

1 **MESO-SCALE PHASE FIELD MODELLING OF REINFORCED CONCRETE**
2 **STRUCTURES SUBJECTED TO CORROSION OF MULTIPLE**
3 **REINFORCEMENTS**

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10 **Abstract**

11 Corrosion-induced concrete cover cracking is one of major deterioration mechanisms for
12 reinforced concrete (RC) structures. Concrete cracking caused by corrosion of multiple
13 reinforcements at the meso-scale involves complex toughening mechanism, stress
14 redistribution and crack interaction. It brings significant challenge to accurately predicting the
15 cover cracking which, in most cases, represents a critical stage of serviceability. This paper
16 aims to develop a meso-scale phase field model for concrete cover cracking induced by
17 corrosion of multiple reinforcements. Concrete is treated as a three-phase heterogeneous
18 material, consisting of aggregates, mortar and interfacial transition zones (ITZ). The developed
19 method is implemented into ABAQUS explicit regime through an in-house VUEL subroutine.
20 The crack patterns and crack width development of concrete induced by corrosion are obtained.
21 The model is also verified against experimental results on the crack width development and
22 crack patterns. Further, a parametric study is carried out to investigate the effects of
23 reinforcement spacing, cover thickness, ITZ fracture properties on concrete cover cracking.
24 Some toughening mechanisms including crack deflection, aggregate/mortar bridging and crack
25 bifurcation in concrete have been captured in the model. ITZ fracture properties significantly
26 affects the crack pattern of concrete cover. The developed method enables high fidelity
27 numerical models with up to tens of millions of degrees of freedom (DOFs), and the completed
28 failure processes of concrete cover are well predicted.

29 **Keywords:** durability; phase field model; corrosion; crack pattern; multiple reinforcements.

30

31 **1. Introduction**

32 Reinforced concrete (RC) structures are widely used in buildings, bridges, piers, tunnels and
33 many other civil engineering applications. During the service life, however, RC structures are
34 subjected to reinforcement corrosion, especially in the chloride-laden and/or carbon dioxide
35 environment. Corrosion of reinforcement can cause spalling or delamination of concrete cover,
36 reduce the bonding strength with concrete and hence decrease the load bearing capacity of the
37 RC structures, bringing great threat to the durability and serviceability of the structures. For
38 instance, it was reported that 70-90% of practical cases of premature deterioration of RC
39 structures were dominated by reinforcement corrosion [1].

40

41 Considerable research has been carried out on the corrosion-induced concrete cracking
42 problems of RC structures [2-9]. Bhargava et al. [10] developed an analytical model to predict
43 the time for cover cracking by considering concrete cracking as a tension-softening process. Li
44 et al. [5] proposed an analytical model to predict the corrosion-induced crack width of concrete
45 based on fracture mechanics. Further, Li and Yang [6] derived a model accounting for the
46 strength of cracked concrete using the concept of fracture energy and predicted the crack width
47 development over time under the combined reinforcement corrosion and applied load. Zhang
48 et al. [9] proposed an analytical model to predict the concrete cracking time in consideration of
49 initial defects in concrete and found an initial defect around concrete surface was more
50 destructive on corrosion-induced concrete cracking than an initial defect inside the concrete.
51 The existing analytical models on predicting corrosion-induced concrete cracking have
52 provided useful tools to assess the serviceability of corrosion-affected RC structures. However,
53 almost all existing analytical models were focused on a single reinforcing bar due to extreme
54 difficulties in addressing the interactions between stress fields and cracks of different
55 reinforcements by analytical methods.

56

57 Within a RC structure, the single rebar corrosion problem or assumption can only provide
58 insight in the localized cover failure; for the whole concrete cover performance under long-
59 term service, the corrosion of multiple reinforcements in the RC structures will have to be
60 considered. In fact, the corrosion of multiple reinforcing bars within the structure can result in
61 different cracking patterns and failure modes as stress fields and cracks can obviously interact
62 [11]. In such cases, numerical approaches bring distinct advantages. Zhang et al. [12] employed
63 a finite element (FE) model to simulate concrete cracking induced by corrosion of two
64 reinforcements and found delamination of cover was more prone to occur for RC structures
65 with a smaller rebar spacing. Cui and Alipour [13] developed a three-dimensional FE model to
66 investigate the concrete cover cracking induced by corrosion of three reinforcements and found
67 more elements were damaged for a thinner concrete cover. Cheng et al. [14] developed a
68 chemical-mechanical coupled model to simulate non-uniform corrosion of multiple
69 reinforcements and concrete cracking, and found that, with the increase of cover thickness, the
70 crack initiation time became longer. Among the above simulations, concrete damage plasticity
71 models were employed to predict the crack patterns of RC beams induced by corrosion.
72 However, corrosion-induced concrete cracking is a typical fracture type problem, i.e., tension-
73 dominated. Therefore, it poses concerns on the accuracy and rationale by using the plasticity-
74 based damage model. Chen et al. [15] developed a lattice model to simulate the crack patterns
75 of concrete cover induced by uniform corrosion of two reinforcing bars. They found that an
76 inner transverse crack connecting two reinforcing bars formed before concrete surface cracking
77 for a small reinforcement spacing. Xi and Yang [16] developed a time-dependent corrosion
78 model and simulated multiple reinforcement corrosion induced concrete cracking through
79 inserting zero-thickness cohesive elements into the FE mesh. Although the lattice model and
80 cohesive crack model can simulate complex concrete cracking problems, the crack

81 propagations are inevitably dependent on the original mesh. Besides, the modelling capability
82 of such methods is limited due to computational expenses and the iteration convergence issue.
83 The computational models reported in the literatures usually have a few tens/hundreds of
84 thousands of degrees of freedom (DOFs).

85

86 Moreover, most existing numerical models treated concrete as homogeneous when simulating
87 the crack propagation induced by the corrosion of multiple reinforcements [11-16]. The
88 homogeneity assumption can only yield an approximate response while concrete is in fact
89 heterogeneous especially at the meso-scale, consisting of aggregates, mortar and interfacial
90 transmission zones between aggregates and mortar (i.e., ITZ). Further, concrete cracking
91 involves toughening mechanisms including micro cracks shielding, crack deflection, aggregate
92 bridging, etc., and ITZ plays an important role in simulating the concrete cracking [17-20].
93 Thus, meso-scale modelling by considering the concrete as a multi-phase quasi-brittle material
94 will provide rational insights in the cracking initiation and propagation in concrete. However,
95 to model arbitrary cracking and crack interactions in concrete induced by corrosion of multiple
96 reinforcements at the meso-scale, a computational model with high fidelity could result in ten
97 million DOFs or more, which has posed a nearly impossible challenge to the existing numerical
98 methods.

