



Multi-physics coupling model of chloride-induced rebar corrosion and concrete cracking in reinforced concrete structure

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ABSTRACT

Chloride-induced rebar corrosion and concrete cracking are complex processes driven by interacting multi-physics mechanisms and multiple contributing factors. This study proposes an innovative multi-physics modeling framework to comprehensively analyze the entire degradation process, from ionic transport to corrosion initiation and cracking induced by corrosion expansion. A multi-ionic transport model is developed to quantify the impact of electrochemical processes and crack propagation on ionic transport. Based on phase-field theory and corrosion kinetics, a corrosion model is then proposed to describe corrosion product loss, filling, and accumulation. A multiphase phase-field cracking model is hence developed to characterize fracture behavior and degradation induced by corrosion product pressure. Third-party data are used to validate the proposed models and framework. Results indicate ignoring multi-ion interactions overestimates pore-solution chloride, while neglecting electromigration distorts local ion distributions. Explicit crack representation generates preferential transport pathways, accelerates ingress, and increases peak current density and electrochemical potential by over 10%. Coupling the displacement field enhances crack-growth predictions and avoids premature or excessive cracking. This work offers a new perspective on cracking and durability deterioration in reinforced concrete by establishing a mechanistic framework that enables more reliable predictions in the cracked state, thereby reducing reliance on empirical formulations.

1. Introduction

Chloride-induced rebar corrosion is a key factor in the durability degradation of reinforced concrete structures [1–3], drawing significant attention in recent decades. It can precipitate premature loss of serviceability, motivating improved mechanistic understanding and durability design strategies [4]. Chloride ions penetrate the concrete cover by diffusion and crack-assisted transport [5], eventually reaching the rebar surface, triggering an electrochemical reaction once a critical content threshold is reached [6,7]. Due to the volume of corrosion products being more than twice that of the reactants [8], these products gradually fill the pore structure near the rebar [9]. The resulting expansive pressure raises tensile stresses; when they exceed the tensile strength of concrete [10], cracking occurs [11–13]. The formation of

cracks, in turn, creates additional pathways for chloride ions and oxygen, further accelerating both corrosion and cracking [14]. Moreover, the infiltration of expansive corrosion products into existing cracks occupies the crack space and exerts pressure, aggravating local damage and promoting further crack widening and propagation [15]. Together, these coupled mechanisms form a self-reinforcing deterioration cycle, ultimately compromising structural integrity and shortening service life [16]. Therefore, understanding the interconnections among the three strongly coupled sub-processes—ionic transport, rebar corrosion, and concrete cracking—is crucial for accurately predicting the performance degradation of reinforced concrete structures.

Previous research in this field has predominantly relied on experimental methods, often involving destructive tests which limits direct observation of time-dependent corrosion evolution and long-term

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deterioration [17]. To address these limitations, various non-destructive techniques have been developed, including acoustic emission (AE) [18], X-ray computed tomography (CT) [19], microscopy-based characterization (e.g., SEM) [20], and electrochemical methods [21–24]. Although these experimental methods have partly enhanced our understanding of corrosion-induced cracking, they are still subject to various limitations, including susceptibility to environmental interference, limited applicability, and an inability to fully elucidate the underlying mechanisms [18,20,25,26]. Furthermore, because corrosion-induced deterioration arises from strongly interacting multi-physics processes, isolating the contribution of each phenomenon experimentally remains challenging.

Compared to experimental methods, numerical methods offer the advantage of integrating multiple factors and efficiently modeling chloride-induced rebar corrosion and concrete cracking, providing a more comprehensive understanding of these interconnected processes. As multi-ionic transport plays a central role in corrosion initiation, it has been a primary focus of recent modeling efforts, with attention to key influences. Temperature and humidity significantly affect the transport process [27,28], while the coexistence of ions with different charges generates electrostatic potentials in the pore solution, influencing both ionic transport and solid–liquid chemical reactions [29]. Concrete heterogeneity and multiphase characteristics also affect transport pathways, as physicochemical reactions can progressively alter the microstructure and consume ions [30]. Cracking introduces preferential pathways that bypass the tortuous pore network and accelerates ionic ingress [31,32], while also providing additional space for corrosion-product accumulation and volumetric expansion, which can further intensify damage development [33]. However, most existing research primarily focuses on limited factors or phenomena, with few integrating them and further examining their combined impact on the deterioration process.

Once the chloride concentration near embedded rebar exceeds a critical threshold, corrosion initiates, generating expansive products that induce internal stresses on the concrete cover. To estimate the distribution of these products, a variety of empirical formulas have been developed. These include partly uniform descriptions [34], linear decay models [35], semi-elliptical, Gaussian, and von Mises distributions that have been reported based on experimental observations [36–39]. Overall, these methods have improved our understanding of the spatial distribution of corrosion products around rebar; however, their temporal evolution is typically imposed via a prescribed corrosion-rate (or mass-loss) history, rather than derived from the underlying transport–reaction processes, which limits predictive reliability across exposure conditions.

As corrosion products accumulate at the rebar–concrete interface, the associated volumetric expansion generates internal tensile stresses that, once exceeding the tensile resistance of the concrete cover, initiate cracking. To capture this mechanism, numerical strategies can be broadly grouped into discrete and continuum fracture formulations. Discrete approaches (e.g., DEM and RBSM) reproduce nonlinear deformation and corrosion-induced cracking; DEM resolves particle interactions, whereas RBSM enables direct crack-width evaluation [40,41]. Continuum-based formulations such as concrete damage plasticity (CDP) describe stress transfer at the rebar–concrete interface while accounting for tensile cracking and compressive crushing [42]. Lattice and peridynamic formulations provide alternative representations of fracture, and have been used to incorporate transport–mechanical coupling or multiscale crack development in corrosion problems [43,44]. Phase-field formulations avoid predefined crack paths and capture crack branching and microcrack evolution [45], which has facilitated progress toward fully coupled multi-physics modeling [46–49]. Nevertheless, existing models often address isolated mechanisms or rely on restrictive assumptions [50], constraining predictive capability for comprehensive modeling of corrosion-induced cracking in reinforced concrete.

Despite the abovementioned progress, most contributions focus on selected links in this chain or adopt narrowly defined corrosion settings, and fully coupled treatments under chloride ingress remain comparatively scarce. As steps toward more complete coupling, German et al. [51] highlighted chloride binding for depassivation-time prediction and verified corrosion products mass via Faraday's law. Wang et al. [52] modeled corrosion-product penetration along crack networks, highlighting the role of product diffusion in cracks, while Van Steen et al. [15] considered the loss of corrosion products and the associated volumetric consequences. Building on these mechanism-level advances, recent studies have introduced phase-field and microstructurally resolved multi-physics frameworks for transport–corrosion–mechanical coupling. Korec et al. [53] targeted impressed-current conditions, focused on the reactive transport and precipitation of dissolved $\text{Fe}^{2+}/\text{Fe}^{3+}$ species, and drove phase-field fracture via a precipitation-induced eigenstrain. To reflect environmental control more explicitly, Wei et al. [54] linked the corrosion products expansion/volumetric straining rate to the dissolved oxygen flux at the rebar–concrete interface within a diffusion–mechanical phase-field setting. Moving to a higher-resolution setting, Pan [55] developed a CT-informed 3D micromechanical multi-physics model coupling chloride transport with thermal–hydraulic–electrical fields, with deterioration quantified by continuous damage and an experimentally based corrosion-current law. Addressing electrochemical chloride removal and subsequent re-corrosion, Fang et al. [56] coupled multi-ionic transport, electrochemical reactions and phase-field cracking at the mesoscale, and implemented corrosion products expansion through a radial interfacial displacement. However, their formulation does not explicitly resolve the redistribution of corrosion products within evolving cracks. These studies represent important advances within their respective target scenarios and coupling scopes. Collectively, these studies provide complementary advances, yet a unified treatment that consistently links the key mechanisms relevant to chloride-induced corrosion and cracking remains challenging.

From the literature review, most existing studies address selected mechanisms or adopt partial coupling; consequently, a fully integrated description from chloride transport to corrosion-induced cracking, together with their mutual interactions, remains limited. To address this gap, we develop a multi-physics framework that couples multi-ionic transport, electrochemical corrosion, and phase-field fracture. The contributions are threefold. First, multi-ionic transport is formulated within the Nernst–Planck framework and consistently coupled with crack evolution, environmental state, and relevant reactions, enabling prediction of ionic migration, consumption, and redistribution. Second, a corrosion-product evolution and redistribution model is introduced to account for product transport and loss into pores and cracks, where crack accommodation is quantified from the phase-field crack measure rather than prescribed geometrically. Third, a fully two-way coupling strategy among ionic transport, corrosion, and cracking is implemented, such that damage evolution continuously updates the transport properties and corrosion driving terms. This framework serves as a reliable tool for understanding corrosion and cracking mechanisms, and for predicting the durability of reinforced concrete structures under chloride exposure.

2. Modeling methodology

In this work, a fully coupled framework is established for chloride-induced corrosion and cracking under natural and laboratory exposure conditions, with an emphasis on circumferentially non-uniform corrosion in a two-dimensional mesoscale cross-sectional domain. As illustrated in Fig. 1, the framework comprises three sub-models: (a) a multi-ionic transport model based on the Nernst–Planck equation, which incorporates ionic reactions, electrochemical potentials, crack-enhanced diffusion, and environmental effects to obtain the concentration distributions of multiple ions (Section 2.1); (b) an electrochemical corrosion

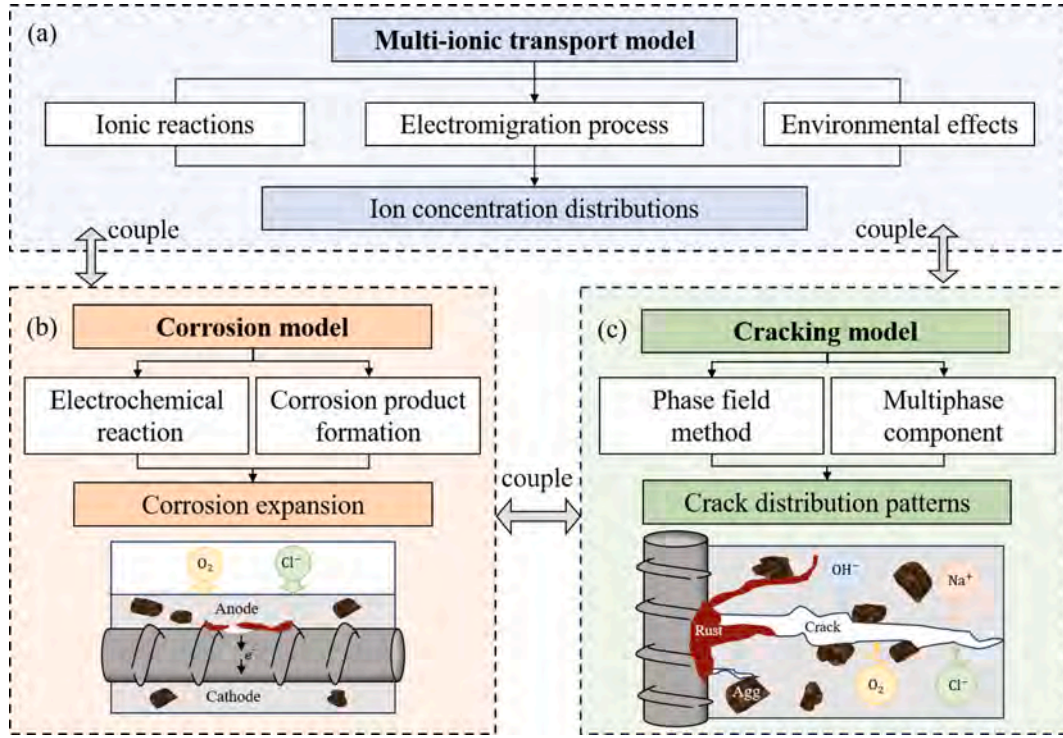


Fig. 1. Integrated framework of the three sub-models: (a) a multi-ionic transport model; (b) an electrochemical corrosion model; (c) a phase-field cracking model.

model that modifies Faraday's law to quantify corrosion products while accounting for product loss, and employs boundary displacement loading to model corrosion-induced expansion (Section 2.2); and (c) a phase-field cracking model using a regularized cohesive-zone formulation to capture crack patterns in multiphase concrete under corrosion-induced expansion (Section 2.3). These sub-models are fully coupled via the dynamic interaction of key variables: ionic concentrations govern electrochemical reactions and product formation; the resulting expansion drives crack evolution; and the evolving damage field feeds back into the transport and corrosion models (Fig. 2).

2.1. Multi-ionic transport in concrete

Rebar corrosion in concrete is governed by the transport of multiple ionic species (such as Ca^{2+} , Na^+ , Fe^{2+} , OH^- , Cl^-) in the pore solution, together with dissolved oxygen, through the pore network [57]. The diffusive and electromigration flux of species k in the pore solution is described by the Nernst–Planck equation [58]:

$$J_k = -D_k \nabla C_k - \frac{z_k D_k F}{RT} C_k \nabla \phi_L \quad (1)$$

where J_k is the ionic flux of species k ($\text{mol}/(\text{m}^2 \cdot \text{s})$), and C_k is its concentration (mol/m^3), D_k is the effective diffusion coefficient, z_k is the ionic charge, F is the Faraday constant, R is the universal gas constant, T is the absolute temperature, ϕ_L is the electrolyte phase potential. The above equation accounts for diffusion and electromigration, but does not explicitly include moisture-driven advection, chloride binding, homogeneous reactions, or crack-enhanced transport [59].

Since concrete is generally unsaturated, moisture transport can strongly influence ionic mobility [60]; under partially saturated conditions, reduced liquid connectivity limits ionic pathways and markedly suppresses transport efficiency [61]. To account for this effect, a convective term is incorporated into Eq. (1), representing moisture-driven ionic transport as follows:

$$J_k = -D_k \nabla C_k - \frac{z_k D_k F}{RT} C_k \nabla \phi_L + \mathbf{v} \bullet C_k \quad (2)$$

where $\mathbf{v}$ is the pore solution velocity, expressed as the product of the humidity-dependent diffusion coefficient $D(h)$ and the gradient of saturation of the concrete interior over time ∇h . The function $D(h)$ follows an S-curve form [62], which is commonly used in concrete transport modeling to capture the nonlinear dependence of moisture diffusivity on saturation in Portland cement-based materials [63], as shown in Eq. (3):

$$D(h) = D_{\text{sat}} \left[\alpha_0 + \frac{1 - \alpha_0}{1 + ((1 - h)/(1 - h_c))^m} \right] \quad (3)$$

where $\alpha_0 = 0.05$, $h_c = 80\%$, and $m = 15$ are empirical parameters [62]. D_{sat} denotes the saturated moisture diffusivity, and is further calculated based on concrete compressive strength f_{ck} :

$$D_{\text{sat}} = \frac{D_{1.0}}{f_{ck}/f_{ck0}} \quad (4)$$

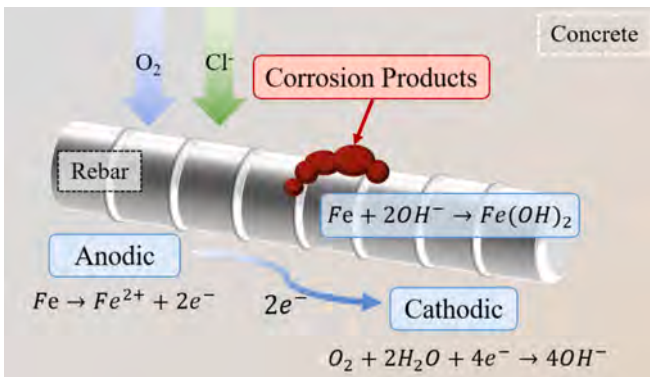


Fig. 2. Electrochemical corrosion mechanism.

where, $D_{1,0}$ denotes the reference moisture diffusion coefficient under standard conditions, with a value of $1.0 \times 10^{-9} \text{ m}^2/\text{s}$, while f_{ck0} represents the reference compressive strength of 10 MPa, f_{ck} is related to the average compressive strength f_{cm} of the specimen, and $f_{ck} = f_{cm} - 8 \text{ MPa}$ [62].

Moreover, it is known that free chloride ions (Cl^-) will interact with hydration products of cement to form bound chloride ions (B_{Cl^-}). This binding effect reduces the availability of free chlorides and thus slows down chloride transport [64]. A Langmuir isotherm is adopted to quantify this process:

$$B_{\text{Cl}^-} = \frac{\alpha C_{\text{Cl}^-}}{w_a(1 + \beta C_{\text{Cl}^-})} \quad (5)$$

where $\alpha = 0.42$ and $\beta = 0.8$ are empirical parameters [65], and w_a is the chemically bound water per unit mass of cement. The parameter w_a depends on the hydration degree ϱ [66], and ϱ is calculated through the water to cement ratio (w/c) [67], see Eqs. (6)–(7):

$$w_a = 0.25\varrho \quad (6)$$

$$\varrho = 0.239 + 0.745 \tanh[3.62(w/c - 0.095)] \quad (7)$$

To integrate chloride binding into the transport model, a correction factor ξ is introduced [68]:

$$\xi = \frac{\alpha}{w_a(1 + \beta C_{\text{Cl}^-})^2} \quad (8)$$

therefore, for chloride ions, the mass balance is written as:

$$(1 + \xi) \frac{\partial C_{\text{Cl}^-}}{\partial t} + \nabla \cdot J_{\text{Cl}^-} = 0 \quad (9)$$

where J_{Cl^-} is given by Eq. (2) with the convective and electromigration terms.

