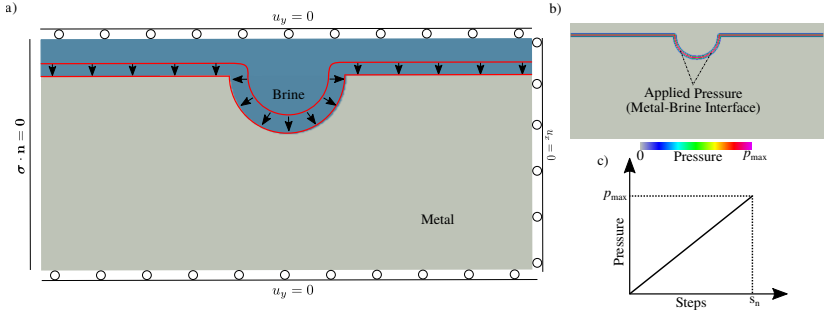


Figure 5.6: Boundary conditions for pressure-induced cracking during pit evolution. (a) Neumann condition on the left face and Dirichlet conditions elsewhere, with pressure applied normal to the brine–metal interface. (b) Pressure distribution across the diffuse interface. (c) Linearly ramped pressure with increment steps. Reproduced from figure 6 in [3].

Table 5.3: Material and simulation parameters for pressure-induced fracture simulations (reported in [3]).

Parameter	Symbol	Value	Unit
Young's modulus	E	210	GPa
Poisson's ratio	ν	0.3	–
Reference crack resistance	G_0	100	N mm ⁻¹
Mesh size	Δx	1	μm
Regularization length scale	ϵ_c	3	μm
Pressure increment	Δp	1	MPa
Kinetic mobility parameter	M_c	10 ⁻³	–
Residual stiffness factor	ϕ_{residual}	10 ⁻¹²	–
Steady-state tolerance	ϵ_{ϕ_c}	5 × 10 ⁻⁵	–
Damage tolerance	ϵ_{damage}	0.02	–

5.2.2.2 Single-phase metal–electrolyte system: Fe–Brine

For the single-phase Fe–Brine system, the normalized critical pressure,

$$\hat{p} = \frac{p_{\text{crit,current}}}{p_{\text{crit,max}}},$$

is evaluated as a function of the pressure-increment steps, with $p_{\text{crit,max}} = 2169$ MPa and $\Delta p = 1$ MPa [3]. Figure 5.7 shows representative early-stage crack growth at $p = 1499$ MPa and later-stage behavior at $p = 2169$ MPa, illustrating how the crack phase-field and the associated driving-force field localize around the pit-induced stress concentrator. The dependence on pit depth is summarized in figure 5.8, where the normalized critical pressure $\hat{p}$ decreases approximately linearly with increasing pit depth. A fitted slope of

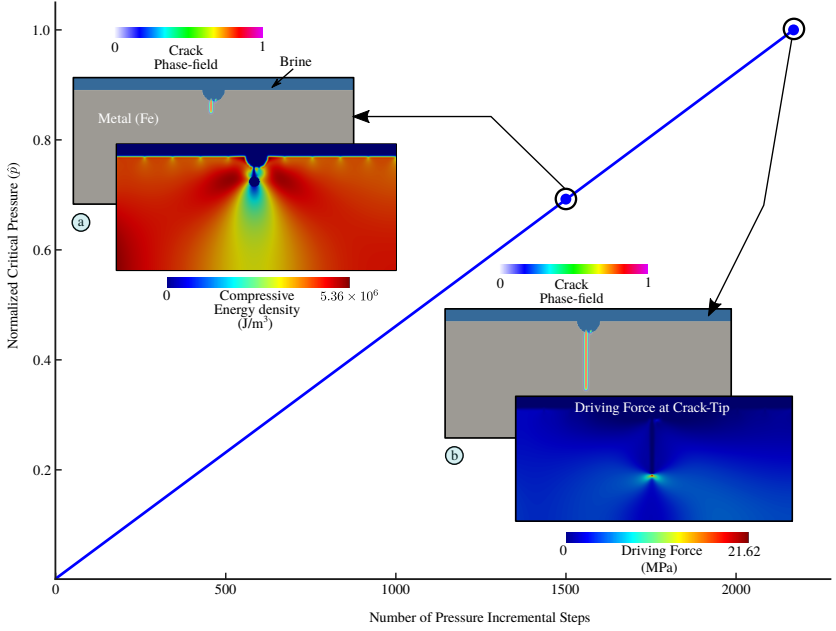


Figure 5.7: Normalized critical pressure, $\hat{p} = p_{\text{crit,current}}/p_{\text{crit,max}}$ ($p_{\text{crit,max}} = 2169$ MPa for Fe–Brine) as a function of pressure increments, $\Delta p = 1$ MPa. (a) Crack phase-field and compressive energy density at $p = 1499$ MPa (early stage). (b) Crack phase-field and driving force at $p = 2169$ MPa (later stage). Reproduced from figure 7 in [3].

$|m| = 0.005 \mu\text{m}^{-1}$ is reported in [3], indicating a clear mesoscale relationship between geometric corrosion severity, as measured by pit depth, and the pressure threshold required for failure in the single-phase reference case, where morphology remains comparatively smooth.