99

100 In the recent years, a phase field model for fracture has been developed and become popular in
101 the community of computational mechanics [21]. The model utilizes crack regularization and
102 the Frankfort-Marigo variational principle [22] to form a non-local damage model, thus has
103 overcome the mesh dependency issue which may exist in other local damage models.
104 Accordingly, the crack initiation, crack propagation, and most importantly, the interaction
105 among multiple cracks can be captured conveniently. The crack trajectory is not necessarily be

106 tracked by using the phase field model, and this has brought great advantages over some of the
107 other widely adopted methods for modelling crack propagation such as the XFEM and cohesive
108 element method [18, 23]. At the meso-scale, phase field model has been applied successfully
109 to fiber-reinforced composites [24] and other heterogeneous materials [25, 26] under the
110 uniaxial tensile and bending loads. Zhang et al. [27] applied the phase field model to multi-
111 phase materials by which both matrix cracking and interfacial debonding can be captured.
112 Zhang et al. [28] further demonstrated that, the explicit phase field model developed in the
113 framework of dynamic mechanics could greatly improve the modelling capability for large
114 sized models with up to 60 million DOFs. To date, the phase field method has not been
115 employed to address the corrosion-induced concrete cracking problem. A meso-scale phase
116 field model with the capacity of simulating arbitrary cracking and crack interactions in concrete
117 will provide new insights into the degradation and failure of RC structures subjected to
118 corrosion of multiple reinforcements.

119
120 This paper establishes a new numerical method to investigate the whole structural cover
121 cracking induced by corrosion of multiple reinforcements, considering concrete as a
122 heterogeneous material. A phase field model for concrete cracking at the meso-scale is first
123 developed and interface regularization is made to address the discontinuity of interfacial
124 properties. A special degradation function is used to consider the rapid change of fracture
125 toughness over the ITZ. The numerical method is implemented into ABAQUS explicit regime
126 through an in-house VUEL subroutine. A non-uniform corrosion model is employed to
127 formulate the rust expansion around the steel reinforcing bars. An example for RC beam with
128 three tensile reinforcements is presented to demonstrate the application of developed method.
129 Repeatability of results and effects of aggregate randomness are also discussed. The model is
130 then verified by comparing the results with those from experiments. Moreover, a parametric

131 study is carried out to investigate the effects of reinforcement spacing, cover thickness, ITZ
 132 fracture properties on the crack pattern and the development of crack width over service time.
 133 Finally, the computational expense and possible ways to reduce the computational expense are
 134 discussed.

135

136 2. Meso-scale Phase Field Model for Concrete Cracking

137 2.1 Dynamic phase field model

138 Considering the domain Ω shown in Figure 1(a), Γ_i and Γ_c represent interface and crack
 139 domains, respectively. An external loading t^* is acting on the boundary $\partial\Omega_t$, whereas the
 140 boundary $\partial\Omega_u$ is subjected to a prescribed displacement. With the introduction of the phase
 141 field $d(\mathbf{x})$, the crack is regularized into a smeared damage zone, according to the theory of
 142 phase field model. The system's Marigo-Francfort potential functional is specified as follows:

$$143 \quad W = \int_{\Omega_{mix}} \omega(d)\psi_\varepsilon dV + \int_{\Omega_{mix}} G_s \gamma(d, \nabla d) dV + \int_{\Omega_{inc}} \psi_\varepsilon dV - W_{ext} \quad (1)$$

144 In the above equation, ψ_ε is the elastic potential density and the first term is the elastic potential,
 145 the second term is the fracture energy, the third term is the aggregate's elastic potential, and
 146 the fourth term is the external work potential. $\omega(d)$ is the degradation function which is used
 147 to account for the elastic property reduction due the damage. The function $\gamma(d, \nabla d)$ is the
 148 surface density function used to calculate the dissipated fracture energy for creating new crack
 149 surfaces. G_s is the critical energy release rate (CERR), also known as fracture energy. It is
 150 assumed that cracks evolve only in the mortar and the interface, so the aggregate is always
 151 intact and the degradation function is not applied to it. In this study, we choose to use a cohesive
 152 phase field model proposed by Wu [29], and the explicit forms of $\omega(d)$ and $\gamma(d, \nabla d)$ are
 153 available in [29]. According to the existing study [22] and the loading condition, it is necessary

154 to split the potential energy into two parts, i.e., the tensile part ψ_ε^+ and the compressive part
155 ψ_ε^- , while only the tensile part contributes to the evolution of damage. In addition, a historic
156 variable H is introduced to prevent the physically unreasonable self-healing phenomenon.
157 With the modifications mentioned above, the first term of Equation (1) can be changed as
158 follows:

$$159 \quad W = \int_{\Omega_{mix}} \omega(d)H + \psi_\varepsilon^- dV, \quad H = \max_{\tau \in [0,t]} \{\psi_b^+(\boldsymbol{\varepsilon}(\mathbf{x}, \tau))\} \quad (2)$$

160 In the framework of dynamics, the system's Lagrange functional consists of potential energy
161 and kinematic energy, specified as follows:

$$162 \quad L(\mathbf{u}, \mathbf{w}, d, \mathcal{D}) = \frac{1}{2} \int_{\Omega} \rho \mathbf{w} \cdot \mathbf{w} dV + \int_T \int_{\Omega} \frac{1}{2} \bar{\eta} \mathcal{D} dV dt - \int_{\Omega_{mix}} \omega(d)H + \psi_\varepsilon^- dV \\
- \int_{\Omega_{mix}} G_s \gamma(d, \nabla d) dV - \int_{\Gamma_c} G_s dS - \int_{\Omega_{inc}} \psi_\varepsilon dV + W_{ext} \quad (3)$$