In addition to the chloride binding phenomena described above, ionic depletion also has an important effect on ionic transport. During the electrochemical corrosion, OH^- and Fe^{2+} in the pore solution are consumed and precipitated as corrosion products. While this dynamic depletion has often been neglected in previous studies, this work introduces a reactive source term to account for the consumption of these ions. Accordingly, Eq. (2) is updated as follows:

$$\frac{\partial C_k}{\partial t} + \nabla \cdot J_k = R_k \quad (10)$$

where R_k accounts for source or sink terms from chemical reactions of species k . In the case of Fe^{2+} and OH^- , R_k corresponds specifically to the

consumption rate of OH^- , k_s is the precipitation rate constant ($\text{m}^7/(\text{mol}^2 \cdot \text{s})$). $H(\mu)$ is the heaviside step function, and μ is a dimensionless index given by:

$$\mu = c_{\text{Fe}^{2+}} \cdot c_{\text{OH}^-}^2 / k_{sp} - 1 \quad (12)$$

where $c_{\text{Fe}^{2+}}$ is the concentration of Fe^{2+} and c_{OH^-} is the concentration of OH^- , the rate constant k_s is set to $3.7 \times 10^{-7} \text{ m}^7/(\text{mol}^2 \cdot \text{s})$ [70].

The electromigration term in the Nernst–Planck flux requires the electrolyte potential ϕ_L , which is obtained by enforcing electroneutrality and charge conservation. Specifically, the electrolyte normal current density i_n at the interface is related to the ionic fluxes by [48]:

$$i_n = F \sum_{k=1}^N z_k (J_k \cdot n) \quad (13)$$

where n is the unit outward normal vector to the interface, N denotes the total number of ionic species considered in the model. The normal current density can also be expressed by Ohm's law as [48]:

$$i_n = -\sigma \nabla \phi_L \cdot n \quad (14)$$

where σ denotes the electrolyte conductivity, which depends on microstructural characteristics, hydrate composition, relative humidity, and temperature. A constant value of $\sigma = 2.5 \text{ S/m}$ is adopted in this study for simplification [49,71], within the environmental and material conditions considered, variations in the effective electrolyte conductivity are expected to be limited. Eqs. (13)–(14), together with charge conservation, are used to obtain the electrostatic potential ϕ_L , which then updates the electromigration contribution in the Nernst–Planck flux.

Moreover, as the electrochemical reaction progresses, the accumulation of corrosion products leads to crack propagation. As cracks develop, the connectivity of the pore network increases, so ionic diffusion in cracked regions becomes much faster than in intact concrete, and a damage function is introduced here to represent this accelerated diffusion:

$$D_k^* = D_k(1 - \omega(d)) + D_{k,c}\omega(d) \quad (15)$$

where D_k^* denotes the effective transport coefficient of cracked concrete that accounts for damage-enhanced transport, and $D_{k,c}$ represents diffusion coefficient in cracked regions. The function $\omega(d)$ is defined in Section 2.3.

Taking all the aforementioned factors into account, Eq. (2) is finally reformulated as Eq. (16), where ξ is set to zero for all species except chloride ions, and the source term R_k is applied only to Fe^{2+} and OH^- to account for their consumption during the corrosion process.

$$\underbrace{\left[1 + \xi\right]}_{\text{Cl}^- \text{ binding}} \frac{\partial C_k}{\partial t} - \underbrace{\nabla \cdot \left(D_k^* \nabla C_k \right)}_{\text{Cracking}} - \underbrace{\nabla \cdot \left(z_k C_k \nabla \phi_L \frac{D_k^* F}{RT} \right)}_{\text{Electromigration}} - \underbrace{\nabla \cdot (D(h) \nabla h C_k)}_{\text{Moisture transport}} = \underbrace{R_k}_{\text{Chemical reactions}} \quad (16)$$

consumption rates associated with the precipitation of $\text{Fe}(\text{OH})_2$, which is formed via the reaction of Fe^{2+} released from rebar dissolution and OH^- ions in the pore solution. This reaction is considered irreversible and occurs when the ionic product exceeds the solubility product of $\text{Fe}(\text{OH})_2$, with solubility product constant $k_{sp} = 7.94 \times 10^{-16} \text{ mol}^3/\text{m}^9$ [69]. The consumption rate of Fe^{2+} and OH^- ions due to precipitation is governed by:

$$2 \times R_{s,\text{OH}^-} = R_{s,\text{Fe}^{2+}} = k_s (c_{\text{Fe}^{2+}} \cdot c_{\text{OH}^-}^2 - k_{sp}) \cdot H(\mu) \quad (11)$$

where $R_{s,\text{Fe}^{2+}}$ means consumption rate of Fe^{2+} , R_{s,OH^-} means

In unsaturated concrete under coupled corrosion–cracking, beyond the convective, diffusive, and electromigration fluxes in the Nernst–Planck formulation, crack-connectivity evolution, chloride binding–release, and electrochemical source–sink reactions can reshape ionic redistribution. Incorporating these processes allows corrosion reactions to modify local ionic fields and crack connectivity to regulate transport pathways, thereby enabling a consistent coupling among ionic transport, corrosion reactions, and crack evolution.

2.2. Electrochemical corrosion of rebar

To characterize the spatial distribution of corrosion products around the rebar, an electrochemical corrosion model is developed. It computes the circumferentially varying corrosion current density and product formation, and further accounts for product loss and an elliptical reconstruction to obtain the local product accumulation.

To quantify the charge transfer kinetics, the electrode potential ϕ is first evaluated as the driving force of the corrosion reaction. According to electrochemical principles, the electrode potential is defined as the difference between the metal phase potential (ϕ_M) and the electrolyte phase potential (ϕ_L) [72].

$$\phi = \phi_M - \phi_L \quad (17)$$

Due to the high electrical conductivity of rebar, the metal-phase potential can be considered spatially uniform; therefore, ϕ_M is set to 0, making the potential ϕ equal to $-\phi_L$.

The corrosion rates of rebars are predominantly influenced by the magnitude of the anodic current density i_{Fe} [73], which is evaluated from the electrode potential using a Tafel-type relation. Since chloride-induced depassivation alters the anodic kinetics, the anodic Tafel slope is corrected to account for the effect of Cl^- [74]:

$$i_{Fe} = i_{Fe}^0 \cdot \exp[2.303 \cdot (\phi - \phi_{Fe}^0) / \beta'_{Fe}] \quad (18)$$

where ϕ_0 Fe (V) is the anodic equilibrium potential, i_0 Fe (A/m²) is the anodic exchange current density, β_{Fe} is the anodic Tafel slope, and β' Fe is the corrected Tafel slope. The depassivation effect of chloride is introduced through a concentration-dependent factor f_{Cl} [75]:

$$\beta'_{Fe} = \beta_{Fe} f_{Cl} \quad (19)$$

$$f_{Cl} = 0.525 C_{Cl}^{-1.126} + 1 \quad (20)$$

where C_{Cl} is the free chloride concentration at the rebar surface (% by mass of binder).

During corrosion, the anodic and cathodic reactions are coupled through current continuity. The cathodic oxygen-reduction current density i_{O_2} is described by a modified polarization relation [76]:

$$i_{O_2} = \frac{i_{O_2}^0 \exp[2.303 \cdot (\phi - \phi_{O_2}^0) / \beta_{O_2}]}{1 + i_{O_2}^0 / i_L \cdot \exp[2.303 \cdot (\phi - \phi_{O_2}^0) / \beta_{O_2}]} \quad (21)$$

where ϕ_0 O₂ (V) is the cathodic equilibrium potential, β_{O_2} (V/dec) is the cathodic Tafel slope, and i_0 O₂ (A/m²) is the cathodic exchange current density. The oxygen diffusion limiting current density i_L is [77]:

$$i_L = \frac{z_{O_2} F D_{O_2} C_{O_2}^s}{a} \quad (22)$$

where $z_{O_2} = 4$ corresponds to the four-electron reduction of oxygen in the cathodic reaction, $C_{O_2}^s$ is the oxygen concentration of concrete surface, and a is the characteristic diffusion distance from the surface.

The net current density at the rebar surface is given by the difference between the anodic and cathodic currents:

$$i_n = i_{Fe} - i_{O_2} \quad (23)$$

This relation is imposed as an interfacial boundary condition, linking the electrode kinetics to the transport fields in the electrolyte (ionic concentrations and potential). The parameters will be introduced in Section 3.1.

As chloride accumulates at the rebar surface and depassivation occurs, the corrosion current density becomes circumferentially non-uniform, leading to localized corrosion. The anodic current density therefore governs the local rebar loss and corrosion products generation; meanwhile, a portion of the generated products can be accommodated

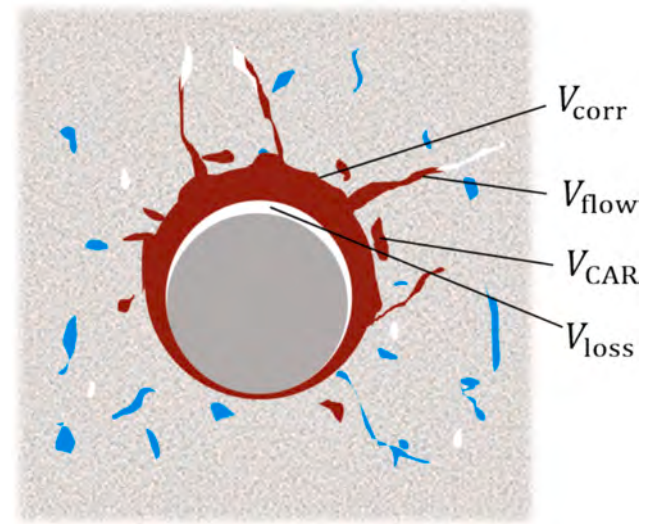


Fig. 3. Representation of the variables of the corrosion process. Note: V_{corr} : theoretical expansion volume; V_{loss} : volume loss; V_{CAR} : corrosion products retained in capillary region; V_{flow} : corrosion products migrated into cracks.

by the steel-loss volume and the available pore/crack space in the surrounding concrete (Fig. 3), which reduces the effective amount accumulating at the rebar–concrete interface. Accordingly, the circumferential corrosion depth $d_{corr}(\theta, t)$ is evaluated from Faraday's law as follows [78]:

$$d_{corr}(\theta, t) = \frac{\int_0^t i_{Fe}(\theta, t) dt \cdot A_{Fe}}{z_{Fe} \cdot F \cdot \rho_{Fe}} \quad (24)$$

where θ is the circumferential coordinate along the rebar surface, and t represents the exposure time, $A_{Fe} = 55.8 \times 10^{-3}$ kg/mol is molar mass of iron, $z_{Fe} = 2$ is the valency of Fe in the anodic reaction, and $\rho_{Fe} = 7860$ kg/m³ is the density of iron. The corresponding volume loss is given by:

$$V_{loss} = \pi [R_0^2 - (R_0 - d_{corr})^2] L_{corr} \quad (25)$$

where L_{corr} denotes the corroded rebar length, $L_{corr} = 1$ is used to evaluate corrosion volume per unit length, R_0 is the radius of rebar. The theoretical expansion volume (V_{corr}) is calculated as:

$$V_{corr} = \eta V_{loss} \quad (26)$$

where η is the volumetric expansion coefficient, which varies with corrosion products and takes values of 2.95 (α -FeOOH), 3.07 (γ -FeOOH), $\eta = 3.53$ (β -FeOOH), and 2.10 (Fe_3O_4), respectively [8]. For simplicity, this study assumes a combination of α -FeOOH and γ -FeOOH, with $\eta = 3$.

In practice, corrosion products influence expansion because they can fill cracks and pores, and they can also occupy the space created by steel loss and the interfacial gap, which reduces the amount of products accumulating at the interface. To account for these effects, the theoretical expansion volume is adjusted by introducing an effective expansion volume $V_{corr,eff}$ [15]:

$$V_{corr,eff} = V_{corr} - V_{loss} - V_{CAR} - V_{flow} \quad (27)$$

where V_{CAR} is the volume of corrosion products retained in the capillary adjustment region, see Eq. (28). V_{flow} refers the volume of corrosion products that have migrated into cracks, see Eq. (29), and the interrelationships of them can be found in Fig. 3. Note that V_{flow} is evaluated from the evolving crack measure V_{crack} obtained from the phase-field description (Section 2.3), thereby coupling crack evolution to the effective expansive driving source. Due to the adopted formulation, precipitation is restricted to the damage-defined domain, rather than

occurring in the real physical space wherever the chemical conditions are satisfied. V_{CAR} can be derived from the capillary porosity of cement paste (ϕ_{cp}) and the matrix volume (V_{CM}):

$$V_{CAR} = \phi_{cp} V_{CM} = \phi_{cp} \pi L_{corr} \left[(R_0 + CAR_{max})^2 - R_0^2 \right] \quad (28)$$

where CAR_{max} is valued at 0.1 mm [79], representing the physical limit of corrosion products accumulation within the pore space between the rebar and concrete. Capillary porosity ϕ_{cp} is evaluated as described in Appendix 1.

Similarly, V_{flow} in Eq. (29) reflects crack filling effect of corrosion products in the crack on the effective expansion volume of corrosion products ($V_{corr,eff}$), which is related to the crack volume (V_{crack}) and the theoretical expansion volume (V_{corr}), with an initial value of zero:

$$V_{flow,s} = V_{flow,s-1} + \begin{cases} \Phi_1 \Delta V_{crack,s}, & \Phi_1 \Delta V_{crack,s} < \Delta V_{corr,s} \\ \Phi_2 \Delta V_{corr,s}, & \Phi_1 \Delta V_{crack,s} \geq \Delta V_{corr,s} \end{cases} \quad s \geq 1 \quad (29)$$

Here, $\Delta V_{crack,s}$ and $\Delta V_{corr,s}$ are the increments of crack volume and corrosion-product expansion volume over the current time step t_s , $V_{flow,s}$ represents the cumulative volume of corrosion products that have migrated into cracks up to time step t_s , Φ_1 controls crack filling at small crack volumes, whereas Φ_2 represents the production-limited regime when cracks become connected. Accordingly, Eq. (35) enforces a physically consistent transition from the Φ_1 -controlled regime to the Φ_2 -controlled regime. In this study, Φ_1 is set to 0.1, while Φ_2 depends on the concrete cover thickness, taking values of 0.2 for cover ≤ 30 mm and 0.5 for covers > 30 mm [15]. The available crack volume is quantified by the crack measure V_{crack} , obtained from the phase-field crack surface density functional following the standard variational phase-field formulation of fracture (Eqs. (42)–(43)), which directly enters Eq. (29) to update V_{flow} and thus modulates $V_{corr,eff}$ in Eq. (27), as detailed in Section 2.3.

After accounting for both loss and filling effects, the effective expansion volume $V_{corr,eff}$ is obtained. As this quantity is volumetric, an additional reconstruction is required to obtain the corrosion-layer thickness along the rebar circumference. Jin et al. [80] found that corrosion products follow an elliptical distribution pattern on the rebar surface. In the present study, this distribution is introduced as an equivalent geometrical reconstruction to represent the corrosion state. Under the thin-annulus approximation ($\mu_1 \ll R_0$), a normalized shape function $f(\theta) = \mu(\theta)/\mu_1$ is introduced, and the maximum thickness u_1 is determined by volume matching:

$$u_1 = \frac{V_{corr,eff}}{R_0 L_{corr} \int_0^{2\pi} f(\theta) d\theta} \quad (30)$$

once μ_1 is obtained, the local rust-layer thickness $\mu(\theta)$ can be reconstructed, as expressed in Eq. (37):

$$\mu(\theta) = \begin{cases} \frac{(R_0 + \mu_1) \cdot (R_0 + \zeta \mu_1)}{\sqrt{(R_0 + \mu_1)^2 \cos^2 \theta + (R_0 + \zeta \mu_1)^2 \sin^2 \theta}} - R_0 & 0 \leq \theta < \pi \\ \zeta \mu_1 & \pi \leq \theta < 2\pi \end{cases} \quad (31)$$

where $\zeta = 1/20$ – $1/30$, is the ratio between minimum and maximum corrosion-layer thickness, reflecting the experimentally observed asymmetry between severely and mildly corroded regions. This step sets the thickness shape around the rebar, while the total volume is still fixed by $V_{corr,eff}$ from electrochemical calculations.

To clarify the coupling strategy (Fig. 4), the corrosion sub-model converts the circumferential anodic current density into rebar loss and corrosion product generation via Faraday's law, and then corrects the resulting expansion volume for steel-loss volume and for product accommodation/loss in pores and evolving cracks (V_{CAR} and V_{flow}), with V_{flow} updated from the phase-field crack volume. The corrected volume $V_{corr,eff}$ is subsequently mapped to a corrosion-layer thickness field through an elliptical, volume-matched reconstruction. This procedure provides a volume-consistent link from electrochemical output to the mechanical expansion source and yields a circumferentially varying corrosion-thickness distribution along the rebar surface.