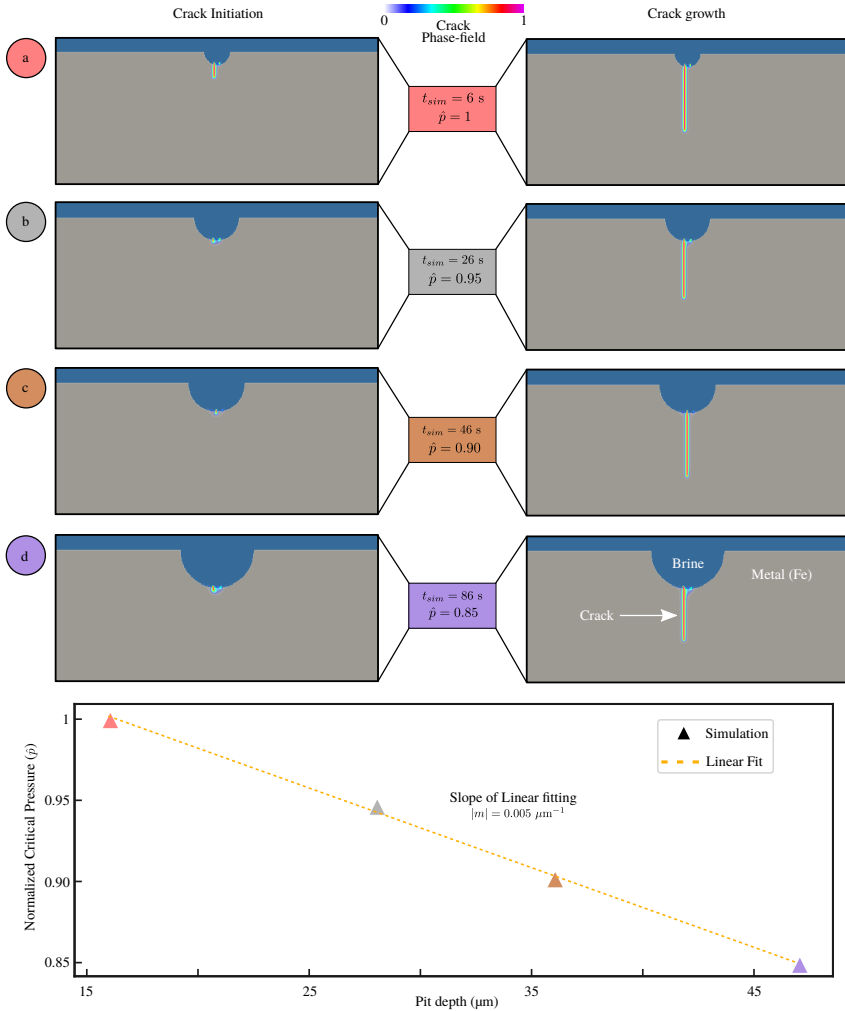


Figure 5.8: a–d) Simulated crack initiation (left) and growth (right) at representative stages of pit evolution in the Fe–Brine system. The plot shows normalized critical pressure versus pit depth (μm), with markers corresponding to stages a–d. The yellow dotted line denotes a linear fit with slope $|m| = 0.005 \mu\text{m}^{-1}$. Reproduced from figure 8 in [3].

5.2.2.3 Dual-phase alloy: Fe–Al in brine environment

Dual-phase Fe–Al systems are examined for horizontal, inclined, and vertical layering configurations. All simulations employ the same pressure-loading setup shown in figure 5.6 and the same mechanical parameter set listed in table 5.3.

In contrast to the single-phase case, where pit morphologies remain comparatively smooth and nearly spherical, the dual-phase systems develop more irregular pit geometries with pronounced high-curvature regions. These features arise from differences in the metal–brine interfacial energies of the constituent phases, which alter the evolving pit shape across phase boundaries, and they act as local stress concentrators that promote crack initiation at lower pressures [3].

An important observation is that the critical pressure varies across configurations during the early stages of pit evolution. In particular, the horizontal configuration exhibits greater resistance when pit growth remains localized within the Fe phase. This distinction, however, progressively diminishes as the pits deepen. At later stages, pit depth becomes the dominant controlling factor, such that the influence of the initial microstructural arrangement becomes secondary. As a result, the critical pressures associated with the different configurations converge once comparable pit depths are reached [3].

It is important to note that the “final” stage represented in the model corresponds to near-complete penetration of the metallic layer, which reduces the critical pressure to negligible values. This behavior should be interpreted as a qualitative trend within a thin representative

layer, rather than as a direct quantitative prediction for the full thickness of a pipe wall [3].

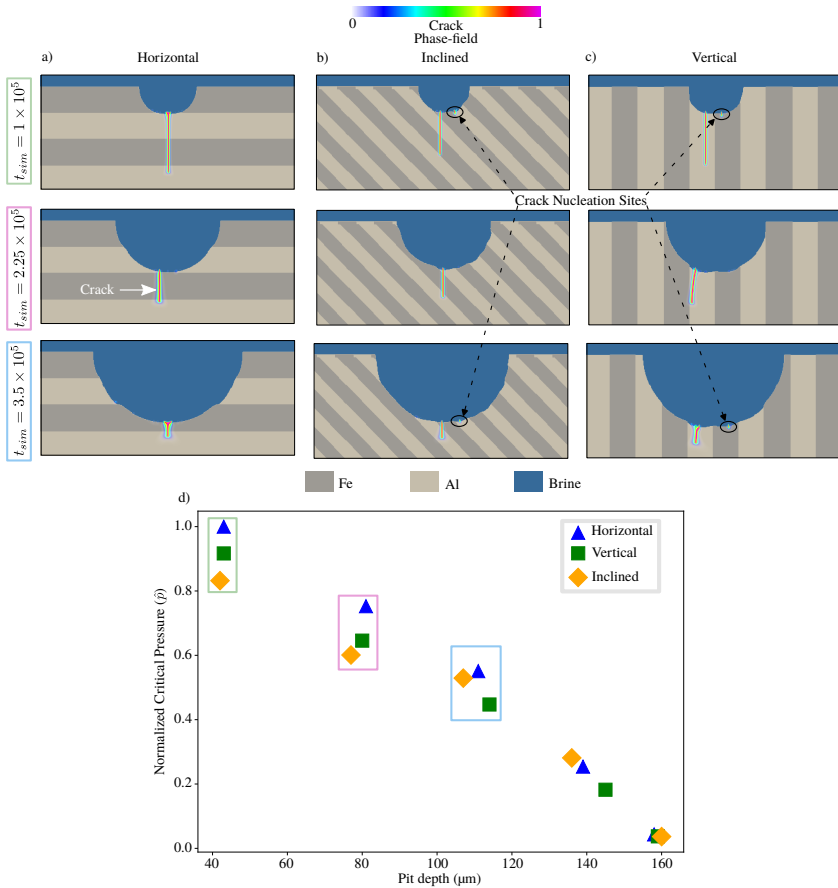


Figure 5.9: Pressure-induced cracking in a two-phase Fe–Al alloy for different phase orientations: (a) horizontal, (b) inclined, and (c) vertical, shown at three time steps. (d) Normalized critical pressure versus pit depth for each orientation. Reproduced from figure 9 in [3].