163 where the first term is the kinematic energy and the second term is the viscosity phase field
164 energy originally introduced in [22]. $\bar{\eta}$ is an artificial viscosity parameter and T is the total
165 time. Let $\mathbf{q} = [\mathbf{u}, d]$ and $\mathcal{Q} = [\mathbf{w}, \mathcal{D}]$, the system's Lagrange equation can be derived through the
166 following equation:

$$167 \quad \frac{d}{dt} \left(\frac{\partial L}{\partial \mathcal{Q}} \right) - \frac{\partial L}{\partial \mathbf{q}} = 0 \quad (4)$$

168
169 The numerical solution of the coupled phase field equation is normally solved with the finite
170 element method, the displacement and phase fields inside an element can be expressed with
171 the nodal values through proper interpolation. The finite element method governing equation
172 of the dynamic phase field model is specified as follows:

$$173 \quad M \ddot{\mathbf{u}}^N = \mathbf{P}_{ext} - \mathbf{P}_{int}, \quad C \dot{\mathbf{d}}^N = \mathbf{Y}(\mathbf{u}, d) \quad (5)$$

174

175 Explicit forms of the matrices are referred to [28]. The equation of displacement is solved by

176 using central difference method while the phase field equation is solved with the forward
 177 difference method. With the aid of the lumped mass matrix M and the lumped viscosity matrix
 178 C , Equation (5) can be solved with the explicit time integration scheme which has
 179 tremendously high efficiency in comparison with the widely used implicit schemes. More
 180 details about the phase field model can be found in our previous studies on modelling fiber-
 181 reinforced composites [24, 28].

182

183 2.2 Meso-scale concrete and interface regularization

184 At the meso-scale, concrete is a typical heterogeneous material that consists of aggregates,
 185 cement mortar and the ITZ. Such a heterogeneous structure of concrete with variation in
 186 mechanical properties can induce some toughening mechanisms during the concrete crack
 187 propagation process, e.g., aggregate bridging, micro-cracks shielding, crack deflection, etc.
 188 [30-32]. Therefore, we establish a three-phase model consisting of aggregates, mortar and ITZ
 189 to simulate the meso-scale concrete cracking. The aggregates are simplified as polygons with
 190 a random size and 4 to 13 sides. For simplicity, only coarse aggregates larger than 2.4 mm are
 191 modelled, while fine aggregates and cement are treated as the mortar phase [17]. The total
 192 fraction of coarse aggregates accounts for about 40% of the whole volume of concrete. A
 193 typical three-segment gradation size distribution [33] in Table 1 is employed to control the
 194 aggregates size distribution. Further, the two-dimensional distribution of aggregates can be
 195 calculated according to the Walraven formula [34, 35]:

$$196 P(D < D_0) = P_k \left(1.065 \left(\frac{D_0}{D_{max}} \right)^{0.5} - 0.053 \left(\frac{D_0}{D_{max}} \right)^4 - 0.012 \left(\frac{D_0}{D_{max}} \right)^6 - 0.0045 \left(\frac{D_0}{D_{max}} \right)^8 + 0.0025 \left(\frac{D_0}{D_{max}} \right)^{10} \right) \quad (6)$$

197 where $P(D < D_0)$ is the probability of the aggregate diameter D in a cross-sectional plane
 198 smaller than D_0 ; D_{max} is the maximum diameter of aggregates. The calculated 2D distribution
 199 of coarse aggregates is also listed in Table 1.

200

201 The change of material properties on the interface (Figure 1a) has brought considerable
202 challenges in the numerical modelling. The thickness of ITZs between aggregates and mortar
203 is normally only tens of microns. Modelling such a small thickness of ITZs will result in very
204 dense meshes or distortions of adjacent elements for mortar and aggregates. There are two
205 common approaches to model ITZs: (1) using zero-thickness interface elements for ITZs [17,
206 18]; (2) setting the thickness of ITZs 0.1-1 mm [36-37]. In this study, we set the ITZ thickness
207 as 0.5 mm. Further, an interface regularization scheme reported in [24, 27] is employed to
208 model the mechanical properties of ITZs. The scheme introduces an auxiliary phase field $\eta(x)$
209 to convert the interface into a smeared strip with certain width, as shown in Figure 1(b). The
210 equivalent material properties are considered smoothly distributed in the smeared zone and are
211 composed of that of the interface and matrix. More details on deriving $\eta(x)$ are referred to [24,
212 27]. The equivalent strength σ_{\max}^s is specified as follows:

$$213 \quad \sigma_{\max}^s(\eta) = \sigma_{\max}^i [1 - h(\eta)] + \sigma_{\max}^m h(\eta) \quad (7)$$

214 whereas the equivalent critical energy release rate (CERR) or fracture energy is given as
215 follows:

$$216 \quad G_s(\eta) = [1 - h(\eta)] \int_0^D \{G_i [1 - h(\eta)] + G_m h(\eta)\} \frac{1}{c_0} \left(\frac{\alpha(d)}{l_0} + l_0 |\nabla d|^2 \right) dx + G_m h(\eta) \quad (8)$$

217 where $D = \pi l_0 / 2$. The subscripts “*i*” and “*m*” represent interface and matrix, respectively and
218 “*s*” represent the equivalent property in the smeared zone. $h(\eta)$ should be chosen to ensure a
219 monotonic change of the material properties. In the previous study, a quadratic form of
220 degradation function was used, as follows

$$221 \quad h(\eta) = (1 - \eta)^2 \quad (9)$$

222 With this degradation function, the fracture energy in Equation (8) changes smoothly but
223 slowly. As a result, any change of the fracture energy with small quantity (especially for the
224

225 interface) may not have a significant impact on the fracture energy, and thus cannot be reflected
 226 in the modelling result. In this study, we propose to use an exponential form of degradation
 227 function, as given by

$$228 \quad h(\eta) = \frac{1 - e^{-k(1-\eta)^n}}{1 - e^{-k}}, \quad k > 0, \quad n \geq 2 \quad (10)$$

229
 230
 231 With the new degradation function, the equivalent CERR is enhanced. As an example, we
 232 assume equivalent CERRs of interface and matrix are 0.02 N/mm and 0.07 N/mm, respectively.
 233 The obtained equivalent CERR is shown in Figure 2. The new degradation function maintains
 234 a short region in which the equivalent CERR is almost equal to the interface, and the value then
 235 has a rapid but smooth transition to that of the matrix. In this way, the change of material
 236 property can be reflected in the modelling result and the mesh density near the ITZ zone can
 237 be relaxed. The length of the front region and the slope of the equivalent CERR shown in Figure
 238 2 can be adjusted by the two parameters, k , n , and in this study we choose
 239 $k = 5000000$, $n = 140$.