2.3. Corrosion-induced cracking of concrete

As corrosion products accumulate, internal pressure increases until concrete cracking occurs [81]. Traditional fracture models typically rely on predefined crack paths or remeshing strategies, which limit their ability to represent complex crack initiation and propagation under evolving boundary conditions. To address this limitation, a phase-field cracking model is adopted to describe continuous damage evolution. Fig. 5 illustrates the classical sharp crack model and the regularized phase-field model. Both models are defined on a solid domain $\Omega \subset \mathbb{R}^{ndim=1,2,3}$. The boundary $\partial\Omega$ is divided into two disjoint parts, $\partial\Omega_u$ and $\partial\Omega_t$. On $\partial\Omega_u$, the displacement boundary condition is prescribed as $u = u^*(x)$, and on $\partial\Omega_t$, the traction boundary condition is prescribed as $t = t^*(x)$. The body force is denoted by b^* .

In Fig. 5(a), the sharp crack S in classical fracture mechanics is modeled as a discontinuity surface, whereas in Fig. 5(b) it is approximated by a smooth damaged region $BC\Omega$, where the phase-field variable d transitions from 0 (undamaged) to 1 (fully damaged). The regularization width of the damaged zone is controlled by the length-scale parameter b . In this study, the phase-field model captures crack growth and stiffness degradation and provides the crack measure

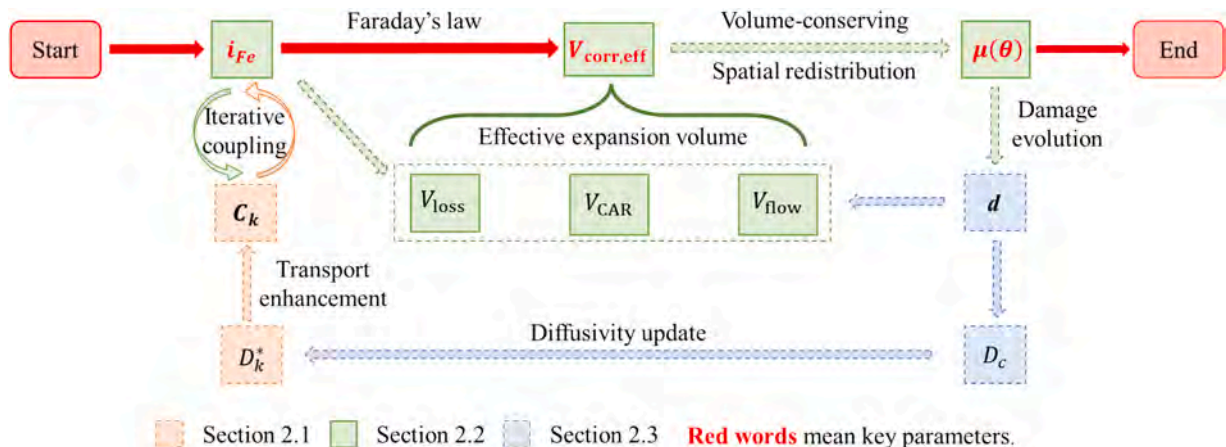


Fig. 4. Schematic of the corrosion model showing key parameter interactions and their links to other models.

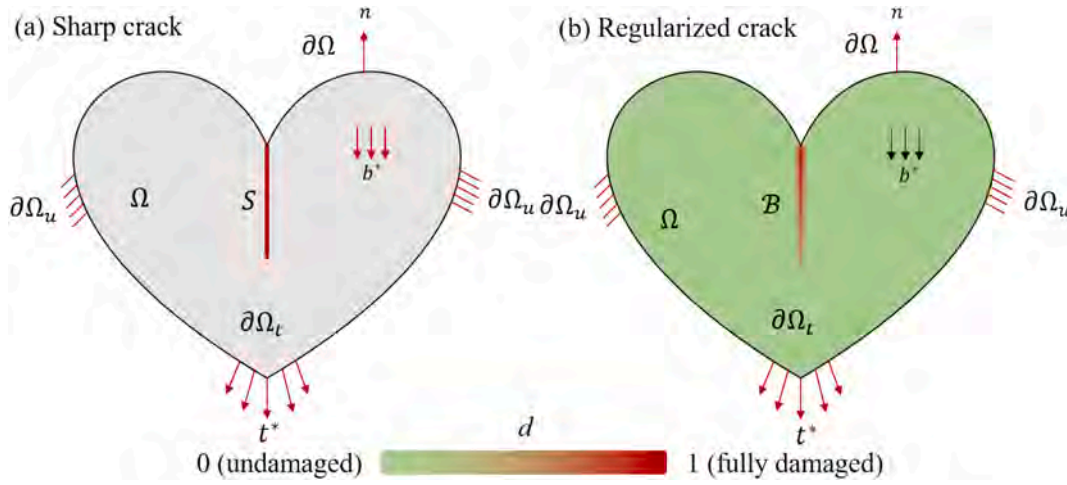


Fig. 5. Illustration of crack representation: (a) Sharp crack; (b) Regularized crack. Note: S in (a) is a sharp crack, B in (b) is smooth damage region.

required for transport–corrosion coupling.

According to phase-field theory, the mechanical behavior of the damaged solid structure is governed by coupled displacement and phase-field equations, which are formulated as:

$$\begin{cases} \nabla \cdot \sigma_s + b^* = 0 & \text{in } \Omega \\ \sigma \cdot n = t^* & \text{on } \partial\Omega_t \end{cases} \quad (32)$$

$$\begin{cases} \nabla \cdot q + Q \leq 0 & \text{in } \Omega \\ q \cdot n \geq 0 & \text{on } \partial\Omega_t \end{cases} \quad (33)$$

where σ_s denotes the stress tensor, q is the flux related to the crack phase-field, and Q represents the phase-field source term. The flux q and source term Q are obtained from the variational phase-field fracture formulation and are given by:

$$\begin{cases} q = \frac{2b}{c_\alpha} G_f \nabla d \\ Q = Y - \frac{G_f}{c_\alpha b} \alpha'(d) \end{cases} \quad (34)$$

where ∇d characterizes the spatial variation of damage, G_f is the fracture energy representing the energy required for crack propagation, and c_α is a normalization constant associated with the crack surface density functional. The crack-driving force Y is defined by:

$$Y = -\omega'(d) \bar{Y} \quad (35)$$

where $\bar{Y}$ denotes the effective driving force for crack evolution and $\omega(d)$ is the energy degradation function describing stiffness reduction. Together with the crack geometry function $\alpha(d)$, which defines the regularized crack surface density, these functions jointly control the evolution of cracks in the phase-field framework. To obtain stable crack growth in concrete and account for softening effects, a viscous phase-field fracture formulation is adopted [82]:

$$\begin{cases} \alpha(d) = \delta d + (1 - \delta) d^2 \\ \omega(d) = \frac{(1 - d)^p}{(1 - d)^p + b_1 d \cdot P(d)}, P(d) = 1 + b_2 d + b_3 d^2 + \dots \end{cases} \quad (36)$$

which satisfy the standard conditions:

$$\alpha(0) = 0, \alpha(1) = 1, \alpha'(d) \geq 0 \quad (37)$$

$$\omega(0) = 1, \omega(1) = 0, \omega'(1) = 0, \omega'(d) \leq 0 \quad (38)$$

where δ denotes the shape parameter and is fixed to 2 [82], so c_α is equal to π according to Eq. (34) and Eq. (36). The parameters in the energy degradation function $\omega(d)$ are calibrated based on the softening curve proposed by Cornelissen et al. [83], the parameter setting ($p = 2$, $b_2 = 1.3868$, $b_3 = 0.6567$) with a high fit degree was obtained, which is also used in this study.

Note that the crack-driving force Y in Eq. (35) may become highly localized during crack propagation, potentially leading to numerical instability. To avoid this, a history-type regularization variable $\mathcal{H}_s$ is introduced and updated at time step t_s . (defined in Section 3.2) as:

$$\begin{cases} \mathcal{H}_0 = \bar{Y}_0 = f_t^2 / 2E, s = 0 \\ \mathcal{H}_s = \max(\mathcal{H}_{s-1}, \bar{Y}_s), s \geq 1 \end{cases} \quad (39)$$

where $\bar{Y}_s$ denotes the effective crack-driving force evaluated at time step t_s , f_t is the uniaxial tensile strength of the material and E denotes the undamaged elastic modulus. This update enforces a non-decreasing driving force and prevents non-physical crack closure.

In addition, the model also accounts for the reduction in material stiffness caused by cracking. This is achieved by modifying the elastic modulus through the degradation function [45]:

$$E^* = E \times \omega(d) \quad (40)$$

where E^* denotes the elastic modulus after cracking. Through this formulation, the evolution of the phase-field damage variable simultaneously governs both the mechanical degradation and the geometric representation of cracks in a thermodynamically consistent manner. Accordingly, once the damage variable evolves, the associated crack opening within the concrete cover can be quantitatively estimated. The crack width is evaluated by integrating the strain field weighted by the damage-induced stiffness reduction [84], see Eq.(49):

$$w_d = \int^L \varepsilon (1 - \omega(d)) dx \quad (41)$$

where ε is the total strain, w_d is the crack width. Beyond the crack opening, the crack geometry itself is further characterized at the continuum level. Following the variational phase-field formulation, the crack geometry is characterized by the crack-surface density $\gamma_l(d, \nabla d)$ [85]:

$$\gamma_l(d, \nabla d) = \frac{1}{c_\alpha b} [\omega(d) + b |\nabla d|^2] \quad (42)$$

The effective cracked-region measure is then defined as

$$V_{\text{crack}} = w_d \int \gamma_i(d, \nabla d) d\Omega \quad (43)$$

Because the present study employs a two-dimensional cross-sectional model with unit out-of-plane thickness, the crack surface measure V_{crack} defined in Eq. (43) is interpreted as an effective cracked volume per unit thickness, i.e., an equivalent geometric measure rather than the true void volume from crack opening displacement.

By introducing phase-field theory and incorporating key mechanisms such as cracking induced transport enhancement and corrosion products accumulation, this study develops a phase-field cracking model that accurately captures concrete cracking behavior. Compared with traditional discrete or sharp crack models, it offers improved numerical stability, better representation of complex crack patterns.

3. Model development and validation

This chapter describes the development of the coupled multi-physics model and its validation. The chapter begins by outlining the adopted parameter settings and the corresponding initial and boundary conditions (Section 3.1), then details the numerical implementation of the transport–electrochemistry–damage coupling (Section 3.2), and finally presents validation results against available experimental observations (Section 3.3).

3.1. Parameter settings

The input parameters adopted in this study are summarized in Table 1 and selected to ensure physical consistency of the coupled multi-physics framework. Initial concentrations and boundary conditions were taken from experimental data [75]; when measurements were

Table 1
Parameters and values.

Parameters	Abbreviation	Unit	Value
Initial concentration of Ca^{2+}	$CO\ Ca$	mol/ m^3	30
Initial concentration of Na^+	$CO\ Na$	mol/ m^3	80
Initial concentration of Fe^{2+}	$CO\ Fe$	mol/ m^3	0
Initial concentration of OH^-	$CO\ OH$	mol/ m^3	140
Initial concentration of Cl^-	$CO\ Cl$	mol/ m^3	0
Initial concentration of O_2	$CO\ O_2$	mol/ m^3	0.268
Diffusion coefficients of Ca^{2+} in uncracked mortar matrix	$D_{Ca,m}$	m^2/s	0.79×10^{-11}
Diffusion coefficients of Na^+ in uncracked mortar matrix	$D_{Na,m}$	m^2/s	1.33×10^{-11}
Diffusion coefficients of Fe^{2+} in uncracked mortar matrix	$D_{Fe,m}$	m^2/s	1.96×10^{-11}
Diffusion coefficients of OH^- in uncracked mortar matrix	$D_{OH,m}$	m^2/s	5.27×10^{-11}
Anodic equilibrium potential	$\phi_0\ Fe$	V	−0.78
Cathodic equilibrium potential	$\phi_0\ O_2$	V	0.16
Anodic exchange current density	$i_0\ Fe$	A/m^2	3×10^{-4}
Cathodic exchange current density	$i_0\ O_2$	A/m^2	1×10^{-5}
Anodic Tafel slope	β_{Fe}	V	$0.09 \times f_{Cl}$
Cathodic Tafel slope	β_{O_2}	V	−0.18
Young's modulus of aggregate	$E_{0,agg}$	MPa	70,000
Young's modulus of mortar	$E_{0,m}$	MPa	35,000
Young's modulus of ITZ	$E_{0,itx}$	MPa	25,000
Poisson's ratio of aggregate	$\nu_{0,agg}$	—	0.2
Poisson's ratio of mortar	$\nu_{0,m}$	—	0.2
Poisson's ratio of ITZ	$\nu_{0,itx}$	—	0.2
Failure strength of mortar	$f_{t,m}$	MPa	6
Failure strength of ITZ	$f_{t,itx}$	MPa	3
Fracture energy of mortar	$G_{f,m}$	N/m	40
Fracture energy of ITZ	$G_{f,itx}$	N/m	20

unavailable, values are adjusted to satisfy charge conservation. Diffusion coefficients were specified by accounting for intrinsic material properties and environmental effects. The transport coefficients for chloride ions and oxygen, including humidity-dependent effects, are provided in Appendix 1. For species without measured diffusivities, free-water diffusion coefficients are first estimated and then converted to effective diffusivities using porosity–tortuosity reduction factors, following established multi-ionic transport models [75,86]. In cracked regions, the effective diffusion coefficient D_k was assigned as $D_{k,c} = 10 D_{k,m}$ (Eq. (15)), with $D_{k,m}$ referring to the uncracked mortar matrix. In the ITZ, it was set as $D_{k,itx} = 3 D_{k,m}$ to account for its higher porosity [87]. Based on these transport models, electrochemical behavior was modeled using electrochemical parameters widely reported in the literature for concrete–rebar systems [88,89]. To capture corrosion-induced mechanical degradation, the phase-field cracking model was employed, with parameters set for different material phases [90,91]. When experimental values are available, they are used directly; otherwise, values are taken from well-established studies on OPC-based concrete under unsaturated conditions and applied consistently throughout the analyses unless stated otherwise.

3.2. Numerical implementation

Based on these basic parameters, a multi-physics coupling framework is developed to comprehensively model the rebar corrosion process, the gradual accumulation of corrosion products, and the resulting concrete cracking caused by chloride ingress. This framework consists of three coupled sub-models: a multi-ionic transport model, a corrosion model, and a cracking model. Based on electrochemical principles, the electric potential is calculated and fed back to adjust ion movement. Using Faraday's law, corrosion products formation and expansion are modeled, which creates internal pressure and causes cracking. The phase-field cracking model then tracks how cracks form and grow, showing their effects on strength, corrosion products accumulation, and transport properties. Fig. 6(a) shows how the three sub-models work together to provide results for ion concentration, electric field, displacement, stress, and cracking. Methodologically, to solve this strongly coupled multi-physics problem, a staggered iteration algorithm is employed in this study, see Fig. 6(b). Compared with a monolithic solution scheme, the staggered iteration improves numerical robustness and reduces memory demand, particularly for strongly nonlinear behaviors such as chloride-induced corrosion–cracking. A representative modeling in the present study (Fig. 7) requires approximately 5–7 h of wall-clock time on a workstation equipped with an AMD Ryzen 9 7950X 16-core CPU. This computational cost reflects the high-fidelity nature of phase-field-based corrosion–cracking analysis and is intended for offline long-term deterioration assessment [92].

As illustrated in Fig. 6(b), the four physical fields involved in the multi-physics system—the diffusion field c , electric potential field e , displacement field u , and phase-field variable g —together with the state variable y , are coupled through a sequential staggered iterative scheme. For each time increment t_s , all variables are initialized using the converged solution from the previous time step t_{s-1} , i.e., $(y_{s-1}, c_{s-1}, e_{s-1}, u_{s-1}, g_{s-1})$. Within the current time step, an inner iteration loop indexed by r is performed. In each iteration, the diffusion field c_r is solved first, followed by the electric field e_r . The mechanical equilibrium equation is then solved for the displacement field u_r , with the phase-field fixed at g_{r-1} , and the phase-field equation is then solved to update g_r . Each sub-problem uses the most recently updated fields as input, allowing nonlinear coupling effects to be captured. Iterations continue until a residual-based tolerance of 0.001 is satisfied for all fields. In addition, a global relative tolerance of 0.01 is enforced at each time step to control coupling drift between successive increments. Once convergence is achieved, the state variable y_s is updated according to its evolution rule, and the converged solution (c_s, e_s, u_s, g_s) is stored and used to initialize the next time step.