5.2.2.4 Polycrystalline alloy: Fe–Al–Mn in brine environment

In the three-phase polycrystalline system, the metallic phases are distributed irregularly, such that no continuous layered pathway extends through the domain and phase boundaries intersect at multiple orientations [3]. The interfacial energies used in these simulations follow the parameter set listed in table 5.2 [3].

The evolving corrosion front develops persistent morphological irregularities, characterized by high-curvature regions that act as recurring stress concentrators. Although multiple crack nucleation sites may arise during the evolution, crack propagation predominantly initiates and proceeds from the most critical location [3].

As shown in figure 5.10, the normalized critical pressure $\hat{p}$ decreases approximately linearly with increasing pit depth, with a fitted slope of $|m| = 0.008 \mu\text{m}^{-1}$. This indicates a stronger depth sensitivity than in the single-phase reference case and is consistent with the persistence of a rough, high-curvature corrosion front that continuously amplifies local stresses during evolution [3].

5.2.2.5 Effect of interfacial mobility ratio on failure response

To examine the effect of kinetic mismatch between phases, the interfacial mobility ratio ($\overline{M}_R$) is introduced,

$$\overline{M}_R := \frac{\overline{M}_{\text{ferrite}}}{\overline{M}_{\text{non-ferrite}}}$$

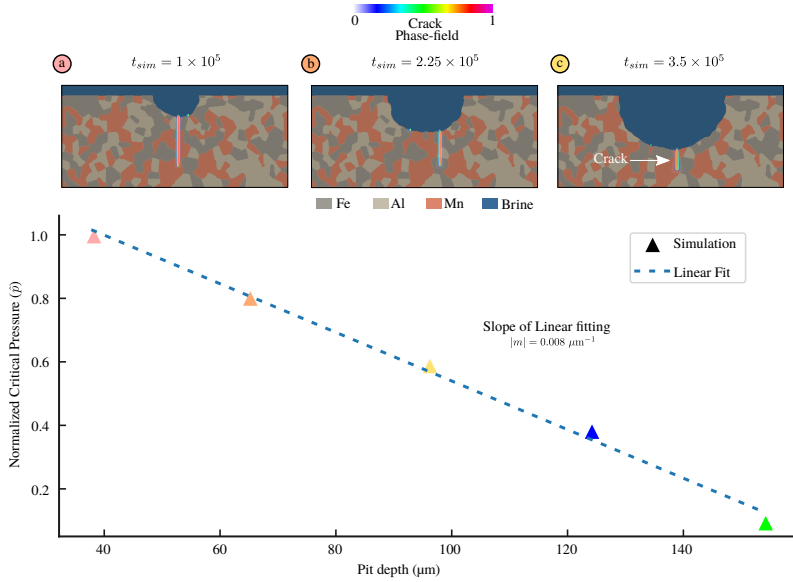


Figure 5.10: a-c) Simulated crack growth at representative stages of pit evolution in the polycrystalline system. (Bottom) Normalized critical pressure versus pit depth (μm) with slope $|m| = 0.008 \mu\text{m}^{-1}$. Reproduced from figure 10 in [3].

and is varied over $\overline{M}_R \in \{1, 2, 4, 8\}$, with the ferrite mobility held constant and the non-ferrite mobility progressively reduced. Increasing $\overline{M}_R$ therefore reduces the corrosion kinetics of the non-ferrite phase, in agreement with experimental observations in Fe–Mn–Al alloys, where ferrite exhibits preferential corrosion due to its lower passivation stability [3, 69].

Figure 5.11 compares four microstructural configurations, i.e., horizontal, vertical, and inclined two-phase arrangements, together with a polycrystalline three-phase system, at an intermediate stage,

$t_{\text{sim}} = 3.5 \times 10^5$. The figure further analyzes the pit depth, normalized critical pressure, and surface-to-volume ratio as functions of the interfacial mobility ratio, $\overline{M}_R$. The configuration-dependent trends can be interpreted mechanistically as follows [3]:

- **Horizontal layers:** Increasing $\overline{M}_R$ suppresses pit growth in the depth direction and promotes lateral widening within the ferrite phase, thereby increasing the surface-to-volume ratio. The normalized critical pressure exhibits a non-monotonic response: at moderate kinetic mismatch ($\overline{M}_R = 2$), the broader and flatter pits distribute stress more uniformly and therefore increase the critical pressure relative to the case $\overline{M}_R = 1$. At higher mobility ratios ($\overline{M}_R = 4, 8$), however, high-curvature regions re-emerge, which intensify local stress concentrations and reduce the critical pressure.
- **Vertical layers:** Corrosion becomes increasingly localized along the vertically aligned ferrite pathway as $\overline{M}_R$ increases, resulting in slightly deeper and narrower pits with limited lateral expansion. The associated increase in curvature near the pit base raises the surface-to-volume ratio and leads to a monotonic decrease in the critical pressure with increasing $\overline{M}_R$.
- **Inclined layers:** This configuration exhibits an intermediate response between the horizontal and vertical cases. With increasing $\overline{M}_R$, corrosion becomes more localized along the inclined ferrite layers, producing narrow groove-like features with pronounced high-curvature regions. Although the pit depth decreases markedly from $\overline{M}_R = 1$ to 2, the simultaneous increase

in curvature offsets the beneficial effect of shallower pits, resulting in comparable critical pressures for these two cases. At higher mobility ratios, the extent of the high-curvature regions increases further, leading to a reduction in critical pressure.

- **Polycrystalline:** Increasing $\overline{M}_R$ suppresses overall pit growth and reduces pit depth, while simultaneously promoting lobe-like pit morphologies and increasing the surface-to-volume ratio. The critical pressure therefore shows a non-monotonic dependence on $\overline{M}_R$: it decreases from $\overline{M}_R = 1$ to 2, despite the lower pit depth, because more pronounced high-curvature regions promote earlier crack initiation. For $\overline{M}_R = 4$ and 8, the lobes become smoother and the pit depth is reduced further, leading to an increase in the critical pressure relative to the $\overline{M}_R = 2$ case.