240 241 **2.3 Numerical implementation**

242 The theory is implemented into ABAQUS EXPLICIT through the users' subroutine VUEL,
 243 and MPI parallel calculation available in ABAQUS. MPI parallel calculation is normally
 244 known inapplicable when a user defined element is used is enabled and in our simulation this
 245 is achieved through programing the VUEL codes with the special consideration of parallel
 246 calculation. One issue when using the explicit integration scheme is the determination of stable
 247 time interval Δt_c . Smaller time intervals can bring additional computational costs but higher
 248 ones could result in unexpected wrong predictions. For central difference method, the critical
 249 stable time interval is

$$\Delta t_u \approx \frac{L_{\min}}{c_d}, c_d = \sqrt{\frac{\lambda + 2\mu}{\rho}} \quad (11)$$

where L_{\min} is the minimum mesh size, c_d is the wave speed, and for isotropic material, ρ is mass density and λ and μ are Lamé constants. For forward difference method, the critical time interval is specified by:

$$\Delta t_d \approx \frac{L_{\min}^2}{2\alpha} \quad (12)$$

where $\alpha = 2l_0 G_s / c_0 \bar{\eta}$, $c_0 = 4 \int_0^1 \sqrt{\alpha(s)} ds$. For the coupled displacement-phase field problem, the adopted time interval is

$$\Delta t_c \approx \kappa \cdot \min \{ \Delta t_u, \Delta t_d \} \quad (13)$$

where $\kappa \in (0,1]$ is a safety parameter and we use $\kappa = 0.5$ in this study.

3. Non-uniform Corrosion Model and Crack Width Calculation

3.1 Non-uniform corrosion model

The reinforcing bar in concrete is normally in passive state due to the alkali environment in concrete. In the chloride-laden environment, the depassivation and corrosion of reinforcing bar can occur once the chloride content near the reinforcement reaches a critical value. Due to the differences in the diffusion routes from different sides of RC structures, the part of steel bar near the concrete cover surface will firstly be corroded and has a higher corrosion rate. Evidently, the corrosion rust development of reinforcing bar in concrete is non-uniform. Considerable experiments and electrochemical corrosion simulations have proved that, more corrosion products accumulate around the half of reinforcing bar near the cover surface while almost no corrosion product can be observed at the other part [38-43]. Therefore, we formulate one of the most widely accepted non-uniform corrosion model, i.e., the semi-elliptical

272 corrosion model [40], to investigate corrosion-induced concrete cover cracking.

273

274 Previous studied [44, 45] have found that, there is a porous zone or corrosion accommodation
275 zone with a thickness of 10-50 μm at the interface between the concrete and reinforcing bar.

276 Corrosion products will first fill into the porous zone without the expansion force. Therefore,

277 the porous zone is considered as a porous circular band in the model. Figure 3 illustrates the

278 distribution of corrosion products around the reinforcing bar. The total amount of corrosion

279 products are divided into three parts: (1) the semi-elliptical band of corroded steel with

280 maximum thickness d_{co-st} ; (2) the porous circular band d_0 ; (3) the semi-elliptical rust band

281 with maximum thickness d_m . The front of the corrosion is in a semi-elliptical shape with the

282 semi-major axis equal to $\phi/2 + d_0 + d_m$ and the semi-minor axis $\phi/2 + d_0$. Considering the

283 boundary of original reinforcing bar, the expansion displacement of rust driving concrete

284 cracking can be expressed as follows:

$$285 \quad r(\theta) = \frac{(\Phi + 2d_0 + 2d_m)(\Phi + 2d_0)}{\sqrt{(2\Phi + 4d_0)^2 + 16d_m(\Phi + 2d_0 + d_m)(\cos\theta)^2}} - \frac{\Phi}{2} - d_0 \quad (14)$$

286 where θ is the location angle of rust in the polar coordinates system ($0 \leq \theta \leq \pi$). Φ is the

287 diameter of the reinforcing bar. The rust expansion function $r(\theta)$ will be the displacement

288 boundary condition in the following numerical models. More details on the semi-elliptical

289 corrosion model can be found in [40, 46].

290

291 Further, the corrosion degree or steel loss ratio can be expressed as follows [11]:

$$292 \quad \eta = \frac{(d_m + 2d_0)\alpha_{rust}\rho_{rust}}{(\rho_{st} - \alpha_{rust}\rho_{rust})\Phi} \quad (15)$$

293 where ρ_{rust} and ρ_{st} are the densities of rust and steel, respectively; α_{rust} is the molecular

294 weight of steel divided by the molecular weight of corrosion products.

295

296 3.2 Determination of crack width

297 Crack width is one of the most significant parameters for the design and assessment of RC
298 structures. For instance, the crack width 0.3 mm is regarded as critical crack width for RC
299 structures exposing in the humidity, moist air, soil conditions [47]. Therefore, a numerical
300 algorithm to calculate the crack opening displacement is proposed to determine the crack width.

301

302 Considering a bar in the region $x \in [0, L]$, the left side is fully fixed, the right side is subjected
303 to tensile loading with specific displacement u^* , as shown in Figure 4(a). Without
304 consideration of body force, the real stress σ_r distributes uniformly along the bar, and the
305 displacement u^* can be represented as follows:

$$306 \quad u^* = \int_0^L \varepsilon dx \quad (16)$$

307 where $\varepsilon = \frac{\sigma_n}{E_0}$ is the total strain, σ_n is the nominal stress, E_0 is the initial elastic modulus. The
308 total strain is assumed to be composed of two parts, i.e., elastic strain and damaged strain.
309 Accordingly, Equation (16) can be rewritten as follows:

$$310 \quad u^* = \int_0^L \frac{\sigma_r}{E_0} dx + \int_0^L \frac{\sigma_n - \sigma_r}{E_0} dx \quad (17)$$

311 According to the phase field model, the real stress can be calculated through $\sigma_r = \omega(d)\sigma_n$; thus
312 Equation (16) can be changed as follows:

$$313 \quad u^* = \int_0^L \frac{\sigma_r}{E_0} dx + \int_0^L \frac{\sigma_n}{E_0} (1 - \omega(d)) dx = \frac{\sigma_r}{E_0} L + \int_0^L \varepsilon (1 - \omega(d)) dx \quad (18)$$