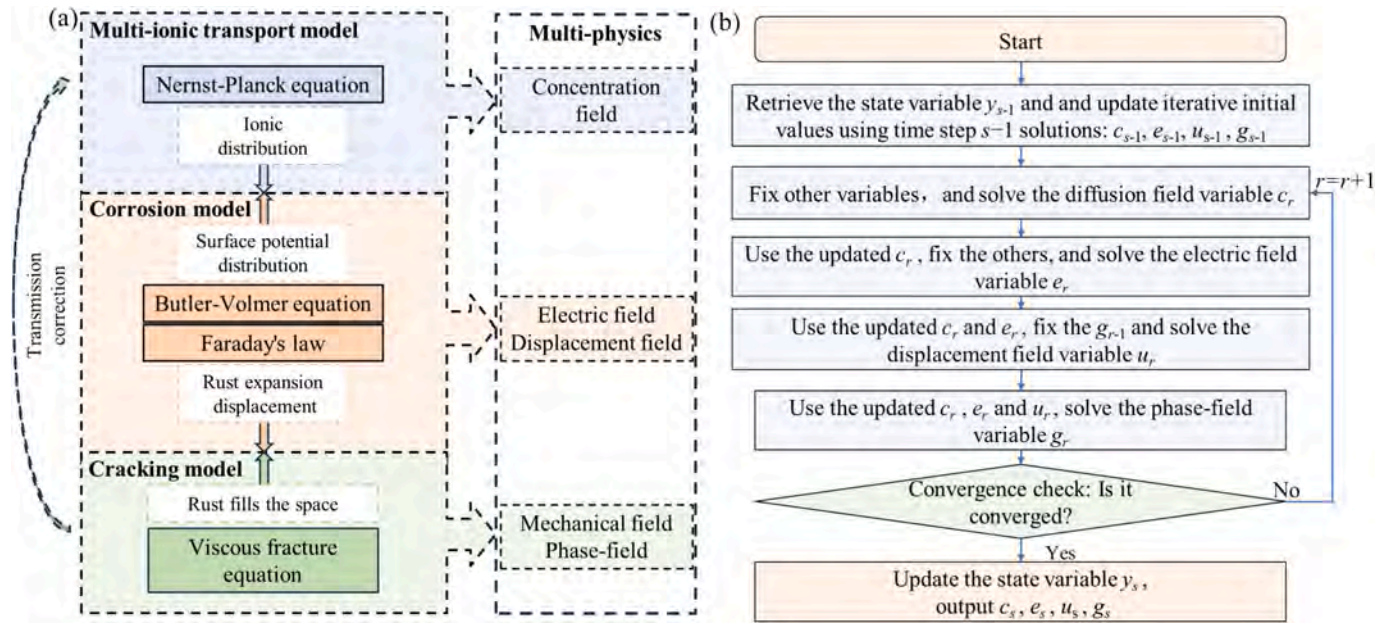


Fig. 6. The flow of the coupling framework and the solution process: (a) Flowchart of the three sub-models; (b) Flowchart of the staggered iterative solution procedure.

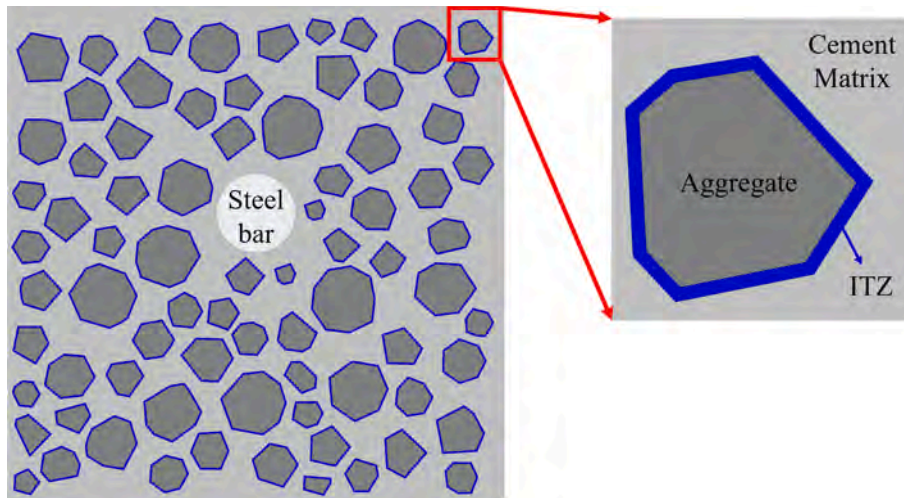


Fig. 7. Multiphase model of concrete.

It should be noted that longitudinal non-uniformity of corrosion and cracking would require an explicit three-dimensional representation. While such effects may influence crack continuity along the reinforcement, they are not expected to change the primary trends of corrosion initiation and crack opening captured by the present two-dimensional framework. Given the computational cost of corrosion-related multiphysics coupling, a two-dimensional cross-sectional model is adopted as a pragmatic compromise; the influence of this assumption is examined in Section 4.3.3. Unless otherwise specified, a 50 mm × 50 mm model is used, as illustrated in Fig. 7. In the model, the blue zone denotes the ITZ, light gray represents the cement matrix, dark gray corresponds to aggregates, and the central white region is the rebar. The geometry is adjusted in model validation to match experimental configurations. To reduce the computational burden of multi-field coupling, the ITZ thickness is set to 0.2 mm [93]. Aggregate-controlled ITZ variability is omitted for computational tractability [94]. Aggregates follow the Fuller grading curve and are randomly distributed as polygons to reflect concrete's heterogeneity [95]. The mesh element size h_e is chosen based on

the criterion $h_e \leq b/5$, where the phase-field length scale parameter b set to 1 mm [95,96], ensuring sufficient resolution for accurate crack modeling. When the mesh size is properly matched to the length parameter, the phase-field formulation yields mesh-objective crack patterns that are insensitive to mesh alignment or further refinement [97].

3.3. Model validation

In this section, the proposed model is validated against published experimental data. Unless otherwise stated, all parameters are kept consistent with those defined in the preceding sections. Validation is conducted using three independent datasets targeting: (1) time-dependent concentration profiles of selected species, (2) the spatial characteristics of rebar corrosion, and (3) the temporal evolution of cracking patterns. For all cases, the predictions are generated using the same coupled governing equations; only the measured observable used for comparison differs.

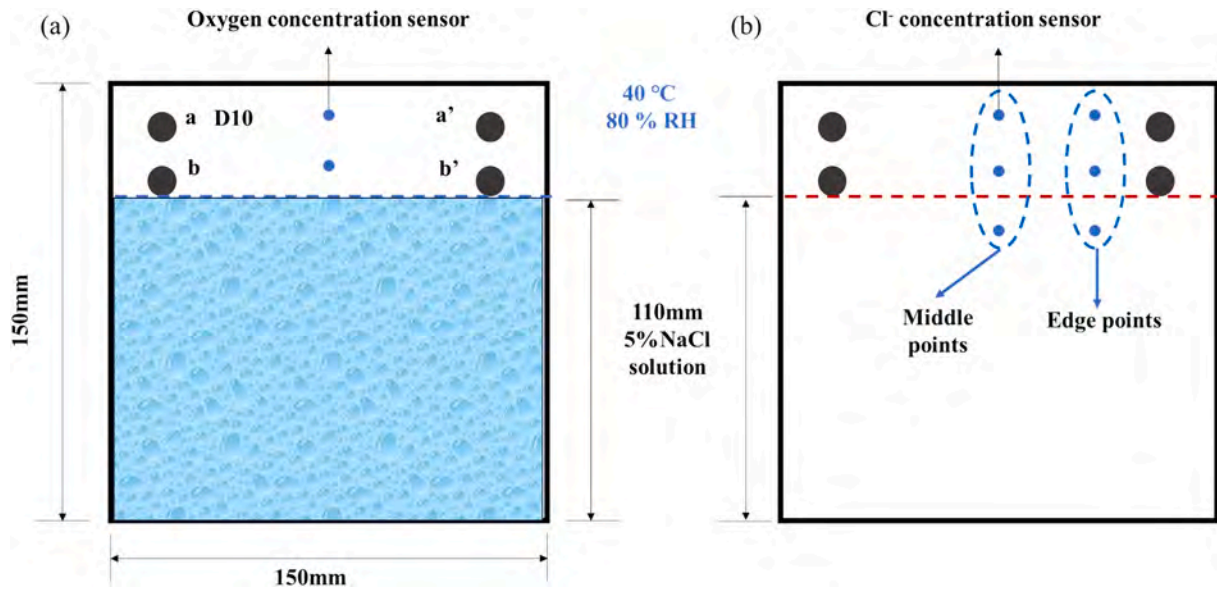


Fig. 8. Position of reinforcement relative to the water level in specimens [98]. (a) Locations of oxygen concentration sensors; (b) Locations of chloride concentration sensors.

Table 2
Modeling parameters used for model validation [98].

Parameter	Value	Parameter	Value
Concrete cover thickness (mm)	10	Chloride diffusion coefficient (m^2/s)	1.2×10^{-11}
Rebar diameter (mm)	10	Surface chloride concentration (wt.% of concrete)	0.677
Concrete section size (height $\times$ width, mm)	150×150	Initial chloride concentration (wt.% of concrete)	0
w/c	0.53	Oxygen diffusion coefficient (m^2/s)	1.64×10^{-9}
Environmental temperature (K)	313	Surface oxygen concentration (mol/m^3)	0.259
Relative humidity (%)	80	Other ions diffusion coefficient	See Table 1

3.3.1. Validation against time-varying oxygen concentration distribution

To validate the accuracy of the multi-ionic transport model,

experimental data from Zhang et al. [98] were adopted. The experimental setup and specimen dimensions are illustrated in Fig. 8. Oxygen concentrations were measured at 1 cm and 3 cm depths in mortar and concrete specimens (Fig. 8(a)). Chloride concentrations were measured at depths of 1, 3, and 5 cm, with two positions defined at each depth:

Table 3
Comparison of oxygen concentration prediction accuracy among models (based on experimental data shown in Fig. 9).

	Source	AM1	AM2	AC1	AC2	Average
MAE (1 cm)	This study	0.0065	0.0054	0.00566	0.00559	0.00579
	Zhang [98]	0.0116	0.0129	0.0113	0.0102	0.0098
MAE (3 cm)	This study	0.00782	0.00651	0.00766	0.00828	0.00757
	Zhang [98]	0.0096	0.0087	0.0112	0.0096	0.0115

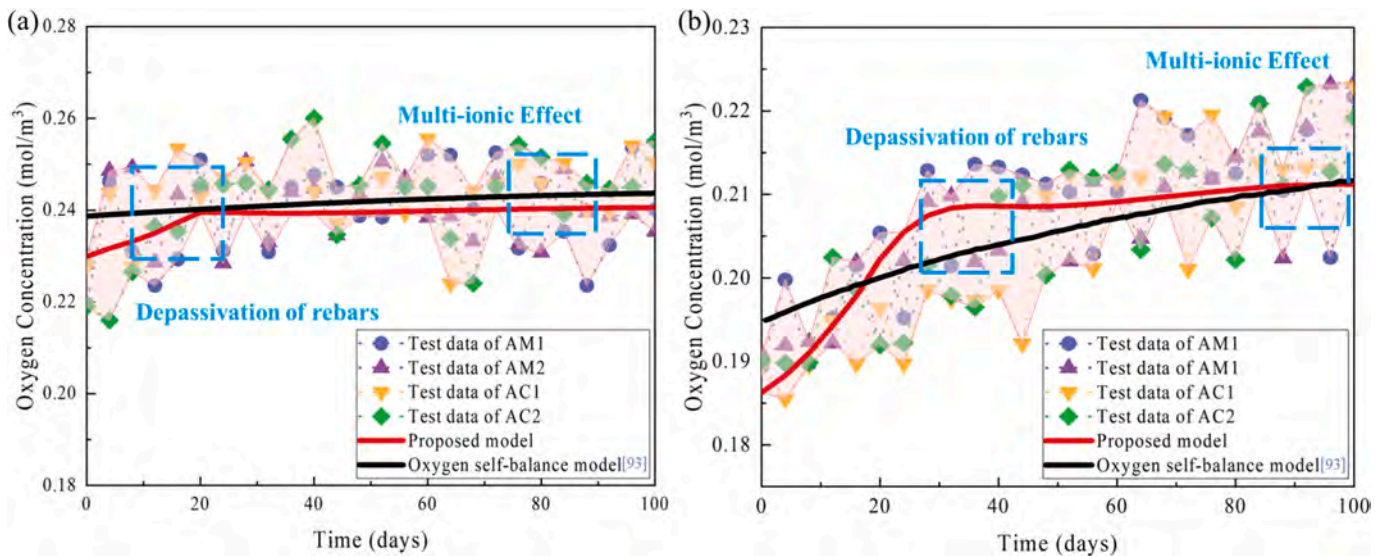


Fig. 9. Comparison of experimental and modeling oxygen concentrations: (a) At 1 cm depth; (b) At 3 cm depth.

middle points located 75 mm from the specimen edge and edge points located 25 mm from the edge (Fig. 8(b)). Specimens were named using a three-character code indicating size (A), material (M for mortar, C for concrete), and sequence number, while each specimen contained four rebars. The modeling parameters derived from experimental conditions are listed in Table 2.

The comparison between experimental measurements and model predictions is shown in Fig. 9, demonstrating good agreement across different depths. Model performance is further assessed by comparing the proposed model with the oxygen self-balance model of Zhang et al. [98], with mean absolute error (MAE) values reported in Table 3. Unlike the oxygen self-balance model, which considers only chloride and oxygen transport, the proposed model accounts for multi-ion migration and electrochemical coupling, enabling a more realistic description of ionic transport in concrete. Two notable differences are observed. First, the turning point in oxygen concentration is more pronounced in the proposed model. Mechanistically, this occurs because once depassivation initiates, the accelerated oxygen consumption associated with active corrosion delays its subsequent increase. Second, around 100 days, the predicted oxygen concentration is markedly lower. This is attributable to the coupling effect, where enhanced chloride ingress intensifies the corrosion current and, in turn, increases oxygen consumption at the rebar surface. A consistent improvement is also observed in the prediction of chloride concentration in mortar, as shown in Fig. 10 and quantified in Table 4. Although both models capture the overall trend of chloride ingress at different depths, the oxygen self-balance model exhibits a systematic underestimation of chloride concentration at edge locations, particularly at later exposure times. In contrast, the proposed model significantly reduces this conservative bias, leading to lower MAE and root mean square error (RMSE) values. At exposed edges, chloride migration is strongly influenced by local moisture conditions, ionic interactions, and corrosion-induced electrochemical reactions. By allowing chloride transport to interact with corrosion-current evolution and ionic redistribution, the proposed model better captures chloride accumulation near the rebar-concrete interface under critical boundary conditions. Collectively, the error metrics indicate improved predictive accuracy for both oxygen and chloride under the tested exposure conditions.

3.3.2. Validation against spatial distribution characteristics of rebar corrosion

Accurately predicting the spatial distribution of corrosion products is essential for modeling corrosion-induced crack initiation and

Table 4

Comparison of Cl^- concentration prediction accuracy among models (based on experimental data of mortar shown in Fig. 10).

Source	RMSE	MAE
This study	0.01169	0.00692
Zhang [98]	0.01250	0.00896

Table 5

Modeling parameters for corrosion validation.

Parameters	Value	Parameters	Value
Concrete cover thickness (mm) [99]	15	Chloride diffusion coefficient (m^2/s)	2.6×10^{-10}
Rebar diameter (mm) [99]	12	Surface chloride concentration (wt.% of cement) [99]	2
Environmental temperature ($^{\circ}\text{C}$)	20	Initial chloride concentration (wt.% of cement) [99]	0
Relative humidity (%)	75	Oxygen diffusion coefficient (m^2/s)	6.2×10^{-9}
Concrete section size (height $\times$ width, mm)	70×60	Surface oxygen concentration (mol/m^3)	0.268
w/c [99]	0.6	Initial oxygen concentration (mol/m^3)	0.156

propagation in concrete. To validate the proposed electrochemical corrosion model, numerical results are compared with the experiments of Ji et al. [37], who studied rebar corrosion under a natural exposure program following salt pre-conditioning. Rectangular specimens ($200 \text{ mm} \times 150 \text{ mm} \times 70 \text{ mm}$) with 12 mm rebar and 15 mm concrete cover were immersed in 10% NaCl at $(20 \pm 2)^{\circ}\text{C}$, followed by outdoor exposure for 4–6 months. Two specimens (A and B), representing different exposure durations and corrosion levels, were selected for validation. Ionic species, boundary conditions, and model parameters follow the preceding sections and relevant literature and are summarized in Table 5.