Figure 5.12 further examines the polycrystalline system by plotting the normalized critical pressure ($\hat{p}$) as a function of pit depth for different values of the interfacial mobility ratio, $\overline{M}_R$. The results show that failure susceptibility cannot be interpreted solely in terms of pit depth. In addition to the progressive weakening associated with deeper pits, the evolving pit morphology exerts a decisive influence on crack initiation. In particular, the formation of high-curvature lobes and notch-like features introduces localized stress concentration sites that can outweigh the effect of reduced pit depth and thereby govern the critical pressure required for failure.

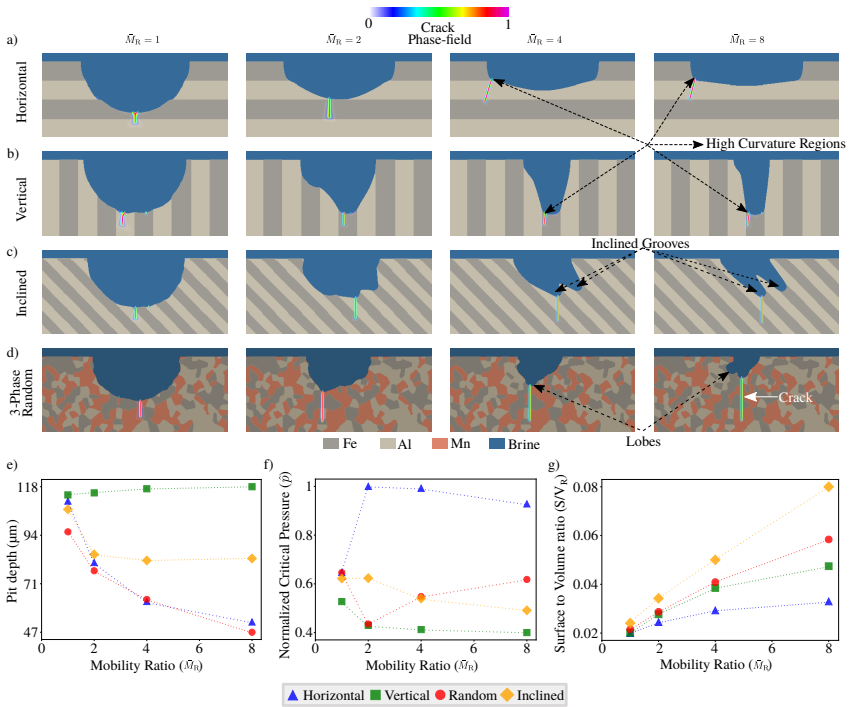


Figure 5.11: Pressure-induced cracking in (a) horizontal, (b) vertical, (c) inclined and (d) three-phase polycrystalline system with varying interface mobility ratio $\bar{M}_R$ for the ferrite-phase metal–brine interface relative to the other metallic phases ($\bar{M}_R = 1, 2, 4, 8$) at $t_{\text{sim}} = 3.5 \times 10^5$, showcasing crack growth. Graphs show (e) pit depth, (f) normalized critical pressure, and (g) surface-to-volume ratio vs mobility ratio for each configuration. Reproduced from figure 11 in [3].

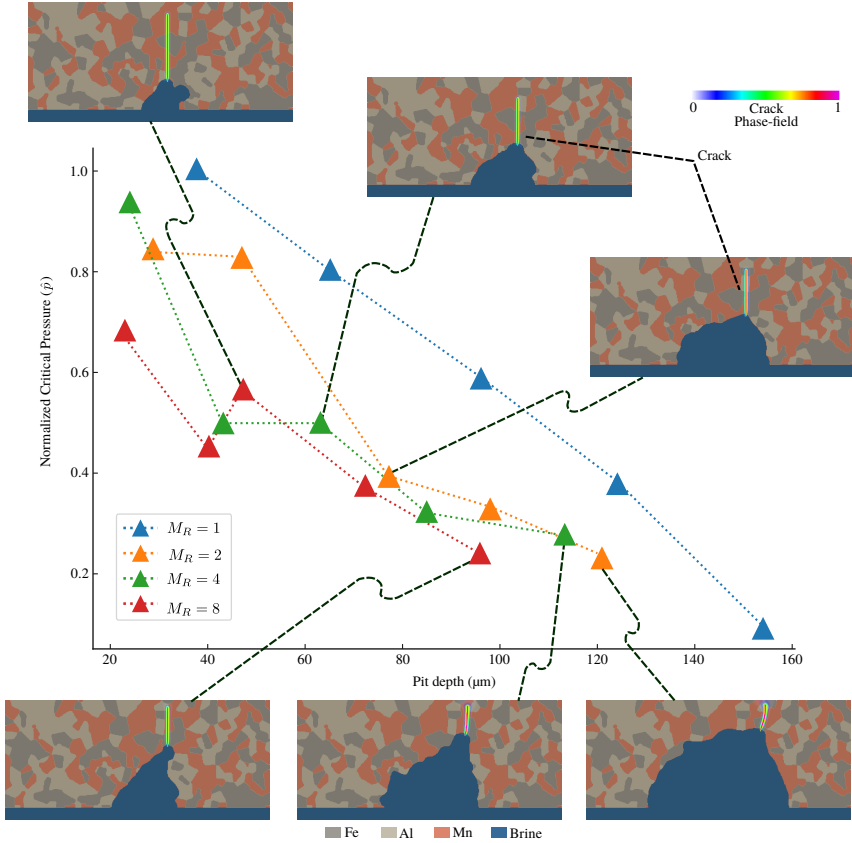


Figure 5.12: Normalized critical pressure ($\hat{p}$) as a function of pit depth (in μm) for mobility ratios $\bar{M}_R = 1, 2, 4, 8$. Upper panel: representative intermediate-stage crack evolution snapshots for $\bar{M}_R = 2, 4, 8$. Lower panel: corresponding later-stage crack propagation for the same mobility ratios. Pressure values normalized w.r.t. the critical pressure $p_{\text{crit}} = 1374 \text{ MPa}$. Reproduced from figure 12 in [3].