314 Obviously, the second term is the crack opening displacement,

$$315 \quad w = \int_0^L \varepsilon (1 - \omega(d)) dx \quad (19)$$

316 We can extend this theory to 2D and 3D cases for calculating the crack opening displacement.

317 Taking a 2D case shown in Figure 4(b) as an example and after obtaining the phase field
 318 distribution, the crack opening displacement along the horizontal direction can be given as
 319 follows:

$$320 \quad w = \sum_{i=1}^4 [u(i+1) - u(i)] \left[1 - \frac{\omega(i+1) + \omega(i)}{2} \right] \quad (20)$$

321

322 **4. Worked Example and Verification**

323 To demonstrate the numerical method, a two-dimensional reinforced concrete beam model
 324 with three tensile reinforcing bars is developed. Figure 5 shows the RC beam model with
 325 dimensions of 400 mm in height and 196 mm in width. The diameter of reinforcement is 12
 326 mm. The cover thickness is 20 mm and the clearing space of reinforcements is 60 mm. To
 327 reduce the computational time, only the top area with the potential of cracking is established
 328 as the heterogeneous model while the other part is taken as homogenous and elastic. All the
 329 basic mechanical and corrosion parameters are given in Table 2. The semi-elliptical non-
 330 uniform corrosion model, i.e., Equation (14), is worked as a displacement boundary condition
 331 in the numerical model. Based on the assumption that chlorides, as well as other essential ions,
 332 such as oxygen and moisture, penetrated through the concrete cover from one side only, e.g.
 333 the splashing wave side, the corroded half of steel bar is facing the top surface of the beam
 334 (shown in Figure 5).

335

336 Figure 6 shows the cracking process of concrete caused by the non-uniform corrosion of
 337 reinforcements. To clearly show the micro and macro cracks in the model, the elements with a
 338 phase field value larger than 0.9 are marked as red. It can be seen that, when the corrosion
 339 degree increases to 0.37%, some micro cracks appear in the interfaces between the aggregates
 340 and mortar. Moreover, surface cracks are first initiated at the top of the two corner
 341 reinforcements. With the development of corrosion, cracks around the middle reinforcement

342 propagate towards the corner reinforcements and cracks around the corner reinforcements
343 propagate towards the middle-located reinforcement (Figure 6b). When the corrosion degree is
344 increased to 0.73% (i.e., Figure 6c), two side cracks appear in the left and right cover of
345 concrete and propagate outwards, which will make a corner spalling failure. Finally, the side
346 cracks will be connected to form a through crack and the delamination of cover will occur
347 (Figure 6d).

348

349 Figure 7 illustrates the energy evolution during the development of corrosion process. The
350 external energy is the total work done by the expansion of corrosion products. The elastic
351 energy is the recoverable deformation energy of concrete. The fracture energy is the energy
352 consumed by concrete cracking. The kinetic energy is associated with dynamic motion. To
353 accurately model a quasi-static problem by ABAQUS/Explicit, the kinetic energy should a
354 small fraction (typically 5–10%) of external energy. It can be seen that, the kinetic energy
355 during the whole simulation is close to zero, which ensures the loading is a quasi-static process
356 in the simulation. The corrosion products expansion transfers to external energy of the beam,
357 of which the elastic deformation energy and fracture energy account most. At the initial
358 corrosion stages (0-0.3%), the fracture energy is close to the elastic energy when lots of micro
359 cracks of concrete appear. After that, the ratio of elastic energy to fracture energy becomes
360 larger when the macro cracks have formed and the crack width is increasing.

361

362 To investigate the effect of aggregate randomness on the numerical results, 10 meso-scale
363 models with the same grading and aggregates fraction are established to simulate corrosion-
364 induced concrete cracking. Figure 8 shows the typical crack patterns of the RC beam caused
365 by the non-uniform corrosion. It can be seen that, the overall failure patterns are very similar,
366 i.e., delamination and corner spalling of concrete cover. As expected, the aggregates in concrete

367 affects the location of micro and macro cracks because the weak interfaces between aggregates
368 and mortar dominates the crack initiation and connections. Moreover, the developed model
369 well reproduces the crack deflection, aggregate/mortar bridging and crack bifurcation
370 phenomena during concrete cracking (e.g., Figure 8). Crack deflection occurs when a potential
371 crack path of least resistance is around an aggregate or a weak interface. Aggregate bridging
372 occurs when two or more cracks propagate along two sides of aggregates and advance beyond
373 the aggregates. Mortar bridging appears when two cracks propagate along the sides of
374 neighboring aggregates. Crack bifurcation appears when a crack deflects into different sides of
375 an aggregate or different aggregates. It can be concluded that, the ITZs in concrete dominate
376 the fracture propagation of concrete at the meso-scale. The developed meso-scale model is
377 advantageous compared with most existing concrete fracture models [16, 39, 48], in terms of
378 capturing toughening mechanisms and arbitrary cracking paths. Figure 9 illustrates the surface
379 crack width developments at the top of two corner reinforcements for the 10 random models.
380 It can be seen that, the surface crack width begins to increase when the corrosion degree reaches
381 to about 0.08%. Then the crack width gradually increases with the development of corrosion.
382 When the corrosion degree is about 0.62-0.75%, the surface crack width reaches 0.3 mm. The
383 numerical results have a good repeatability for different random models.

384

385 To verify the developed numerical method on the crack width development, experimental
386 results from Ye et al. [38] are used for comparison. In the experiment, the rust distribution of
387 C20 specimens was non-uniform and the crack width development as a function of corrosion
388 degree was given. The geometric and mechanical parameters are listed in Table 3. Figure 10
389 shows the crack width developments from numerical and experimental results. It can be seen
390 that, the numerical results have a good agreement with the experimental results. It should be
391 mentioned that, the crack width from experiments are obtained by using a binocular lens with

392 a measuring precision of 0.01 mm [38]. Therefore, the error when measuring a very small crack
393 width could result in the differences between experimental and numerical results at the initial
394 stage (crack width smaller than 0.02 mm).

395

396 To verify the developed numerical method on the crack patterns induced by multiple
397 reinforcement corrosion, experimental results from Zahid et al. [49] are used for comparison.