As shown in Fig. 11, the circumferential distribution of corrosion products thickness after 4–6 months of exposure was compared between the model values and the experimental results. For specimen A, results from the present model are compared with both the experimental profile and the model of Cheng et al. [100]; for specimen B, only the present model is compared with the measurements because Cheng et al. did not report corresponding numerical results. Cheng et al.'s model is primarily transport-driven (chloride-focused) and does not account for corrosion-

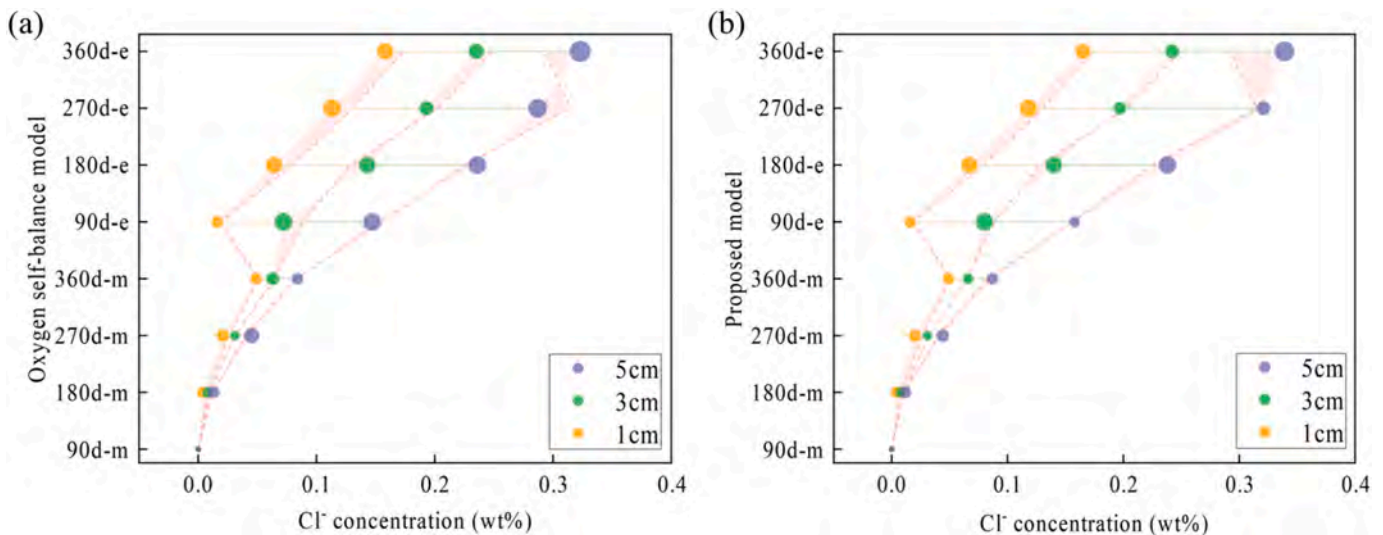


Fig. 10. Comparison of chloride concentration predictions (mortar): (a) Oxygen self-balance model [98]; (b) Proposed model. Note: Vertical axis: 90d-m (middle) and 90d-e (edge) measurements; horizontal axis: depth (1, 3, 5 cm). Marker size = error magnitude; red shade = error range.

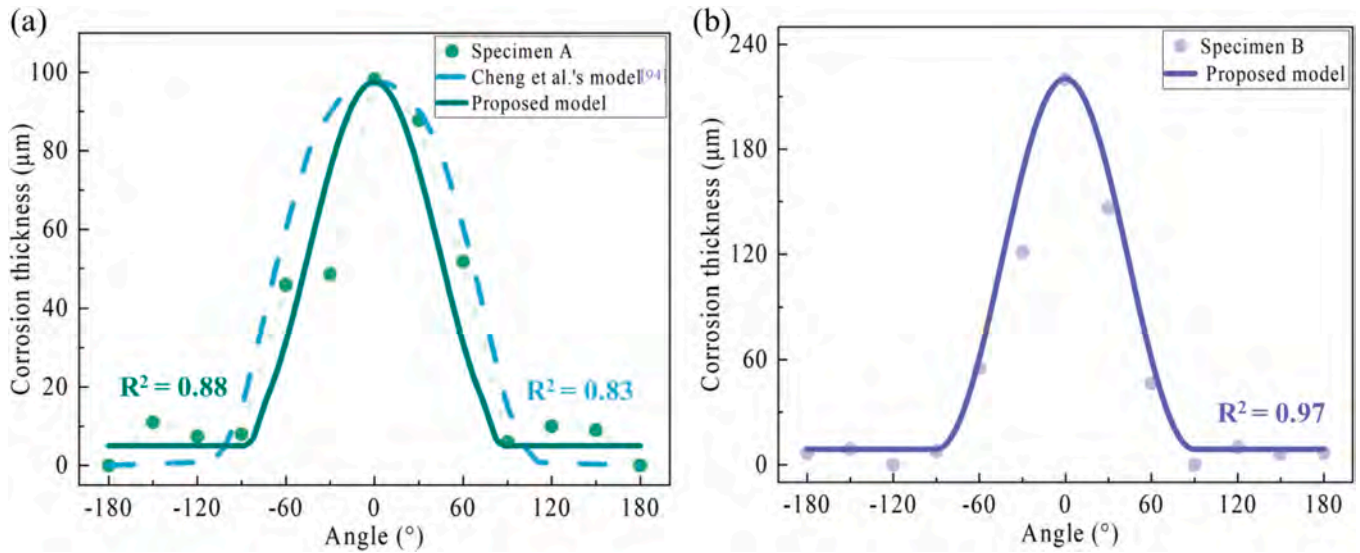


Fig. 11. Comparison of modeled and measured corrosion products thicknesses. (a) Specimen A; (b) Specimen B.

product redistribution and thickness reconstruction. By contrast, the present study integrates these factors, enabling a more comprehensive representation of the corrosion process. As illustrated in Fig. 11(a), incorporating modifications to the corrosion product distribution enables the proposed model to more accurately reproduce asymmetric accumulation, particularly the increased thickness of corrosion products on the opposite side where chloride ions enter. As can be observed in Fig. 11(b), the modeling results for specimen B also exhibit good agreement with the experimental data, indicating that the proposed model captures well the evolution of corrosion product thickness over time. From a mechanistic perspective, the proposed model provides a more realistic description of ion migration and corrosion-product deposition, which together influence redistribution around the reinforcement. Multi-ionic transport under natural exposure can accelerate corrosion, and including rebar volume loss improves the prediction of corrosion-layer thickness. The elliptical distribution reflects non-uniform transport conditions around the bar, leading to uneven accumulation in localized regions. The ability of the framework to reproduce this spatial pattern supports its capability to capture both the rate and the shape of corrosion-product formation.

3.3.3. Validation against crack propagation patterns

3.3.3.1. Validation considering aggregate distribution and ITZ effects. The accumulation and volumetric expansion of corrosion products generate internal stresses, leading to concrete cover cracking. To validate the proposed phase-field cracking model and assess the effects of aggregate distribution and ITZ properties, numerical results were compared with experimental data from Pedrosa et al. [101]. The specimens (150 mm × 150 mm) included 16 mm rebars and 20 mm covers. The model assumed uniform corrosion and applied boundary constraints to restrict lateral and bottom displacements. Material properties and phase-field parameters are listed in Table 6. Aggregates were randomly placed in the models, while CAD-based reconstruction was used to approximate the actual experimental configurations. For computational efficiency, the number of aggregates was reduced and the ITZ thickness was uniformly

set to 0.3 mm. Model predictions of crack evolution are presented in Fig. 12.

Fig. 12 compares cracking behavior with and without explicit aggregates/ITZ and with the experimental observation. The damage factor distribution ranges from dark blue (no damage) to red (complete failure), with a value of 1 indicating full cracking and structural failure. The model without heterogeneity (Fig. 12(a)) reproduces the overall crack trend, whereas incorporating aggregates and an explicit ITZ (Fig. 12(b)) yields closer agreement with the experimental crack morphology (Fig. 12(c)), indicating the importance of multiphase heterogeneity in corrosion-induced cracking. From a mechanical perspective, regions aligned with the rebar are more prone to cracking due to concentrated maximum principal stress. Cracks initiating from both sides of the rebar and extending toward the concrete cover. Such horizontal cracks can lead to delamination, threatening structural integrity and long-term performance. The inclusion of aggregate morphology and ITZ in the model accurately reproduces crack initiation and propagation. By treating the ITZ as a weak interface relative to the surrounding matrix, the model captures preferential crack propagation along these weak zones [103].

3.3.3.2. Validation against multi-rebar corrosion experiments at structural scale. To further assess the generalization capability of the proposed numerical framework, the model was applied to modeling corrosion-induced cracking in reinforced concrete members with a more complex reinforcement layout and a substantially larger structural scale than those considered previously. For this purpose, independent experimental results reported by Zahid et al. [90] were adopted as a benchmark. The panels measured 600 × 600 × 150 mm and contained five longitudinal rebars with a diameter of 19 mm and a concrete cover of 30 mm. Electrochemically accelerated corrosion was applied to all five rebars for 45 days. The concrete had a coarse aggregate volume fraction of ~ 40%, with a measured compressive strength of 42 MPa and an elastic modulus of 35 GPa. The corresponding geometric configuration and mechanical parameters implemented in the numerical model are summarized in Table 7.

Table 6
Material parameters for phase-field cracking model [84,91,102].

Material	Mortar				ITZ				Aggregate	
Parameter	$E_{0,m}$ (GPa)	$G_{f,m}$ (N/m)	$\nu_{0,m}$	$f_{t,m}$ (MPa)	$E_{0,itz}$ (GPa)	$G_{f,itz}$ (N/m)	$\nu_{0,itz}$	$f_{t,itz}$ (MPa)	$E_{0,agg}$ (GPa)	$\nu_{0,agg}$
Value	25	40	0.2	2.6	18	20	0.2	1.3	70	0.2

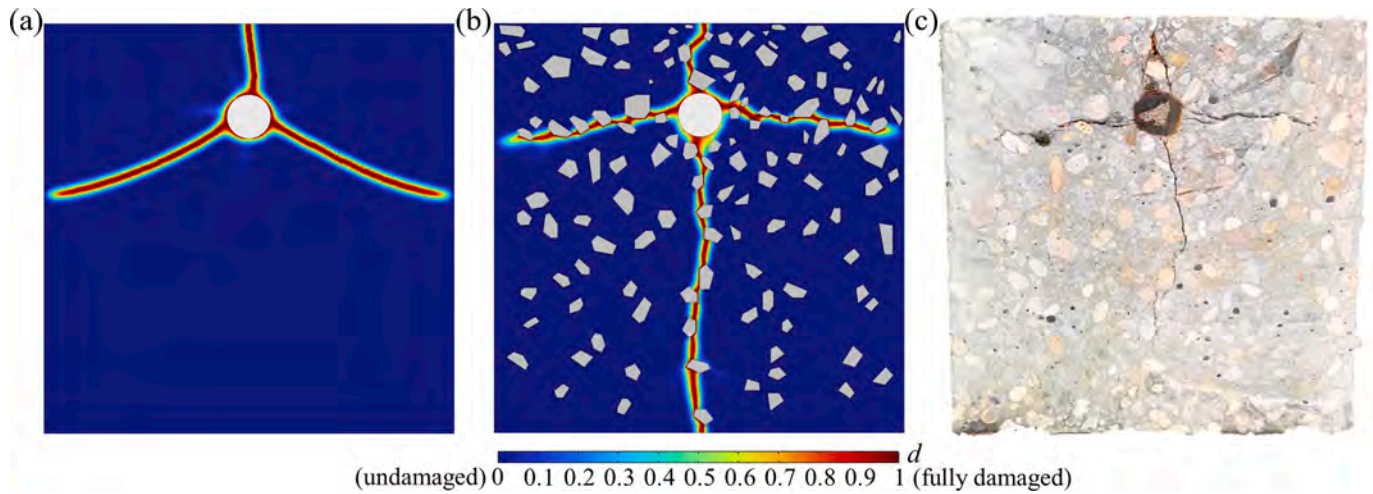


Fig. 12. Comparison between numerical and experimental crack patterns: (a) No consideration of multiphase; (b) Consideration of multiphase; (c) Experiment [101].

Table 7

Material parameters for phase-field cracking model [84,90,91,102].

Material	Mortar				ITZ				Aggregate	
Parameter	$E_{0,m}$ (GPa)	$G_{f,m}$ (N/m)	$\nu_{0,m}$	$f_{t,m}$ (MPa)	$E_{0,itz}$ (GPa)	$G_{f,itz}$ (N/m)	$\nu_{0,itz}$	$f_{t,itz}$ (MPa)	$E_{0,agg}$ (GPa)	$\nu_{0,agg}$
Value	25	60	0.2	6	12.5	30	0.2	3	70	0.2

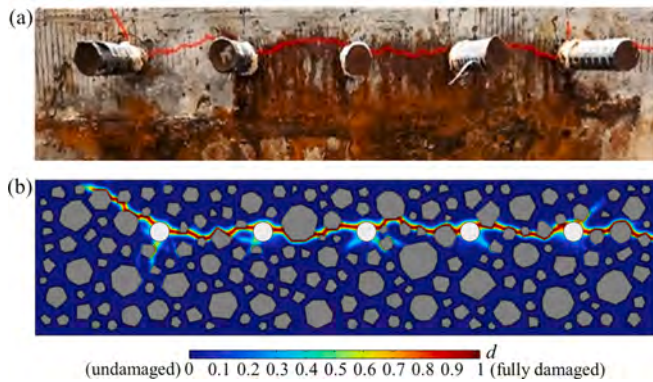


Fig. 13. Comparison between numerical and experimental crack patterns: (a) Experiment [90], (b) Modeling.

Fig. 13 compares the experimentally observed cracking pattern with the corresponding numerical prediction. In the experiment, corrosion of multiple adjacent rebars results in a dominant horizontal crack connecting neighboring rebars, together with several secondary cracks locally around individual bars. This pattern reflects the interaction between corrosion-induced expansion and the heterogeneous concrete microstructure. The numerical model well reproduces these key features. Local crack deflection and branching are also captured in modeling, particularly where aggregates interrupt the direct crack path, resulting in a tortuous crack trajectory similar to that observed experimentally. Overall, the agreement indicates that the framework captures both the global cracking mode associated with multi-rebar interaction and the local crack-path modulation induced by material heterogeneity.

4. Results and discussion

This chapter presents the main results and discussion of the proposed coupled framework. It begins with an overview of the key outputs (Section 4.1), then examines the effect of multi-physics coupling on

corrosion-cracking behavior, including the roles of crack evolution, multi-ionic interactions, and corrosion-product redistribution (Section 4.2). Followed by a sensitivity analysis that identifies the parameter groups most critical to transport, electrochemical response, and cracking predictions (Section 4.3).

4.1. Overview

This study systematically investigates rebar corrosion and concrete cracking under chloride attack. Before the parametric analysis, we examined the core multi-physics coupling effects: crack evolution, multi-ionic interactions, and corrosion product distribution. Building on these findings, extensive parametric studies assessed how material and structural properties influence the corrosion process. Unless noted otherwise, initial ion concentrations follow the reference values in Table 1. For computational efficiency, the internal concrete temperature is set to 290.5 K and the relative humidity to 78%, reflecting stable environmental conditions. Diffusion coefficients for O_2 and Cl^- are calculated using Eq. (A.9) to accurately represent the involved transport processes. The methods for determining diffusion coefficients in the ITZ and aggregates remain consistent with the previous section.

The model's boundary conditions reflect real-world engineering scenarios. The top surface is defined as a material flux boundary to model chloride or oxygen ingress, while the bottom surface is fixed to prevent vertical displacement, ensuring stability. In the following sections, unless otherwise specified, the baseline scenario adopts the following parameters: 8 mm rebar diameter, 12 mm concrete cover, 0.4 w/c ratio, 300 mol/m³ surface chloride concentration, 0.35 aggregate content, and 0.2 mm ITZ thickness.

4.2. Effect of the multi-physics coupling

4.2.1. Role of crack evolution in transport-corrosion coupling

The durability of reinforced concrete under chloride exposure is closely linked to crack evolution, which accelerates ion ingress. Traditional models often simplify cracking effects and estimate diffusion coefficients through empirical relations [104], which limits their ability to

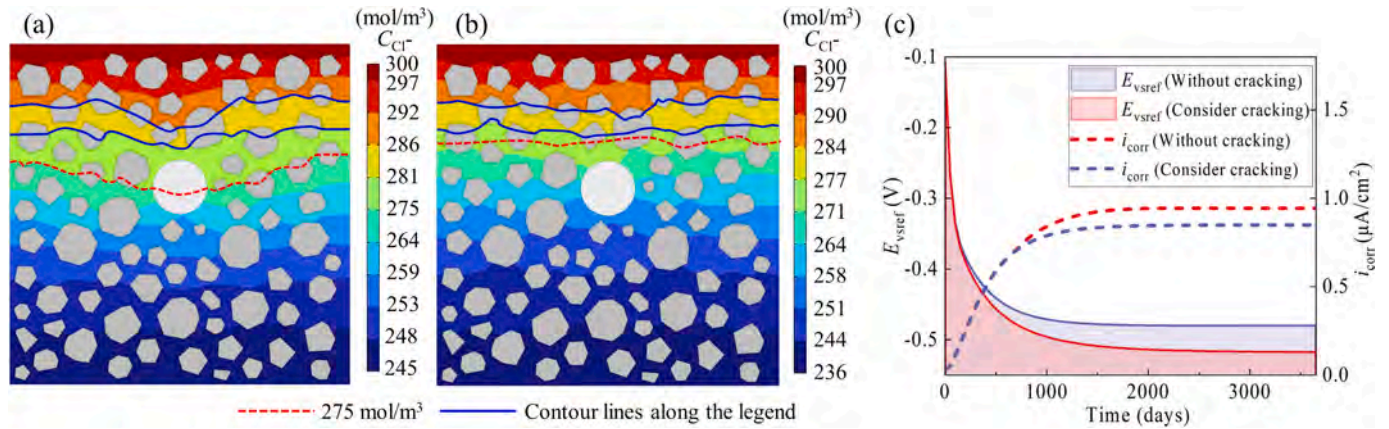


Fig. 14. Effect of crack evolution on chloride concentration fields and electrochemical response: (a) Coupled transport with crack evolution; (b) Uncoupled transport (without cracking); (c) Time histories of i_{corr} and E_{vsref} for cases with and without cracking. Note: The blue curves denote iso-concentration contours corresponding to the colorbar levels, and the red dashed curve highlights the $C_{Cl^-} = 275 \text{ mol/m}^3$ contour.

predict long-term degradation. As shown in Fig. 14(a)-(b), the proposed coupled model incorporating crack evolution predicts significantly deeper chloride ingress and a more pronounced redistribution of ionic species compared with the uncoupled case. Crack growth provides preferential pathways and increases the effective transport capacity, leading to steeper local concentration gradients, particularly at the rebar-concrete interface where chloride accumulation governs corrosion initiation.