5.3 Concluding remarks

This chapter validated and applied the corrosion-to-failure framework introduced in chapter 2 to quantify how evolving pitting morphologies transition into pressure-induced cracking [3]. The pseudo-1D and 2D benchmark cases demonstrate that the corrosion model captures diffusion-controlled pit growth trends in good agreement with established reference solutions and the experimental datasets used for model benchmarking. In addition, the Euler–Bernoulli beam and spherical hydrostatic benchmark problems confirm that the diffuse-interface pressure boundary condition provides a convergent and robust approach for applying mechanical loads to evolving internal interfaces without the need for explicit geometry tracking.

Across all investigated microstructures, pit growth leads to a systematic reduction in the critical pressure required for crack initiation. At the same time, the results show that the failure threshold is not governed by pit depth alone, but is strongly influenced by pit morphology, particularly by the persistence of high-curvature surface features that act as stress concentrators [3]. This effect is most pronounced in heterogeneous and polycrystalline systems and becomes strongly configuration-dependent when kinetic mismatch between phases is introduced. The mobility-ratio analysis further demonstrates that, although kinetic mismatch may suppress pit deepening, it can simultaneously promote the formation of lobes and notch-like features that lower the critical pressure, thereby producing non-monotonic failure behavior.

From the perspective of infrastructure integrity, these findings highlight the need for risk metrics that incorporate both pit depth and morphological descriptors, such as curvature-based measures or surface-to-volume ratio, rather than relying on pit depth alone. This is particularly important for multiphase alloys operating in corrosive brine environments, where microstructural heterogeneity can significantly amplify morphology-driven failure mechanisms. The critical pressures reported here should therefore be interpreted primarily as comparative, mechanistic indicators of microstructural failure rather than as direct design values for full-scale well casings or pipelines, while the identified trends provide a basis for future upscaling toward component-level integrity assessment.

6 Conclusion

This thesis investigated interface-controlled processes in geological subsurface systems and related installations using phase-field methodology. The central objective was to understand how microscale interface evolution governs macroscopic consequences such as pore-space creation, pore-space closure, permeability evolution, and mechanically critical degradation. Although the three application areas considered in this thesis differ in material system and physical context, namely K-feldspar dissolution, clay-mediated quartz cementation, and pitting corrosion with pressure-induced cracking, they share a common mechanistic foundation: evolving interfaces, controlled by thermodynamics, kinetics, anisotropy, microstructure, and transport or mechanical fields, determine the emergent system response.

A unified methodological framework was developed and applied across these three problems. The phase-field approach provided a natural basis for resolving evolving solid–fluid interfaces without explicit front tracking. This was essential for capturing topological changes such as etch-pit coalescence, pore-throat occlusion, corrosion-pit growth, and crack initiation from irregular pit morphologies. The methodology combined thermodynamically consistent multiphase-field formulations, anisotropic interfacial-energy and mobility descriptions, pore-scale flow characterization, grand-potential-based corrosion modeling,

diffuse-interface pressure loading, and phase-field fracture. Together, these ingredients enabled microstructure-resolving simulations in which interface morphology emerged from the governing physics rather than being imposed geometrically.

In Chapter 3, the framework was applied to crystallographically controlled K-feldspar dissolution. The model reproduced experimentally observed etch-pit characteristics on the K-feldspar surface, including faceted pit geometries, inclination angles, and anisotropic retreat kinetics. This demonstrated that the combined capillary and kinetic anisotropy formulation is capable of representing the essential physics of etch-pit formation. The simulations further showed that dissolution does not proceed as uniform grain shrinkage. Instead, localized etch-pits nucleate, expand laterally, interact, and coalesce into elongated intragranular channels. This morphology-driven evolution modifies grain topology and creates new hydraulic pathways before substantial bulk mineral loss occurs.

The sandstone-scale simulations in Chapter 3 established a direct link between grain-scale dissolution morphology and permeability evolution. Through the grain-wise local refinement and re-embedding workflow, high-resolution etch-pit dissolution within individual K-feldspar grains could be transferred into larger digital sandstone geometries without globally refining the entire computational domain. The resulting pore-scale flow analysis showed that permeability enhancement is controlled primarily by connectivity transitions rather than by porosity increase alone. Feldspar volume fraction and crystallographic orientation were shown to influence the timing and strength of these transitions. Favorably oriented grains promoted earlier channel integration and stronger permeability enhancement,

whereas less favorable orientations delayed connectivity development. These results demonstrate that anisotropic etch-pit growth acts as a topology-modifying mechanism in reactive porous media.

In Chapter 4, the thesis addressed the complementary process of pore-space reduction through quartz cementation. A multiphase-field model for syntaxial quartz overgrowth was extended to account for clay-coated quartz grains. The introduced digital coating-generation workflow enabled controlled variation of coating thickness, coverage, and spatial pattern on quartz grains and grain packs. This made it possible to isolate the influence of coating attributes in a way that is difficult to achieve in natural samples, where coating coverage, mineralogy, continuity, and grain orientation are often coupled.

The cementation simulations showed that clay coatings strongly influence both the amount and spatial localization of quartz overgrowth. Coating coverage was identified as the dominant control on cement volume and reservoir-quality preservation because it directly limits the reactive quartz–fluid surface area. Increasing coating coverage reduced net cement volume and helped preserve porosity and permeability. However, the simulations also demonstrated that coverage alone is not sufficient to predict reservoir-quality evolution. Coating pattern and crystallographic orientation introduce secondary but important controls by determining where cement can nucleate, how growth localizes, and when pore-throat bridging occurs. Since permeability is governed by a limited number of connected pathways, local suppression or redirection of cement growth can preserve permeability disproportionately relative to porosity. The comparison with natural sandstone samples and field-based coating–cement trends supported the physical realism of the approach.

Together, Chapters 3 and 4 provide a coherent pore-space evolution narrative for reactive porous media. K-feldspar dissolution creates pore space through anisotropic, topology-modifying etch-pit growth, whereas clay-mediated quartz cementation reduces pore space through anisotropic precipitation and pore-throat bridging. The two processes act in opposite directions, but both demonstrate that pore-scale morphology and connectivity are more informative than bulk mineral volume change alone. This highlights the importance of morphology-resolving simulations for understanding reservoir-quality evolution in diagenetic systems.