398 In their experiments [49], concrete panels of dimensions $600 \times 600 \times 150$ mm with five
399 reinforcements of 19 mm in diameter were made for corrosion tests. The cover thickness of
400 Panels 1 and 2 are 30 mm. Electrochemical accelerated corrosion was applied to five
401 reinforcements in Panel 1 for 45 days and middle three reinforcements in Panel 2 for 56 days.

402 The volume proportion of coarse aggregates for the concrete specimens are about 40%. The
403 compressive strength and elastic modulus of the concrete specimens are 42 MPa and 35 GPa,
404 respectively. The geometric and mechanical parameters in the numerical model are listed in

405 Table 4. Consistent with the experiment set-up, corrosion expansions for all five reinforcements

406 are modelled for Panel 1 while only the middle three reinforcements corrosion is modelled for

407 Panel 2. Figure 11 shows the crack patterns from experimental and numerical results. It can be

408 seen that the numerical results have a good agreement with experimental results. For Panel 1

409 with five reinforcement corrosion, a through crack is formed and connected to make concrete

410 delamination. Only two vertical surface cracks form at the top of two side reinforcements. This

411 is because the through crack releases stress concentration and stops concrete surface cracking

412 at the top of middle reinforcements. For Panel 2 with only middle three reinforcement corrosion,

413 two vertical cracks form at the top of corroded side reinforcements. Experimental and

414 numerical results both show that, surface cracking is more prone to form for corroded corner

415 reinforcement.

416

417 **5. Parametric Study and Discussion**

418 The clearing space of reinforcement is an important parameter for the design of RC structures.
419 Figure 12 shows the crack patterns of concrete for the clearing spaces of reinforcements, 30
420 mm, 60 mm and 90 mm, respectively. It can be seen that, delamination failure of concrete cover
421 occurs for the three cases but the smaller the clearing space of reinforcements is, the more
422 complex the crack network is. For the clearing space 30 mm, the aggregate bridging and
423 parallel cracks occur at the middle of concrete cover. While for the relatively large clearing
424 space of reinforcements (i.e., 60 and 90 mm), the side cracks are more prone to connect to form
425 a through crack. Figure 13 illustrates the surface crack width development for different clearing
426 space of reinforcements. It can be found that, the larger the clearing space is, the larger the
427 surface crack width is. A significantly drop of the surface crack width occurs when the through
428 crack is formed for the clearing space 90 mm. Therefore, the through crack will affect concrete
429 surface crack development. Figure 14 shows the effect of the clearing space on the ratios of
430 fracture energy to external energy and elastic energy to external energy. Generally, the larger
431 the clearing space is, the larger the energy ratio is. Therefore, more external energy caused by
432 corrosion is transferred to elastic energy for the RC structures with a smaller reinforcement
433 clearing space. Therefore, it is helpful for reducing the clearing space of reinforcements to
434 maximize the using of materials and prolong the service life of RC structures under corrosive
435 environments.

436

437 Figure 15 shows the crack patterns of concrete for cover thicknesses 20 mm, 30 mm and 40
438 mm. It can be seen that, the crack patterns of concrete are all delamination and corner spalling,
439 i.e., a horizontal through crack make the middle part of concrete delaminate, and top and side
440 cracks around the corner rebar make corner spalling. For non-uniform corrosion of
441 reinforcements, more corrosion products accumulate around the half of reinforcement facing

442 concrete cover, which produces concentrated tensile stress to make cover delaminate. Figure
443 16 illustrates the crack width developments for different cover thicknesses. It can be found that,
444 the smaller the cover thickness is, the smaller the corrosion degree to surface cracking is. The
445 initial surface crack width (<0.1 mm) is larger for a smaller cover thickness. With the crack
446 width increasing, the difference of crack width for different cover thicknesses becomes
447 negligible.

448

449 It is very challenging to measure the fracture properties of ITZ, especially fracture energy,
450 through experiments [50-52]. Moreover, the tensile strength and fracture energy of ITZ are
451 dependent on the aggregate type, roughness and curing conditions [52-54]. Therefore, it is
452 worthy to investigate the effect of ITZ fracture properties on corrosion-induced concrete
453 cracking. Figure 17 shows the crack patterns of concrete for tensile strengths of ITZ 0.1 MPa,
454 0.25 MPa and 1 MPa which are about 1/20-1/2 of mortar tensile strength with reference to [52-
455 52]. The other parameters including fracture energy of ITZ keep the same as those in the
456 worked example (see Table 2). It can be seen that, two failure modes (i.e., delamination and
457 corner spalling) occurs for the concrete beam with different ITZ strengths. With a lower ITZ
458 strength, the top crack is less likely to form and the concrete cover is more prone to be
459 delaminated by corrosion-induced horizontal through cracks. Therefore, the ITZ strength
460 significantly affects the failure mode of corrosion-induced concrete beam cracking, which also
461 proves the necessity and value of modelling corrosion-induced concrete beam cracking at the
462 meso-scale. Figure 18 illustrates the crack width development for different ITZ strengths. It
463 can be seen that, for low ITZ strengths, the top surface crack firstly increases to about 0.03 mm
464 then gradually decreases to about zero. The lower the ITZ strength is, the faster the top surface
465 crack closes. This is because the side crack releases stress concentration on the top of concrete
466 cover and the side crack propagates faster for a lower ITZ strength. Figure 19 shows the crack

467 patterns of concrete cover for different fracture energies of ITZ. The ITZ fracture energies are
468 chosen as 0.00525 N/mm, 0.0105 N/mm and 0.021 N/mm which are about 0.07-0.3 time of
469 mortar fracture energy after previous experimental results [52]. The other parameters including
470 tensile strength of ITZ keep the same as those in the worked example (see Table 2). It can be
471 seen that, horizontal through cracks form in the concrete cover for the three values of ITZ
472 fracture energy, which makes the middle of concrete covers delaminate. However, for the
473 smallest fracture energy (see Figure 19a), the left upper surface crack does not appear. Figure
474 20 illustrates the crack width developments for different fracture energies of ITZ. It can be seen
475 that, for ITZ fracture energy 0.00525 N/mm, the crack width at the left top surface of the beam
476 firstly increases to 0.02 mm but gradually decreases to about zero. For other cases, the ITZ
477 fracture energy has little effect on the crack width development. Therefore, fracture energy of
478 ITZ can also change the corrosion-induced cracking pattern. The stronger the ITZ is (i.e., larger
479 strength and fracture energy), the corner spalling of concrete cover is more likely to occur for
480 RC beam with multiple reinforcements.