Fig. 14(c) further illustrates that the presence of cracks results in a marked increase in corrosion current density (i_{corr}) and a more negative rebar reference potential (E_{vsref}) over time. This response is not only due to faster chloride delivery: enhanced multi-ionic transport requires the potential field to adjust to satisfy charge balance, which strengthens potential gradients and increases the migration contribution, thereby further reshaping interfacial ionic conditions consistent with the observed increase in i_{corr} and E_{vsref} . Quantitatively, the current density is elevated by approximately 15% and the potential shows an additional $\sim 10\%$ negative shift (normalized by the uncoupled value) at the end of the analyzed period. Kato et al. [105] similarly recognized the role of cracks in accelerating ionic transport. However, their approach treated cracks as static geometries with empirically prescribed diffusion coefficients, without capturing the time-dependent evolution of crack morphology or the two-way coupling between mechanical degradation

and electrochemical processes. In contrast, the present study integrates the dynamic progression of cracks and their feedback effects on ionic transport and corrosion kinetics within a multi-physics coupling framework, providing a more mechanistic and temporally consistent representation of how crack evolution influences the corrosion process.

4.2.2. Role of electromigration and multi-ionic coupling in transport

Understanding how multi-ionic transport and electrochemical fields shape ionic migration in cement-based materials is crucial for accurately modeling chloride-induced corrosion. Under actual service conditions, multi-ionic coexist and interact through diffusion, electromigration, and chemical reactions [106]. Fig. 15(a) therefore compares the predicted corrosion-related response obtained from a multi-ionic Nernst-Planck formulation that includes electromigration with that from a simplified chloride-oxygen transport model in which electromigration and multi-ionic coupling are omitted. Compared with the reduced model, the coupled model predicts a faster early-stage increase and a slightly higher plateau of C_{Cl^-} at the rebar-concrete interface, while the incremental increase gradually diminishes as the driving gradients decay and the transport pathway becomes more resistive. Consistent with Liu et al. [106], the chloride build-up exhibits a time-dependent accumulation accompanied by a reduced incremental transport efficiency.

Fig. 15(b) illustrates the spatial distribution of Ca^{2+} ions at 3000

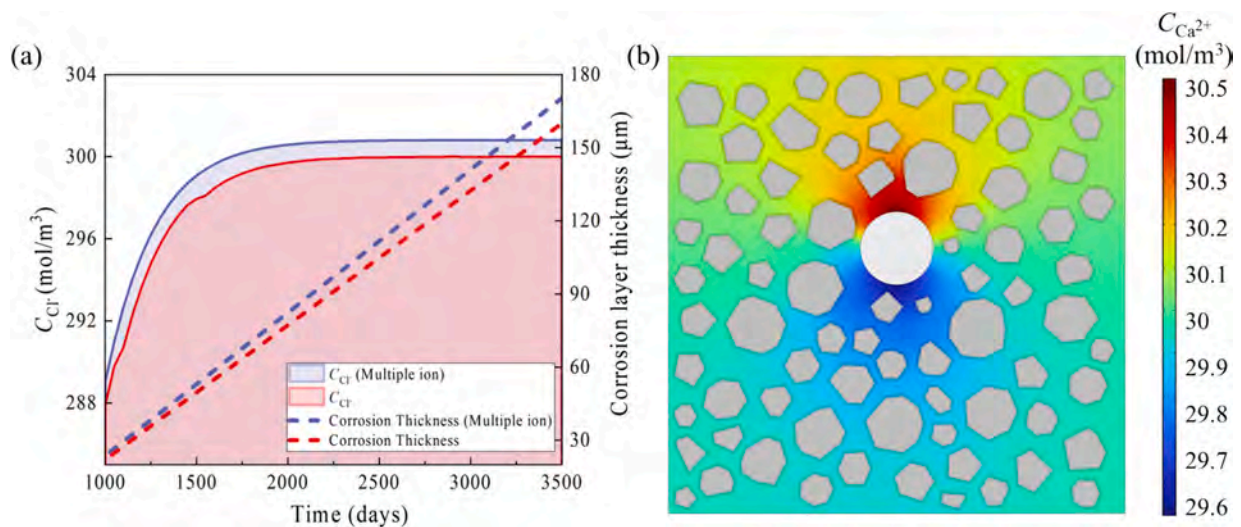


Fig. 15. Effects of multi-ionic electromigration on interfacial chloride accumulation and corrosion-product growth: (a) C_{Cl^-} and corrosion-layer thickness versus time (multi-ion vs. chloride-oxygen-only); (b) Distribution of Ca^{2+} concentration over 3000 days.

days, with pronounced enrichment on one polarized side of the rebar and depletion on the opposite side, indicating field-driven electromigration rather than diffusion alone. This redistribution highlights the inadequacy of conventional transport models that neglect electrical driving forces, and it can modify the local electrochemical microenvironment near the rebar surface [107]. Moreover, the coupled model predicts an enhancement of corrosion-product growth, yielding an $\sim 6\%$ increase in the ultimate corrosion-product layer thickness (evaluated at the end of the analyzed period). This response stems from the concurrent migration of multiple charged species driven by electrochemical-potential gradients, which can reduce ionic resistance and promote corrosion-product accumulation, in agreement with Meng et al. [58], who demonstrated that electromigration of various ions can enhance chloride transport efficiency in cementitious systems. These results demonstrate that multi-ion coupling with electromigration is essential for capturing corrosion-related transport in concrete.

4.2.3. Role of corrosion-product redistribution in crack development

The spatial-temporal distribution of corrosion products plays a critical role in cracking, yet traditional models often assume uniform expansion or rely on empirical relations, while in practice, corrosion products form and move in a non-uniform way, which causes local pressure and stage-dependent crack development. Fig. 16 presents a comparison between the conventional Faraday-based expansion model and the proposed multi-physics coupling framework. As shown in Fig. 16(a)–(b), the traditional model predicts earlier and more severe cracking because it assumes a constant corrosion-product loss ratio and a prescribed non-uniform distribution (e.g., an elliptical pattern), which can overestimate the effective expansion volume and thus the internal pressure driving damage. Consequently, cracking becomes more widespread with multiple possible paths, whereas the coupled model yields a more localized main crack pattern. In contrast, Fig. 16(c)–(e) demonstrate that the proposed model captures the complete evolution of

corrosion-induced cracking across three distinct temporal phases. During the latent phase (0–600 days), internal stresses progressively accumulate without visible cracking, reflecting progressive microstructural degradation. In the initiation phase (600–1200 days), a dominant crack emerges along the ITZ [94], aligning with the principal tensile stress direction. This is consistent with the findings of Peng et al. [40], who identified the ITZ as the preferential site for corrosion-induced damage initiation. The rapid rise in the ITZ damage index, exceeding that of the cement matrix (Fig. 16(f)), further supports this localized vulnerability. Finally, in the stable propagation phase (>1200 days), non-uniform rust expansion promotes secondary cracks and progressive crack connectivity, which enhances ionic transport and accelerates electrochemical degradation. Du et al. [108] reported similar three-stage behavior, but their model mainly emphasized corrosion ratio and expansion volume, without explicitly linking an evolving corrosion front and rust redistribution to damage localization through coupled multi-physics interactions.

Notably, the non-uniform distribution of corrosion products governs both the timing of crack initiation and the spatial characteristics and propagation mechanisms of cracking. This indicates that corrosion-induced cracking is a dynamic process driven by the synergistic interaction of electrochemical, transport, and mechanical fields.

4.3. Sensitivity analysis

4.3.1. Influence of crack diffusivity enhancement

To examine the influence of the diffusivity enhancement in cracked regions, the diffusivity in the cracked zone was set to 5 $\times$, 10 $\times$, and 20 $\times$ that of the intact concrete (denoted as 5 $\times$, 10 $\times$, and 20 $\times$). The top surface of the specimen is prescribed as a chloride ingress boundary with a constant chloride concentration of 500 mol/m³. The chloride concentration distributions at 450 days after crack formation are shown in Fig. 17. All three enhancement factors accelerate chloride transport

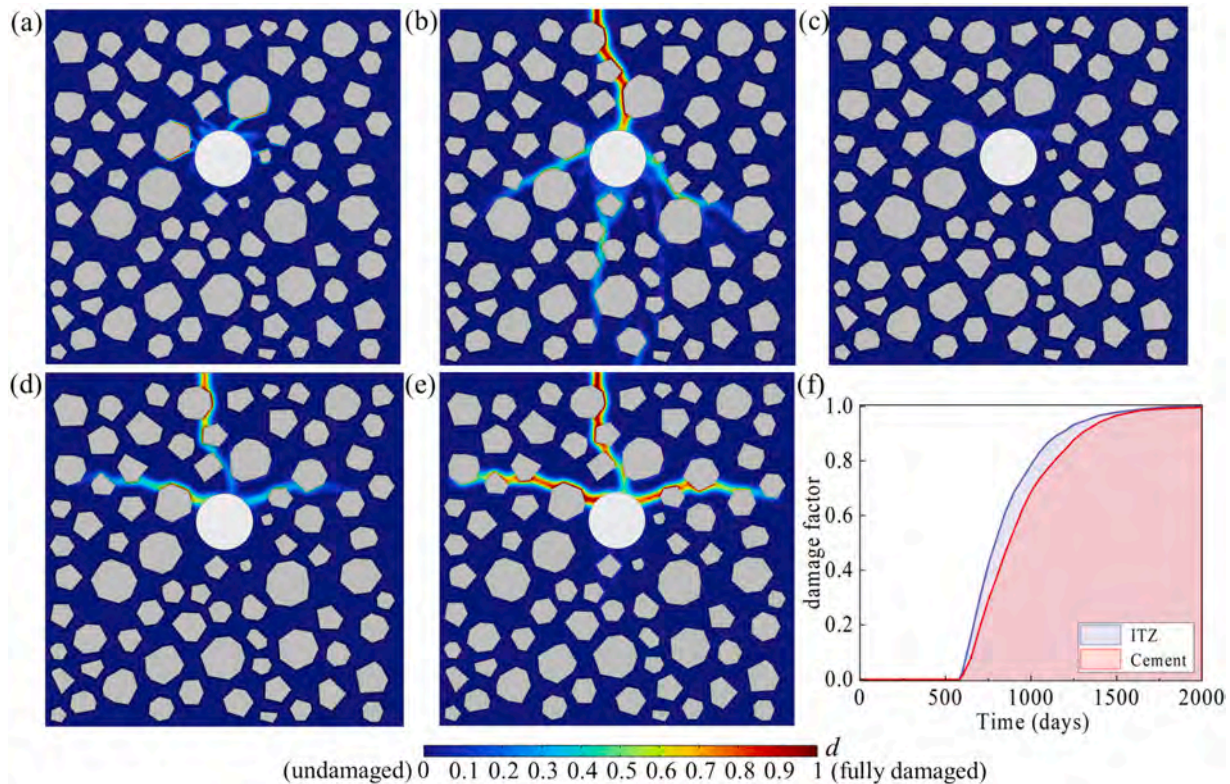


Fig. 16. Influence of corrosion products distribution on cracking evolution: (a–b) Crack morphology at 100 and 450 days under traditional Faraday's law; (c–e) Crack evolution over 600, 1200, and 2400 days under chloride exposure using the proposed framework; (f) Time-history of peak damage factors in the ITZ and cement matrix.

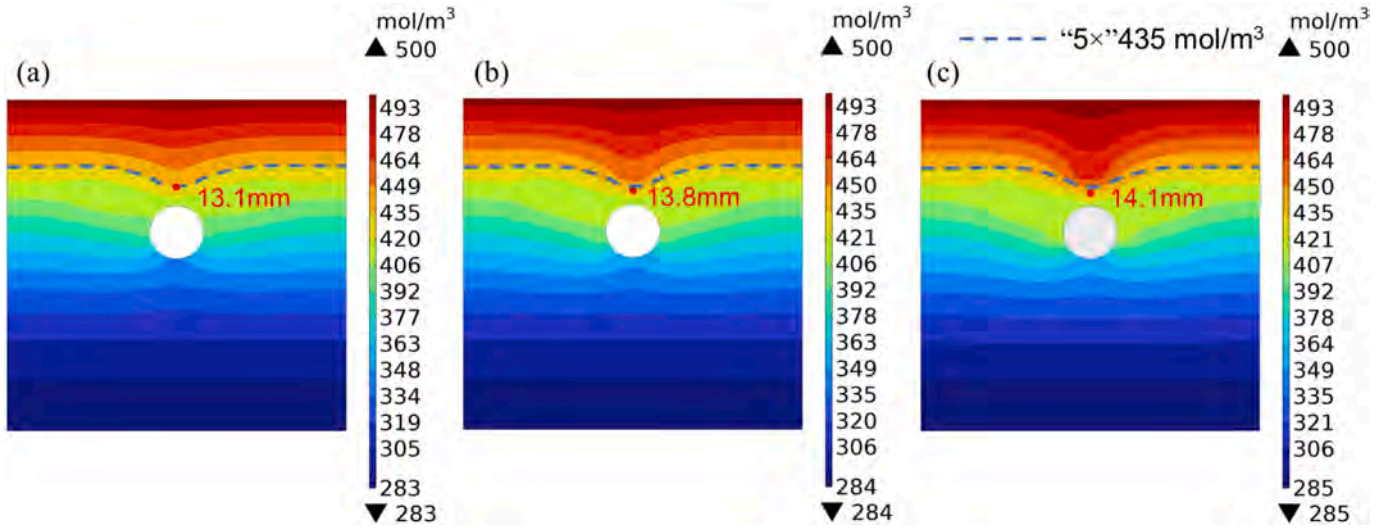


Fig. 17. Sensitivity of chloride concentration distribution to the diffusivity enhancement factor in cracked regions: (a) $5 \times$ enhancement factor; (b) $10 \times$ enhancement factor; (c) $20 \times$ enhancement factor. Note: Red markers indicate the chloride penetration depth at a concentration of 435 mol/m^3 . The blue dashed line denotes the 435 mol/m^3 isoline from the $5 \times$ case.

along the cracked region, whereas the overall concentration fields in the intact concrete remain nearly similar, indicating a limited sensitivity of the global field to the exact factor. Quantitative comparison of the chloride penetration front defined by the $C_{\text{Cl}^-} = 435 \text{ mol/m}^3$ contour shows that the difference in penetration depth between the $5 \times$ and $10 \times$ cases is within 5.4%, while the difference between the $10 \times$ and $20 \times$ cases is less than 2.2%. This suggests that the factor mainly influences local concentration gradients near the crack rather than the surrounding matrix.

Regarding the concentration patterns, higher enhancement factors (e.g., $20 \times$) lead to concentration patterns characteristic of wide and well-connected cracks, while lower values (e.g., $5 \times$) are more representative of narrow or micro-cracks with limited transport enhancement. Accordingly, $10 \times$ is adopted as a practical compromise to capture the dominant crack-assisted effect without unrealistically strong localization, consistent with previous studies on crack-assisted transport in cementitious materials [44]. Ideally, the diffusivity enhancement factor should vary with crack width and connectivity; however, using a constant value of $10 \times$ provides a stable and reasonable approximation within the present framework.

4.3.2. Influence of phase-field length scale

Mesh resolution and the phase-field length scale are critical for

accurate crack modeling. Here, we assess the sensitivity to the phase-field length scale b and the associated mesh resolution. A simplified $30 \text{ mm} \times 30 \text{ mm}$ concrete specimen was considered, with an aggregate volume fraction of 0.35 and an embedded rebar of 5 mm radius. Three phase-field length scales were examined: $b = 1.0 \text{ mm}$, $b = 1.25 \text{ mm}$, and $b = 1.5 \text{ mm}$. A graded mesh was adopted, with finer discretization applied to the ITZ and rebar-adjacent regions to resolve stress concentrations and capture crack initiation, and coarser elements used where the stress field varies smoothly. For all cases, the maximum element size satisfied $h_e \leq b/5$ throughout the domain, with smaller values in the ITZ.