In Chapter 5, the phase-field framework was extended from geological porous media to metallic subsurface installations. A grand-potential phase-field model was used to simulate pitting corrosion in single-phase, dual-phase, and polycrystalline alloy systems. The corrosion model was first validated against pseudo-one-dimensional and two-dimensional benchmark configurations, showing agreement with established pit-growth trends. A diffuse-interface pressure boundary condition was then validated against analytical elasticity solutions, demonstrating that pressure can be applied to evolving internal interfaces without explicit interface tracking. This was a key methodological step because it enabled mechanical loading of complex corrosion-pit morphologies generated by the phase-field corrosion model.

The corrosion-to-failure simulations demonstrated that pit depth systematically reduces the critical pressure required for crack initiation. However, the results also showed that pit depth alone is not sufficient to characterize failure susceptibility. Pit curvature, asymmetry, phase

arrangement, interfacial energy contrast, and interfacial mobility mismatch all influence the local stress concentration and therefore the pressure threshold for crack initiation. In multiphase and polycrystalline systems, corrosion fronts developed irregular morphologies with persistent high-curvature regions. These features acted as stress concentrators and could lower the critical pressure even when pit depth was not maximal. The mobility-ratio analysis further showed that kinetic mismatch between phases can produce non-monotonic failure behavior: suppressing pit deepening may still increase failure susceptibility if it promotes lobe-like or notch-like pit shapes.

The results of Chapter 5 therefore demonstrate that corrosion-induced failure should be interpreted through morphology-aware descriptors rather than through pit depth alone. Surface-to-volume ratio, curvature-based measures, pit asymmetry, and microstructural phase arrangement provide additional mechanistic information about failure risk. The reported critical pressures should be understood as comparative microstructural failure indicators rather than direct component-scale design values. Nevertheless, the identified trends provide a mechanistic basis for future upscaling toward integrity assessment of full-scale well casings, pipelines, and geothermal installations.

Across all three application areas, the thesis establishes several overarching conclusions. First, interface morphology is a controlling variable in subsurface processes. Whether the interface represents a dissolving mineral surface, a growing cement front, or a corroding metal–electrolyte boundary, the shape and connectivity of the evolving interface determine the macroscopic response. Second, anisotropy

is essential for capturing realistic microstructure evolution. Crystallographically controlled etch-pits and faceted quartz overgrowth cannot be represented adequately by isotropic surface-recession or growth models. Third, microstructural heterogeneity modifies interface evolution in a nonlinear way. Mineral distribution, coating coverage, phase arrangement, and grain orientation all influence where reactions localize and how morphology develops. Fourth, transport and mechanical consequences are strongly topology-dependent. Permeability enhancement, permeability loss, and crack initiation are governed by connectivity transitions and stress localization rather than by volume change alone.

The main scientific contribution of this thesis is therefore the development and application of a microstructure-resolving phase-field modeling strategy that links local interface physics to macroscopic functional properties. For reactive porous media, this link is expressed through porosity–permeability evolution. For metallic installations, it is expressed through the transition from localized corrosion morphology to pressure-induced cracking. The thesis does not attempt to provide universal reservoir-scale or component-scale predictions directly. Instead, it resolves the mechanisms that must be understood before such predictions can be made reliably. In this sense, the thesis provides a mechanistic bridge between experimental observations, digital microstructure analysis, and future upscaled models.

Overall, the thesis demonstrates that phase-field methodology is a versatile and physically consistent approach for studying interface-driven processes in geological subsurface systems and installations. By capturing dissolution, precipitation, corrosion, and fracture within a common modeling philosophy, the work contributes to a more

unified understanding of how microscale interfacial transformations control reservoir quality and infrastructure integrity. This provides a foundation for future developments in reactive-transport coupling, multiscale upscaling, uncertainty quantification, and predictive assessment of subsurface materials under chemically and mechanically demanding conditions.

7 Outlook

This thesis demonstrates that phase-field methodology provides a flexible and physically consistent framework for studying interface-controlled processes in geological subsurface systems and related installations. The models developed in this thesis resolve key mechanisms of pore-space creation, pore-space closure, and corrosion-induced failure at the pore or microstructure scale. At the same time, several extensions are required before such simulations can be used directly for predictive reservoir-scale or component-scale assessment. Future developments should therefore focus on increasing the physical completeness of the models, improving the treatment of coupled transport and mechanical effects, and establishing systematic pathways for upscaling.

A first important direction concerns reactive-transport coupling in mineral dissolution and cementation. In the K-feldspar dissolution model developed in chapter 3, dissolution is driven by a prescribed chemical driving force representing a sustained undersaturated fluid environment. This assumption is appropriate for isolating the role of crystallographic anisotropy and etch-pit morphology. However, natural feldspar dissolution is influenced by evolving fluid composition, local saturation state, pH, ion activity, and transport limitations [70–73]. A natural extension would therefore be to couple the anisotropic

phase-field formulation to explicit solute transport and local reaction kinetics, such that the chemical driving force evolves dynamically with the local fluid composition. This would make it possible to investigate feedbacks between etch-pit geometry, reactive surface area, concentration boundary layers, and evolving permeability.

A similar extension is relevant for clay-mediated quartz cementation. In chapter 4, quartz overgrowth is represented under prescribed supersaturation, enabling controlled investigation of coating coverage, coating pattern, and crystallographic orientation. In natural diagenetic systems, however, quartz cementation depends on silica supply, temperature history, pressure solution, fluid flow, and the evolving saturation state of the pore fluid [18, 74, 75]. Future work should therefore incorporate explicit silica transport and supersaturation-dependent growth laws. This would allow clay coatings to be studied not only as geometrical barriers to quartz overgrowth, but also as local modifiers of transport, attachment kinetics, and silica availability within connected pore networks.

The treatment of clay coatings can also be refined. In this thesis, the coating phase is treated as inert and non-growing, which captures the essential masking effect of coatings on quartz overgrowth. Natural coatings, however, may consist of chlorite, illite, smectite, kaolinite, or mixed-layer clays, each with different morphology, stability, surface chemistry, and influence on quartz cementation [17, 21–23]. Future models should therefore distinguish between clay mineral types and include mineral-specific properties such as coating permeability, surface reactivity, attachment kinetics, and possible coating transformation during burial. A further step would be to model coating formation dynamically instead of prescribing the coating

geometry as an initial condition. This would improve the connection between pore-scale simulation and petrographic observations of natural sandstone samples.