481

482 **6. Computational expense**

483 Considering that the corrosion induced concrete fracture is a quasi-static process and the
484 present explicit phase field model is developed under the framework of dynamic mechanics,
485 the loading speed should be kept as small as possible to eliminate the dynamic effect. The
486 computational expense, DOFs and results for the worked example are provided in Figure 21.
487 There are 2,495,106 triangle elements for mortar and ITZs, 953,863 triangle elements for
488 aggregates and 737,696 triangle elements for homogeneous concrete in the model. Each node
489 for mortar and ITZs elements has three displacement DOFs and one phase field DOF. The node
490 for elastic aggregate and homogeneous concrete only has three displacement DOFs. The total
491 DOF in the worked example is 40,090,626. The mesh size for the interested meso-scale part is

492 0.1 mm. Here we compare three different ways utilizing less consumed time, i.e., (1) using less
 493 loading time to model the same physical process (the standard loading time is 0.05s which is
 494 used as the reference and we use 0.01s in this case. Time is fictitious here; (2) using less loading
 495 time and using artificial damping to the system and; (3) using a digital filter (low pass
 496 Butterworth filter) to remove high frequency components from the results in (1). The definition
 497 of the damping is specified by

$$498 \quad (\sigma_{vis})_j = \begin{cases} b_1 \rho c_d L_e \dot{\varepsilon}_j - \rho [b_2 L_e \langle \dot{\varepsilon}_j \rangle_-]^2, & \text{for } j = 1, 2 \\ 0, & \text{otherwise} \end{cases} \quad (21)$$

499 where $\dot{\varepsilon}_j = \partial \varepsilon_j / \partial t$, c_d is the wave speed, L_e is the characteristic length of the element, and
 500 b_1 and b_2 are viscosity parameters, here we use $b_1=0.12$ and $b_2=2.4$.

501

502 From the result in Figure 21 (a) and (b), all the three approaches have reduced the consumed
 503 time since the total load time step is reduced. Approach (1) has brought significant dynamic
 504 responses, as demonstrated by the waves in the curve. Approach (2) is closer to the result with
 505 more loading time. Approach (3) is closer to approach (1) and the curve is flatter. The dynamic
 506 response might contain contributions from both low and high frequencies, and the viscosity
 507 added to the system has attenuated the dynamic response. However, the filter only removed the
 508 high frequency's contribution. The filter could be used in case that the mechanics response is
 509 well understood and the parameters are well calibrated, as illustrated by the right half of the
 510 curve from approach (3) which is close to the reference.

511

512 7. Conclusions

513 In this paper, a meso-scale phase field model for concrete cover cracking under simultaneous
 514 corrosion of multiple reinforcements has been developed. A three phase (i.e., aggregates,
 515 mortar and interfaces) heterogeneous concrete model was considered and a regularization

516 method was proposed to address interface properties when incorporated into the phase field
517 model. The numerical model was implemented into ABAQUS EXPLICIT through an in-house
518 VUEL subroutine. A non-uniform corrosion model based on previous experimental results was
519 employed and a numerical algorithm was proposed to calculate the crack width. A concrete
520 beam with three tensile reinforcements was presented to demonstrate the developed numerical
521 method which was also verified through comparison with experimental results from the
522 literature. It has been found that the developed model can well simulate arbitrary cracking and
523 complex crack interactions. Some toughening mechanisms including crack deflection,
524 aggregate/mortar bridging and crack bifurcation in concrete were captured. Further, parametric
525 studies were carried out to investigate effects of reinforcement spacing, cover thickness and
526 ITZ properties on concrete cover cracking. The larger the reinforcement spacing is, the
527 horizontal through crack is more prone to connect and more external energy caused by
528 corrosion is transferred to fracture energy. The fracture properties of ITZ significantly affects
529 the cracking patterns of concrete cover. The stronger the ITZ is (i.e., larger strength and fracture
530 energy), the corner spalling of concrete cover is more likely to occur. The numerical model
531 presented in the paper can be used to simulate the meso-scale fracture of RC structures
532 subjected to non-uniform corrosion of multiple reinforcements.

533

534

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539

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- 671

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677 Table 4 Values for variables used for comparison and validation of crack patterns [49]

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682

Table 1 Three-segment gradation of aggregate size distribution [33-35]

| Aggregate size (mm) | 3D fraction in concrete | 2D fraction in concrete |
|---------------------|-------------------------|-------------------------|
| 2.40-4.67 | 8.08% | 6.2% |
| 4.76-9.52 | 15.96% | 8.7% |
| 9.52-19.05 | 15.96% | 9.8% |

683

684

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686

Table 2 Basic mechanical and corrosion parameters in the worked example [16, 17, 55]

| Description | Values |
|------------------------------|-------------------------|
| Young's modulus of concrete | 46 GPa |
| Poisson's ratio of concrete | 0.22 |
| Young's modulus of aggregate | 80 GPa |
| Poisson's ratio of aggregate | 0.16 |
| Young's modulus of mortar | 23 GPa |
| Poisson's ratio of mortar | 0.22 |
| Tensile strength of mortar | 2.2 MPa |
| Fracture energy of mortar | 0.072 N/mm |
| Young's modulus of ITZ | 18 GPa |
| Poisson's ratio of ITZ | 0.2 |
| Tensile strength of ITZ | 1 MPa |
| Fracture energy of ITZ | 0.021 N/mm |
| Density of steel | 7.85 mg/mm ³ |
| Density of rust | 3.6 mg/mm ³ |
| Molecular weight ratio | 0.57 |

687

688

689 Table 3 Values for variables used for comparison and validation of crack width development

690 [11, 38]

| Description | Values |
|------------------------------|-----------|
| Top cover thickness | 10 mm |
| Edge cover thickness | 20 mm |
| Diameter of steel bars | 10 mm |
| Poisson's ratio of aggregate | 0.16 |
| Length of specimen | 100 mm |
| Height of specimen | 100 mm |
| Young's modulus | 18.82 MPa |
| Poisson's ratio | 0.18 |
| Tensile strength | 5.725 MPa |
| Fracture energy | 0.12 N/mm |

691

692

693 Table 4 Values for variables used for comparison and validation of crack patterns [49]

| Description | Values |
|------------------------------|----------|
| Young's modulus of concrete | 35 GPa |
| Poisson's ratio of concrete | 0.2 |
| Young's modulus of aggregate | 70 GPa |
| Poisson's ratio of aggregate | 0.2 |
| Young's modulus of mortar | 25 GPa |
| Poisson's ratio of mortar | 0.2 |
| Tensile strength of mortar | 6 MPa |
| Fracture energy of mortar | 60 N/m |
| Young's modulus of ITZ | 12.5 GPa |
| Poisson's ratio of ITZ | 0.2 |
| Tensile strength of ITZ | 3 MPa |
| Fracture energy of ITZ | 30 N/m |

694

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698 for the interface and the matrix are 0.02 N/mm and 0.07 N/mm, respectively.