As shown in Fig. 18, the predicted crack patterns are nearly identical for all three values of b , indicating that the global cracking pattern is insensitive to b under the present discretization criterion. Increasing b leads to more diffuse damage and reduced crack localization, whereas decreasing b produces sharper and more localized cracks. This improved resolution comes at a computational cost because mesh refinement increases the number of degrees of freedom; in the present setting, reducing the characteristic mesh size by 0.1 mm results in an approximately twofold increase in runtime. Therefore, b and the mesh size should be chosen so that the ITZ and the rebar-adjacent region remain well resolved, while avoiding unnecessary refinement in the bulk matrix where gradients are mild.

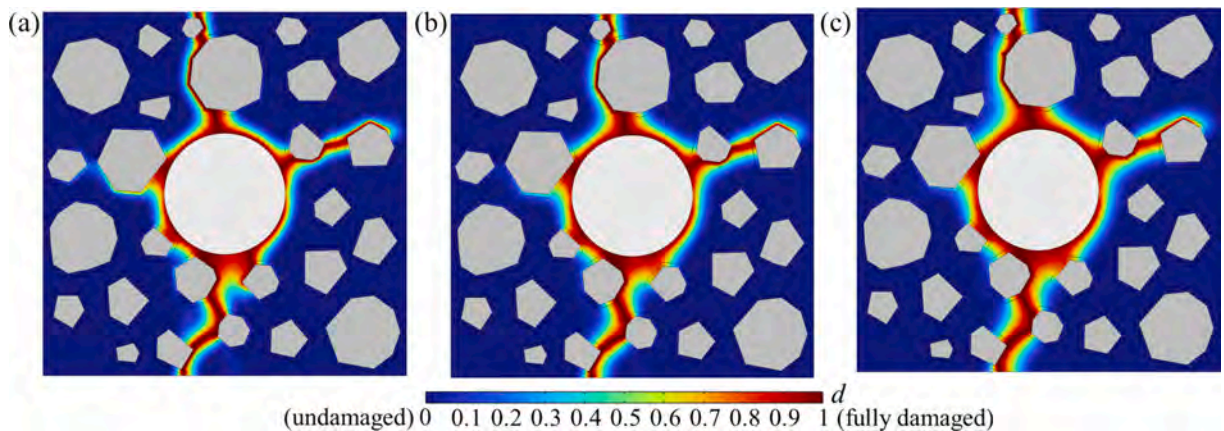


Fig. 18. Influence of phase-field length scale on crack patterns and damage localization. (a) Crack pattern for $b = 1.0 \text{ mm}$; (b) Crack pattern for $b = 1.25 \text{ mm}$; (c) Crack pattern for $b = 1.5 \text{ mm}$.

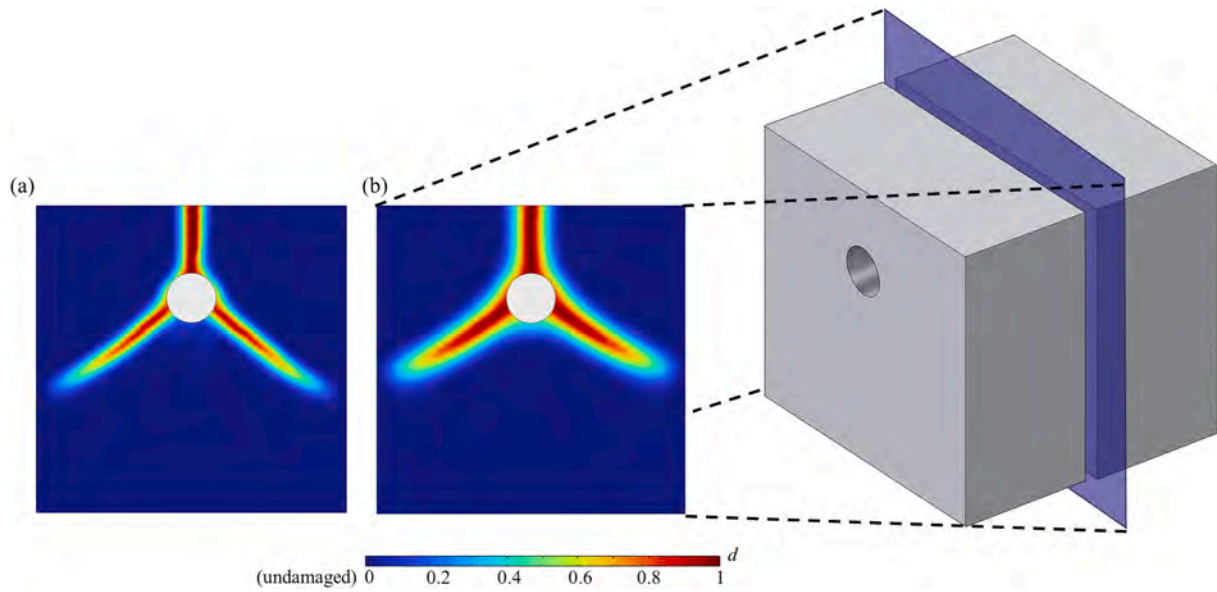


Fig. 19. Comparison between two-dimensional and three-dimensional phase-field crack predictions under identical conditions: (a) crack pattern predicted by the 2D phase-field model; (b) corresponding 3D slice extracted from the 3D model.

4.3.3. Influence of dimensional representation

Previous experimental and numerical studies support the use of a two-dimensional representative cross-section to investigate corrosion-induced cracking mechanisms. Zhang et al. [109] reported that initial surface cracks typically form directly above the reinforcing bar and subsequently propagate and coalesce into longitudinal cracks. Similarly, experimental studies by Alonso et al. [110] and Vidal et al. [111] demonstrated that crack initiation and propagation are primarily governed by the radial expansion of corrosion products and the tensile resistance of the surrounding concrete, indicating that the dominant fracture mechanisms are largely controlled by local cross-sectional processes.

To further assess the applicability of the proposed formulation beyond two dimensions, Fig. 19 compares phase-field damage patterns obtained from a 2D model and a representative slice extracted from the three-dimensional geometry under identical loading and material

conditions. The results show that the formulation can be applied in 3D and that the cracking pattern predicted on the extracted 3D slice agrees well with the corresponding 2D model. This agreement suggests that, for cases where material distribution and boundary conditions are approximately uniform in the out-of-plane direction, 2D models can provide a representative description of the three-dimensional cracking response. Nevertheless, even for the 3D slice model shown in Fig. 19(b) requires more than $10 \times$ the computational effort of the corresponding 2D case in Fig. 19(a), and is more prone to convergence difficulties.

Moreover, when structural geometry, corrosion intensity, or material heterogeneity varies markedly along the reinforcement length, a single 2D cross-section is no longer sufficient to characterize the overall cracking behavior. In such cases, crack initiation and propagation tend to localize along mechanically weaker planes or regions with unfavorable geometric or material features. To address this, a practical strategy involves first identifying critical sections via coarse 3D analysis and

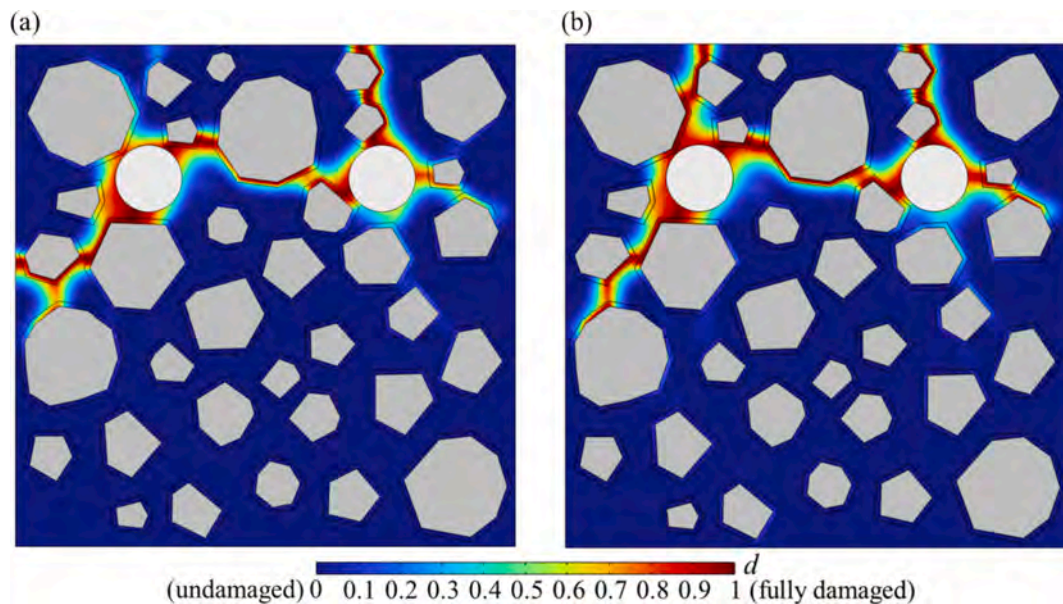


Fig. 20. Sensitivity of corrosion-induced cracking patterns to ITZ tensile strength: (a) $f_{t,ITZ} = 0.5$ MPa; (b) $f_{t,ITZ} = 1.0$ MPa.

subsequently conducting targeted 2D phase-field crack analyses on these vulnerable planes. This hybrid approach captures key three-dimensional effects while avoiding the prohibitive computational cost of fully resolved 3D phase-field fracture models. Accordingly, the present 2D modeling framework should be viewed as an efficient approximation within its intended scope, rather than as a full substitute for comprehensive 3D analysis.

4.3.4. Influence of ITZ fracture properties

The mechanical properties of the interfacial transition zone (ITZ), particularly tensile strength and fracture energy, are difficult to measure directly and are known to vary with aggregate type, surface roughness, and curing conditions [112]. To assess the influence of uncertainties in ITZ fracture properties on corrosion-induced cracking, a sensitivity study is performed on a representative concrete specimen (30×30 mm) with a centrally embedded rebar (diameter = 4 mm).

Two cases are examined by assigning the ITZ tensile strength as $f_{t,itz} = 0.5$ MPa and 1.0 MPa [112], respectively, while keeping the ITZ fracture energy unchanged. The resulting phase-field damage distributions are shown in Fig. 20. Reducing the ITZ tensile strength promotes preferential cracking along the ITZ network and increases the tendency for near-rebar horizontal cracking, thereby facilitating cover delamination (Fig. 20(a)). In contrast, a stronger ITZ delays crack initiation along the interface and leads to a more distributed cracking response, in which cracks are less constrained to propagate along the ITZ and are more likely to cut through the surrounding matrix (Fig. 20(b)).

The influence of ITZ fracture energy is further examined by selecting two representative values, $G_{f,itz} = 7$ N/m and 30 N/m, within experimentally reported ranges for Portland cement-based materials [112]. Variations in ITZ fracture energy have a limited effect on the global cracking mode but markedly influence the spatial distribution of damage. For the lower fracture energy case (Fig. 21(a)), cracking becomes more strongly confined to the ITZ network, with more pronounced fine cracking within the concrete interior. By contrast, a higher ITZ fracture energy (Fig. 21(b)) promotes a more even distribution of cracks between the matrix and interface regions, resulting in less ITZ-dominated crack paths. Overall, these results highlight the importance of explicitly accounting for *meso*-scale heterogeneity in corrosion–cracking analyses.

4.3.5. Influence of electrochemical equilibrium potentials

To evaluate the sensitivity of the predicted cracking behavior to

electrochemical parameters, a comparative analysis was performed by varying the anodic and cathodic equilibrium potentials while keeping all other model inputs unchanged. The aggregate volume fraction was fixed at 0.4, the concrete cover thickness was 17 mm, and a constant chloride concentration of 300 mol/m^3 was imposed at the external boundary. The phase-field damage distributions corresponding to the two sets of electrochemical equilibrium potentials are shown in Fig. 22. In Fig. 22(a), the anodic and cathodic equilibrium potentials were set to -0.4 V and 0.4 V, respectively, whereas in Fig. 22(b) they were adopted as -0.78 V and 0.16 V, which are commonly adopted for rebar corrosion in alkaline pore solutions [75]. Compared with Fig. 22(b), the electrochemical parameter set in Fig. 22(a) delays crack initiation by approximately 300–400 days, indicating a lower corrosion rate and a slower accumulation of corrosion products. This delay is attributed to the reduced effective overpotential associated with the equilibrium potentials adopted in Fig. 22(a), which leads to smaller corrosion current densities and postpones the development of critical expansive stresses in the surrounding concrete.

Notably, despite the difference in crack initiation time, the overall crack morphology remains largely consistent between the two cases. In both scenarios, cracking initiates near the reinforcing bar and preferentially propagates along mechanically weakened paths governed by the aggregate distribution and ITZ properties, resulting in similar dominant crack pattern.

4.3.6. Sensitivity ranking and dominant controls

By varying key model inputs and quantitatively comparing the overlap of the resulting crack patterns, we identify the parameters that most strongly control crack morphology. Within the investigated ranges, the ITZ tensile strength is the most influential factor, resulting in a 23.4% difference in crack morphology, whereas the ITZ fracture energy has a secondary effect (5.46%). By contrast, variations in electrochemical parameters and switching between 2D and 3D models induce comparatively minor changes in crack geometry, with crack-pattern differences consistently below 5%.

In addition, we performed a quantitative screening of time-to-cracking by introducing a normalized sensitivity index S [113], defined as the relative change in cracking time induced by a relative perturbation of a given input parameter. This normalization enables meaningful comparisons across heterogeneous parameters. Based on the available sensitivity cases, electrochemical parameters exert the

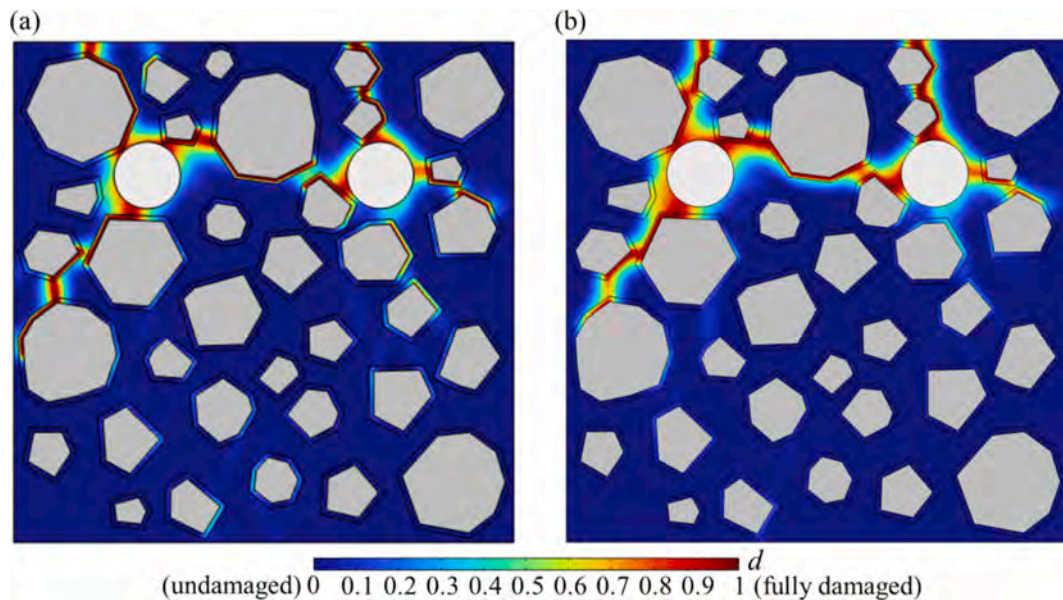


Fig. 21. Sensitivity of corrosion-induced cracking patterns to ITZ fracture energy: (a) $G_{f,itz} = 7$ N/m; (b) $G_{f,itz} = 30$ N/m.

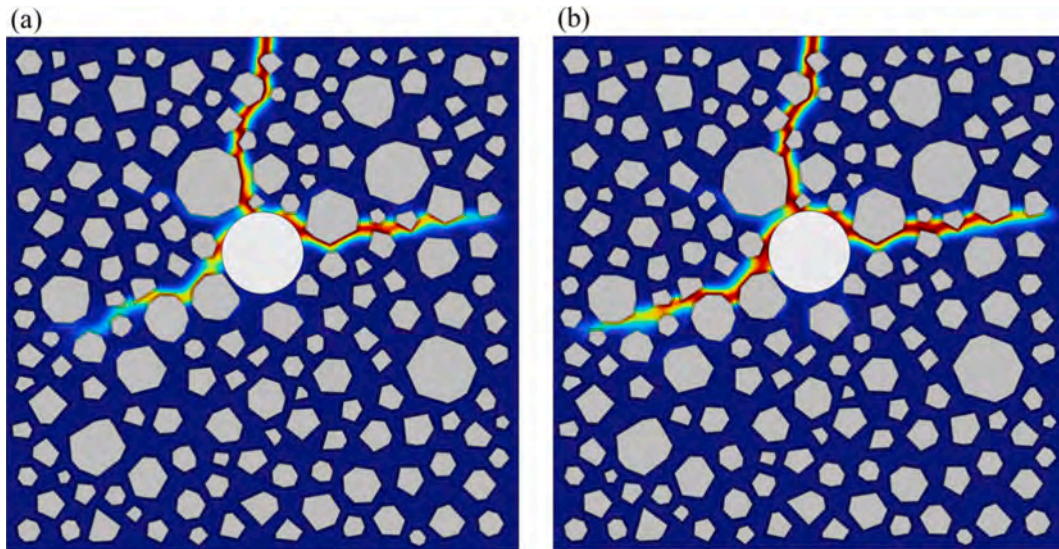


Fig. 22. Sensitivity of corrosion-induced cracking behavior to electrochemical equilibrium potentials. (a) Anodic and cathodic equilibrium potentials of -0.4 V and 0.4 V; (b) Anodic and cathodic equilibrium potentials of -0.78 V and 0.16 V.

strongest influence on cracking time ($S = 1.06$), followed by the non-uniformity of rust-expansion distribution ($S \approx 0.68$). In contrast, the crack-zone diffusivity enhancement factor shows only a minor effect on the cracking-time scale ($S \approx 0.1$), consistent with its primary role in modifying local chloride gradients rather than governing global crack-initiation timing.