A particularly promising extension of the present framework lies in the direction of carbon capture, utilization, and storage (CCUS). During CO₂ injection into saline porous media, dry or under-saturated CO₂ can evaporate water from the brine phase, increase local salt concentration, and eventually induce salt crystallization. Such precipitation can obstruct pore throats, alter flow pathways, and reduce injectivity, making it a critical pore-scale process for geological CO₂ storage [76–78]. The methodology developed in this thesis provides a natural foundation for this problem because it already resolves evolving interfaces, pore-space morphology, and transport-property changes. Future work can therefore extend the reactive porous media framework toward sequentially coupled CO₂–brine flow, evaporation, solute transport, supersaturation-driven halite nucleation, and crystal growth. In such a workflow, microfluidic observations can guide pore-scale simulations of CO₂ invasion, brine-film retention, concentration buildup, and salt precipitation. The resulting halite phase could then be reintroduced into the pore geometry as an immobile solid phase to quantify changes in porosity, permeability, and injectivity. Beyond such reactive-flow extensions, future subsurface storage models should increasingly account for thermo-hydro-mechanical-chemical-biological (THMCB) coupling. This is particularly relevant for geological CO₂ and H₂ storage, where temperature and pressure changes, multiphase flow, mineral reactions, deformation, and microbial activity may jointly influence injectivity, storage security, and long-term energy utilization. Extending pore-scale and phase-field-based workflows

toward THMCB-informed multiscale models would therefore support more realistic assessment of subsurface energy-storage systems.

For corrosion-induced failure, this thesis uses a sequential strategy in which corrosion morphologies are first generated and selected pit geometries are subsequently transferred to a mechanical model for pressure-induced crack analysis. This approach is computationally efficient and well suited for identifying how pit morphology controls critical pressure. However, in real materials, corrosion and mechanical damage may evolve simultaneously. Stress can influence dissolution rates, crack opening can expose fresh reactive surfaces, and local chemistry inside pits or cracks may evolve as damage progresses [26, 28, 43]. A future extension should therefore move toward a more tightly coupled corrosion–fracture formulation in which corrosion, stress redistribution, crack initiation, and crack propagation interact continuously. This would be particularly relevant for stress corrosion cracking, hydrogen-assisted degradation, and corrosion fatigue, where mechanical loading and electrochemical reactions are not separable in time.

Another important step is the inclusion of more realistic mechanical heterogeneity in multiphase alloys. In chapter 5, the metallic phases are assigned identical elastic properties so that the influence of corrosion morphology can be isolated. Future simulations should incorporate phase-dependent elastic stiffness, plasticity, fracture toughness, and mechanical jump conditions at phase boundaries [62, 79]. This would allow the model to distinguish between failure controlled primarily by corrosion-pit morphology and failure influenced by mechanical contrast between phases, precipitates, inclusions, or grain

boundaries. In addition, cyclic pressure loading should be considered, since geothermal and subsurface installations often experience operational pressure fluctuations. Coupling corrosion morphology to fatigue-sensitive phase-field fracture would provide a more realistic basis for assessing long-term damage accumulation.

The simulations presented in this thesis are intentionally pore-scale or microstructure-scale. This resolution is necessary to capture etch-pit coalescence, pore-throat bridging, corrosion-pit curvature, and crack initiation. However, reservoir and installation assessments require predictions at much larger scales. Future work should therefore establish systematic upscaling strategies that translate phase-field-resolved morphology into continuum-scale descriptors. For reactive porous media, this includes porosity, permeability, tortuosity, reactive surface area, pore-throat statistics, and connectivity measures [6, 80–82]. For corrosion-induced failure, it includes morphology-aware descriptors such as pit curvature, surface-to-volume ratio, notch sharpness, pit asymmetry, and phase-interface topology. The results of this thesis show that such descriptors are often more informative than volume change or pit depth alone.

Finally, future work should address parameter uncertainty and computational cost. The models developed here involve parameters such as interfacial energies, kinetic mobilities, diffusion coefficients, coating properties, corrosion mobilities, and fracture toughness, many of which are difficult to determine uniquely. Sensitivity analysis and uncertainty quantification would help identify which parameters most strongly control permeability evolution or critical pressure. At the same time, high-resolution phase-field simulations remain computationally demanding, especially in three dimensions and for coupled

corrosion–fracture or CCUS crystallization problems. Reduced-order models, surrogate models, and machine-learning-assisted workflows could therefore support faster parameter exploration and multiscale prediction. Such approaches should complement, rather than replace, physics-based modeling by using simulation data to identify dominant mechanisms and accelerate repeated evaluations.

Overall, the future development of this work should move from mechanism-resolving simulations toward predictive multiscale workflows. For mineral reactions, this means coupling phase-field models with reactive transport and geological time-temperature histories. For cementation, it means incorporating mineral-specific coating behavior and dynamic coating evolution. For CCUS, it means extending the framework to CO_2 –brine flow, evaporation-induced concentration buildup, and salt crystallization with direct quantification of injectivity impairment. For corrosion-induced failure, it means coupling corrosion, fracture, fatigue, and mechanical heterogeneity under realistic loading histories. Across all these directions, the central message remains the same: macroscopic subsurface behavior cannot be understood from volume change alone. It depends critically on how interfaces move, how morphology evolves, and how local topology controls transport or stress concentration. Phase-field methodology provides a powerful route to resolve these mechanisms explicitly and to build predictive tools for reservoir-quality assessment, CCUS operations, and infrastructure integrity in chemically and mechanically demanding subsurface environments.