Overall, the sensitivity is output-dependent: crack morphology is governed primarily by tensile strength, whereas the time-to-cracking is controlled mainly by electrochemical parameters.

5. Conclusions

This study establishes a multi-physics coupling framework to investigate chloride-induced rebar corrosion and the resulting concrete cracking. The framework incorporates moisture migration, chemical transport, electrochemical reactions, and mechanical damage to capture the interactions among environmental exposure, electrochemical processes, and structural degradation. The key findings are summarized as follows:

- 1) The developed framework, validated against experimental data, accurately reproduces ion concentration distributions, corrosion-layer growth, and crack propagation in chloride-exposed reinforced concrete. Its predictions demonstrate reliable agreement with experimental measurements for chloride and oxygen concentrations ($\text{MAE} < 0.008$), corrosion-layer thickness ($R^2 > 0.85$), and cracking morphology across both single-rebar and multi-rebar configurations.
- 2) By integrating multi-ionic interactions, electrochemical effects, and crack evolution, the framework offers a more comprehensive representation of coupled deterioration than conventional approaches. It captures both crack initiation and the transition from stable to progressive growth, thereby clarifying the feedback between cracking and electrochemical processes.
- 3) Model-predicted parametric trends indicate that neglecting multi-ion effects or electromigration underestimates chloride ingress, whereas explicitly accounting for crack-induced transport increases peak current density and electrochemical potential by over 10%. Furthermore, considering the spatially non-uniform distribution of corrosion products mitigates errors such as premature or overly intensified cracking.
- 4) Sensitivity analyses demonstrate that model outputs are parameter-dependent: mechanical parameters (especially ITZ tensile strength)

govern crack morphology, resulting in a 23.4% difference in crack patterns, whereas electrochemical parameters primarily control the time-to-cracking with a normalized sensitivity index of $S = 1.06$.

From an engineering perspective, the proposed framework facilitates durability-oriented design by delivering quantitative outputs—such as ion transport behavior, corrosion-layer growth, crack initiation and propagation, and electrochemical responses. For service-life assessment, the analyses further identify the key factors governing corrosion development and cracking progression. Consequently, the framework serves as a mechanism-based complement to conventional code-based durability design, rather than a direct replacement for empirical design rules.

It should be emphasized that the present study is developed for unsaturated chloride transport in OPC-based concrete without wet-dry cycling. Moisture effects and chloride binding are included, and corrosion is modeled as spatially non-uniform under the local ionic and electrochemical fields. Within this scope, the experimentally supported conclusions are limited to ion transport behavior, corrosion, and cracking morphology. Parametric trends and any conclusions drawn beyond this scope should be viewed as model-based mechanistic insights. Moreover, the validation uses multiple datasets that focus on separate processes; a single fully integrated experimental validation covering the entire deterioration chain—from chloride ingress to corrosion initiation and subsequent crack propagation—is not yet available and remains an important direction for future work.

Beyond the validated scope discussed above, several aspects warrant further investigation. While the present study focuses on a specific modeling framework, certain parameters are adopted from established literature rather than independently calibrated for all material compositions and exposure conditions; consequently, a comprehensive global sensitivity or uncertainty analysis falls outside the current scope. Although key transport processes account for temperature and humidity effects through their influence on chloride and oxygen diffusivities, the independent, time-varying impacts of these environmental factors are not explicitly explored and require dedicated future study [114]. Additional considerations—such as time-dependent environmental boundary conditions, uncertainties in moisture-retention parameters, aggregate heterogeneity, fully resolved three-dimensional crack development, and detailed corrosion-product characteristics—remain critical avenues for future research. Addressing these aspects will enhance the engineering applicability of the proposed framework for service-life

assessment and may complement conventional code-based durability design approaches.

CRediT authorship contribution statement

Panyue Gao: Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Xuan Gao:** Writing – review & editing, Methodology, Data curation. **Liang-yu Tong:** Writing – review & editing, Investigation, Formal analysis. **Zhaozheng Meng:** Writing – review & editing, Software, Formal analysis. **Qing-xiang Xiong:** Writing – review & editing, Investigation, Formal analysis. **Liberato Ferrara:** Writing – review & editing, Investigation, Formal analysis. **Qing-feng Liu:** Writing – review & editing, Supervision, Resources, Project administration, Methodology, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial

interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix 1. Calculation of diffusion coefficients for chloride ions and oxygen taking into account the effect of temperature and humidity

Based on the GEM theory, the relationship between the transport properties of cement paste and capillary porosity can be characterized by electrical conductivity, where the cement paste is composed of the solid phase and the pore solution [115–117]. According to the Nernst-Einstein [118,119] relation, the relative diffusion coefficient (D_s/D_0) equals the relative electrical conductivity (σ_{solid}/σ_0), which leads to the solid phase relative diffusivity [120]:

$$\frac{D_s}{D_0} = 0.00357 \times \left[1 - \frac{1}{1 + (2\phi)^{5.85}} \right] \quad (A.1)$$

where D_s (m^2/s) is the chloride diffusivity in the cement paste solid phase, and D_0 is the chloride diffusivity in the concrete pore solution, which is $2.032 \times 10^{-9} \text{ m}^2/\text{s}$. The relative diffusivity of chloride ions in cement paste ($D_{Cl,p}/D_0$) can be calculated from the solid phase relative diffusivity (D_s/D_0) [120]:

$$\frac{D_{Cl,p}}{D_0} = \left\{ m_{\phi_{cp}} + \sqrt{m_{\phi_{cp}}^2 + \frac{\phi_c}{1 - \phi_c} \left(\frac{D_s}{D_0} \right)^{\frac{1}{\tau_1}}} \right\}^{\tau_1} \quad (A.2)$$

where $m_{\phi_{cp}}$ is a coefficient related to porosity and concrete composition [118]:

$$m_{\phi_{cp}} = \frac{1}{2} \left\{ \left(\frac{D_s}{D_0} \right)^{\frac{1}{\tau_1}} + \frac{\phi_{cp}}{1 - \phi_c} \bullet \left[1 - \left(\frac{D_s}{D_0} \right)^{\frac{1}{\tau_1}} \right] - \frac{\phi_c}{1 - \phi_c} \right\} \quad (A.3)$$

For different concrete compositions, τ_1 varies, being 2.7 for Portland cement paste and 4.5 for cement paste with silica fume [119]. ϕ_c represents the critical porosity for pore network percolation, approximately 0.18 for various w/c in cement-based materials [121]. ϕ_{cp} is the capillary porosity of cement paste, which can be calculated using a modified Powers model [118]:

$$\phi_{cp} = 1 - \frac{1 + 1.31\theta}{1 + 3.2w/c} \quad (A.4)$$

Oxygen, as a key reactant in the cathodic reaction, has a diffusion coefficient at 25°C [122]:

$$D_{O_2,p} = 1.92 \times 10^{-6} \times \phi_{cp}^{1.8} \quad (A.5)$$

Considering the effects of temperature and humidity on material diffusivity, this study introduced temperature and humidity correction factors. The humidity impact factor for chloride ion diffusivity is given by [123]:

$$F_{Cl}(H) = \left[1 + \frac{[1 - H(t)]^4}{(1 - H_c)^4} \right]^{-1} \quad (A.6)$$

where $F_{Cl}(H)$ represents the humidity impact factor for chloride ion diffusivity, $H(t)$ is the humidity of the internal environment over time, and $H_c = 0.75$ is the critical humidity [123]. The humidity impact factor for oxygen diffusivity is expressed as [122]:

$$F_{O_2}(H) = [1 - H(t)]^{2.2} \quad (A.7)$$

The temperature impact factor on material diffusivity is described by the Arrhenius law [123].

$$F_j(T) = \exp\left\{\frac{E_a}{R} \times \left[\frac{1}{T_0} - \frac{1}{T(t)}\right]\right\} \quad (\text{A.8})$$

where $F_j(T)$ represents the temperature impact factor, with j represents different diffusing substances (Cl^- or O_2). $T(t)$ is the temperature of the concrete internal environment over time, E_a (kJ/mol) is the activation energy for material diffusion, $T_0 = 296$ K is the reference temperature for chloride ions [124], and the reference temperature for oxygen is 298.15 K [122]. The activation energy is related to the w/c and the amount of mineral admixtures, with values for ordinary Portland cement listed in Table A1 [125,126]:

Table A1

Relationship between activation energy (E_a) and the w/c .

w/c	Activation energy of oxygen (kJ/mol)	Activation energy of chloride (kJ/mol)
0.4	19.0 ± 0.5	41.8 ± 4.0
0.5	22.0 ± 2.4	44.6 ± 4.3
0.6	14.9 ± 2.8	32.0 ± 2.4

This energy parameter governs the temperature dependence of ionic transport, influencing the diffusion rates of corrosive agents such as chloride and oxygen in concrete. To ensure accurate modeling under varying environmental conditions, practical applications should consider the temperature and humidity conditions, which are adjusted to match the experimental setup, ensuring consistency with the conditions under which the measurements were obtained. Building on this, the final diffusion coefficient can be expressed as follows [28]:

$$D_j(t) = D_{j,p} \times F_j(T) \times F_j(H) \quad (\text{A.9})$$

Appendix 2. Summary of parameters and corresponding abbreviations used in this study

Parameters	Abbreviation	Parameters	Abbreviation
C_k	Ionic concentration of species k	J_k	The ionic flux of species k
z_k	The ionic charge	F	Faraday constant
R	The universal gas constant	T	Absolute temperature
ϕ	The electrostatic potential	v	The pore solution velocity
$D(h)$	Humidity-dependent diffusion coefficient	∇h	The gradient of saturation
α_0	Empirical parameters	h_c	Empirical parameters
m	Empirical parameters	D_{sat}	The saturated moisture diffusivity
f_{ck}	Concrete compressive strength	$D_{1,0}$	The reference moisture diffusion coefficient
f_{ck0}	The reference compressive strength	f_{cm}	The average compressive strength
B_{Cl^-}	Bound chloride ions	C_{Cl^-}	Free chloride ions
β	Empirical parameters	α	Empirical parameters
w_a	The chemically bound water per unit mass of cement	ϱ	The hydration degree
w/c	The water to cement ratio	ξ	Correction factor
R_k	Source or sink terms from chemical reactions	k_{sp}	Solubility product constant
$R_{s,\text{Fe}^{2+}}$	Consumption rate of Fe^{2+}	R_{s,OH^-}	Consumption rate of OH^-
k_s	Precipitation rate constant	$H(\mu)$	The heaviside step function
n	The unit outward normal vector to the interface	N	The total number of ionic species
μ	A dimensionless index	σ	Conductivity of the electrolyte conductivity,
D_k	Effective diffusion coefficient	$D_{k,c}$	Corresponding value in cracked regions
D_k^*	The effective transport coefficient of cracked concrete	$\phi_0 \text{ Fe}$	Anodic equilibrium potential
ϕ_M	The metal phase potential	ϕ_L	Electrolyte phase potential
i_{Fe}	Anodic current density	β_{Fe}	Anodic Tafel slope
β_{Fe}	Corrected Tafel slope	$i_0 \text{ Fe}$	Anodic exchange current density
C_{Cl^+}	Free chloride concentration at the rebar surface	f_{Cl}	Concentration-dependent factor
i_{O_2}	Cathodic current density	$\phi_0 \text{ O}_2$	Cathodic equilibrium potential
$i_0 \text{ O}_2$	Cathodic exchange current density	β_{O_2}	Cathodic Tafel slope
z_{O_2}	The four-electron reduction of oxygen in the cathodic reaction	i_L	Oxygen diffusion limiting current density
CS O_2	Oxygen concentration of concrete surface	a	The vertical diffusion distance from the concrete surface
θ	The circumferential coordinate along the rebar surface	t	The exposure time
$d_{\text{corr}}(\theta, t)$	The corrosion depth	A_{Fe}	Atomic mass of Fe
L_{corr}	The corroded rebar length	ρ_{Fe}	The density of Fe
η	The volumetric expansion coefficient	V_{corr}	Theoretical expansion volume
V_{CAR}	The volume of corrosion products retained in the capillary adjustment region	$V_{\text{corr,eff}}$	The effective expansion volume of corrosion products
$\Delta V_{\text{crack},s}$	The increments of crack volume over the current time step t_s	V_{flow}	The volume of corrosion products that have migrated into cracks
ϕ_{cp}	The capillary porosity of cement paste	$V_{\text{flow},s}$	The cumulative volume of corrosion products that have migrated into cracks up to time step t_s
CAR_{max}	The physical limit of corrosion products accumulation within the pore space between the rebar and concrete	$\Delta V_{\text{corr},s}$	The corrosion-product expansion volume over the current time step t_s
Φ_2	The fraction of production-limited condition	V_{CM}	The matrix volume
$f(\theta)$	The dimensionless shape function	Φ_1	The fraction of newly formed crack volume
μ_1	The maximum corrosion-layer thickness	$\mu(\theta)$	The local corrosion-layer thickness
σ_s	Stress tensor	ζ	The ratio between minimum and maximum corrosion-layer thickness
Q	The phase-field source term	q	The flux related to the crack phase-field

(continued on next page)

(continued)

Parameters	Abbreviation	Parameters	Abbreviation
∇d	Spatial variation of damage	b^*	Force per unit volume applied to the domain
G_f	The fracture energy	b	The length scale parameter
$\partial\Omega$	Outer boundary	Y	The driving force
$u^*(x)$	Displacement	$\partial\Omega_u$	The displacement boundary condition
$\partial\Omega_t$	The traction boundary condition	$t^*(x)$	Traction
δ	Shape parameter	$\bar{Y}$	The effective crack-driving force
P	Parameter in the energy degradation function	$\omega(d)$	The energy degradation function
b_2	Parameter in the energy degradation function	$a(d)$	The crack geometry function
$\mathfrak{H}_s$	History-type regularization variable at time step t_s	c_α	Normalization constant
$\bar{Y}_s$	The effective crack-driving force at time step t_s	b_1	Parameter in the energy degradation function
f_t	The uniaxial tensile strength	b_3	Parameter in the energy degradation function
E^*	The elastic modulus after cracking	t_s	The time at the s -th time step
w_d	Crack width	$\mathfrak{H}_0$	Initial value of history-type regularization variable
V_{crack}	Crack surface measure	E	Undamaged elastic modulus
$CO\ k$	Initial concentration of species k	ε	Total strain
$D_{k,m}$	Diffusion coefficients of species k in the uncracked mortar matrix	$\gamma_l(d, \nabla d)$	The phase-field crack surface density functional
$D_{k,itx}$	Diffusion coefficients of species k in the uncracked ITZ	$E_{0,agg}$	Young's modulus of aggregate
g	Phase-field variable	$E_{0,m}$	Young's modulus of mortar
u	Displacement field	$E_{0,itx}$	Young's modulus of ITZ
D_0	Chloride diffusivity in the concrete pore solution	$\nu_{0,agg}$	Poisson's ratio of aggregate
σ_0	Relative electrical conductivity in the concrete pore solution	$\nu_{0,m}$	Poisson's ratio of mortar
$m_{\phi cp}$	Coefficient related to porosity and concrete composition	$\nu_{0,itx}$	Poisson's ratio of ITZ
ϕ_c	The critical porosity for pore network percolation	$f_{t,m}$	Failure strength of mortar
$F_{Cl}(H)$	The humidity impact factor for chloride ion diffusivity	$f_{t,itx}$	Failure strength of ITZ
H_c	The critical humidity	$G_{f,m}$	Fracture energy of mortar
$F_f(T)$	The temperature impact factor	$G_{f,itx}$	Fracture energy of ITZ
$T(t)$	The temperature of the concrete internal environment	c	The diffusion field
T_0	Reference temperature	e	Electric field
k	Ion/gas species	D_s	Chloride diffusivity in the cement paste solid phase
S	Sensitivity index	σ_{solid}	Relative electrical conductivity in the cement paste solid phase
i_n	Normal current density	$D_{Cl,p}$	Effective chloride diffusivity in cement paste
E_a	Activation energy for material diffusion	τ_1	Empirical exponent
y	The state variable	$D_{O_2,p}$	Oxygen diffusion coefficient at 25°C
R_0	The radius of rebar	$H(t)$	The humidity of the internal environment
h_e	The mesh element size	$F_{O_2}(H)$	The humidity impact factor for oxygen diffusivity

Data availability

The data that has been used is confidential.

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