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List of own publications

Peer-reviewed journal publications

[1] **Kumar, A.**, Prajapati, N., Späth, M., Busch, B., Schneider, D., Hilgers, C., & Nestler, B. (2023). Qualitative Dissolution Modeling of Etch-Pit Formation on the K-Feldspar Surface Through Phase-Field Approach. *Journal of Geophysical Research: Solid Earth*, 128(4), e2022JB025749. <https://doi.org/10.1029/2022JB025749>

[2] **Kumar, A.**, Späth, M., Prajapati, N., Busch, B., Schneider, D., Hilgers, C., & Nestler, B. (2025). Impact of clay coating on sandstone reservoir quality: A multiphase-field investigation by numerical simulation. *Petroleum Exploration and Development*, 52(3), 715–730. [https://doi.org/10.1016/S1876-3804\(25\)60598-2](https://doi.org/10.1016/S1876-3804(25)60598-2)

[3] **Kumar, A.**, Prajapati, N., Reder, M., Jeela, R. K., Schneider, D., & Nestler, B. (2026). A grand-potential phase-field approach for modeling pitting corrosion and pressure-driven cracking in multiphase alloys. *Journal of Materials Research and Technology*, 42, 8726–8747. <https://doi.org/10.1016/j.jmrt.2026.05.130>

[4] Chakraborty, R., Späth, M., **Kumar, A.**, Busch, B., Nestler, B., Mantani, M. A., & Hilgers, C. (2025). Petrophysical Characterization of Metamorphic Rocks using X-ray micro-CT data—Implications for fluid flow. *Journal of Structural Geology*, 191, 105338. <https://doi.org/10.1016/j.jsg.2025.105338>

Conference, workshop, and seminar contributions

[5] **Kumar, A.**, Prajapati, N., Weichel, M., Reder, M., Schneider, D., Cheng, C., Hilgers, C., & Nestler, B. (2026, May 26). Pore Scale Modeling of Evaporation Induced Salt Crystallization for CO₂ Storage and Utilization. *JpGU-AGU Joint Meeting 2026*, Chiba, Japan, May 24–29, 2026. <https://doi.org/10.5445/IR/1000194581>

[6] **Kumar, A.**, Prajapati, N., Reder, M., Jeela, R. K., Schneider, D., & Nestler, B. (2026, March). Sequential Chemo-Mechanical Phase-Field Modeling of Corrosion-Induced Cracking in Geothermal Pipes. *2nd GeoLaB Scientific Workshop*, Karlsruhe, Germany, March 12–13, 2026. <https://doi.org/10.13140/RG.2.2.36823.74409>

[7] Epp, F., Prajapati, N., Reder, M. D., **Kumar, A.**, & Nestler, B. (2025). Quantitative Modeling of Thermo-Hydraulic Transport in Geothermal Fractures: A Diffuse Interface Perspective. *AGU Fall Meeting 2025*, New Orleans, LA, USA, December 15–19, 2025. In

press.

[8] Prajapati, N., **Kumar, A.**, & Nestler, B. (2025, August 28). CO₂ Cycle: Experimentally-informed Simulation Workflows for Injection, Storage, and Utilization in a Circular Economy. *Circular Economy Seminar*, Bordeaux, France, August 28–29, 2025.

[9] **Kumar, A.**, Prajapati, N., Reder, M. D., Koeppe, A. H., Schneider, D., Selzer, M., & Nestler, B. (2025, June 16). Data-Driven and Physics Based Modeling for Corrosion-induced Cracks. *Künstliche Intelligenz für effizienten Korrosionsschutz*, Frankfurt am Main, Germany, June 16–17, 2025. <https://doi.org/10.5445/IR/1000190670>

[10] **Kumar, A.**, Prajapati, N., Schneider, D., Busch, B., Hilgers, C., & Nestler, B. (2025). Revealing the Hidden Dynamics of Clay-Coated Quartz Grains in Sandstone with Multiphase-Field Modeling. *EGU General Assembly 2025*, Vienna, Austria, April 27–May 2, 2025. <https://doi.org/10.5194/egusphere-egu25-3471>

[11] **Kumar, A.**, Prajapati, N., Späth, M., Schneider, D., Nestler, B., & Busch, B. (2024, December 5). Qualitative modeling of etch-pit formation (dissolution) on the K-feldspar surface through phase-field approach. *Seminar am Institut für Angewandte Geowissenschaften*, Karlsruhe, Germany, December 5, 2024. <https://doi.org/10.5194/egusphere-egu24-4571>

[//doi.org/10.5445/IR/1000190682](https://doi.org/10.5445/IR/1000190682)

[12] **Kumar, A.**, Späth, M., Schneider, D., & Nestler, B. (2024). Uncovering the Influence of Crystal Growth, Dissolution, Crack Propagation, and Vein Formation on Earth's Subsurface: A Phase-field Investigation. *Deformation Mechanisms, Processes and Fabric Analysis in Earth Materials from the Global to the Nano Scale – Methods and Applications*, Kharagpur, India, February 26–28, 2024. <https://doi.org/10.5445/IR/1000180959>

[13] **Kumar, A.**, Späth, M., Schneider, D., Busch, B., Hilgers, C., & Nestler, B. (2024). Decoding the Dynamic Impact of Clay-Coated Quartz Grains in Sandstone through Multiphase-Field Modeling. *37th International Geological Congress*, Busan, South Korea, August 25–31, 2024. <https://doi.org/10.5445/IR/1000180957>

[14] **Kumar, A.**, Späth, M., Schneider, D., & Nestler, B. (2023). Unraveling the Influence of Clay Coating in Sandstone on Reservoir Quality through 3D Multiphase-Field Investigation. *AGU Fall Meeting 2023*, San Francisco, CA, USA, December 11–15, 2023. <https://doi.org/10.5445/IR/1000180958>

[15] **Kumar, A.**, Prajapati, N., Späth, M., Schneider, D., Busch, B., Hilgers, C., & Nestler, B. (2022, July). Qualitative modeling of etch-pit formation (dissolution) on the K-feldspar surface through

phase-field approach. *15th World Congress on Computational Mechanics and 8th Asian Pacific Congress on Computational Mechanics*, Online, July 31–August 5, 2022. <https://doi.org/10.5445/IR/1000158330>

Magazine article

[16] Weichel, M., Jeela, R. K., **Kumar, A.**, Reder, M., Prajapati, N., Schneider, D., & Nestler, B. (2024). Die Gestaltung einer nachhaltigen Zukunft: Der Einfluss von KI-basierten Simulations- und Datenmanagementsystemen auf die Weiterentwicklung von Post-Lithium-Ionen-Batterien, Brennstoffzellen und geothermischer Energie. *Mitteilungen*, 24(4).