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701 way of estimation of the crack opening displacement in a 2D mesh.

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704 (c) 0.73%; (d) 0.81%.

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708 (a) left top surface (b) right top surface.

709 **Figure 10** Comparison of surface crack width from numerical and experimental results [38].
710 The differences at the initial stage may be caused by the measurement error from a binocular
711 lens with a precision of 0.01 mm.

712 **Figure 11** Comparison of crack patterns from numerical and experimental results [49]. (a) and
713 (b) show the experimental and numerical results for all five reinforcement corrosion,
714 respectively. (c) and (d) show the experimental and numerical results for the middle three
715 reinforcement corrosion.

716 **Figure 12** Crack patterns for different clearing spaces of reinforcements: (a) 30 mm; (b) 60
717 mm; (c) 90 mm.

718 **Figure 13** The crack width developments affected by the clear spacing of reinforcement: (a)
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720 through crack forms for the clear spacing 90 mm.

721 **Figure 14** The energy ratio developments for different reinforcement spacing: (a) fracture
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723 by corrosion is transferred to elastic energy for the RC structures with a smaller reinforcement
724 clearing space.

725 **Figure 15** Crack patterns for different thicknesses of concrete cover: (a) 20 mm; (b) 30 mm;
726 (c) 40 mm.

727 **Figure 16** The crack width developments for different thicknesses of concrete cover: (a) left
728 top surface (b) right top surface.

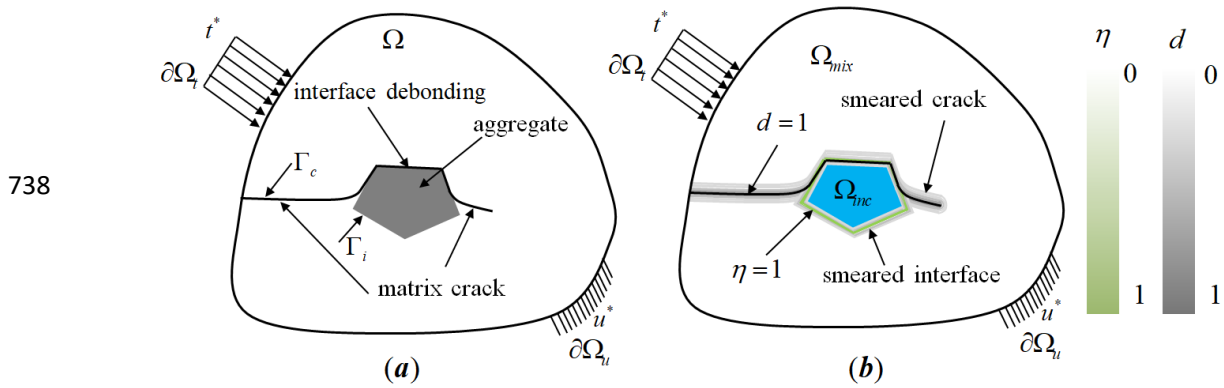
729 **Figure 17** Crack patterns for different strengths of ITZ: (a) 0.1 MPa; (b) 0.25 MPa; (c) 1 MPa.

730 **Figure 18** The crack width developments for different strengths of ITZ: (a) left top surface (b)
731 right top surface.

732 **Figure 19** Crack patterns of concrete for different fracture energies of ITZ: (a) 0.00525 N/mm
 733 (b) 0.0105 N/mm; (c) 0.021 N/mm.

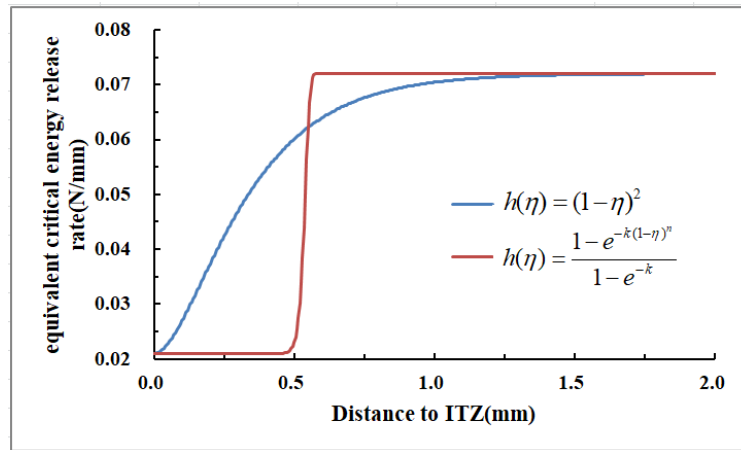
734 **Figure 20** The crack width developments for different fracture energies of ITZ: (a) left top
 735 surface (b) right top surface.

736 **Figure 21** Expended time (a) and the modelling results (b) with different modelling approaches.
 737



739 Figure 1 Representation of cracks and the interface (a) discrete model (b) smeared model.

740



741
 742 Figure 2 Equivalent Critical Energy Release Rate ($k=5000000$; $n=140$). The values of CERR
 743 for the interface and the matrix are 0.02 N/mm and 0.07 N/mm, respectively.

744

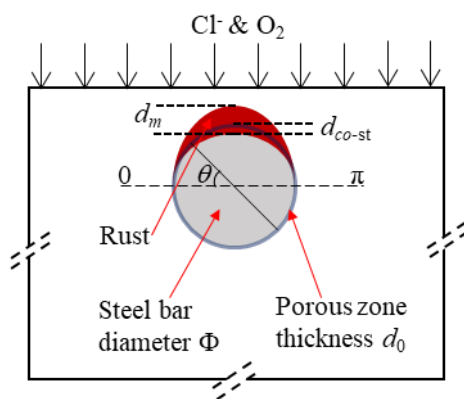
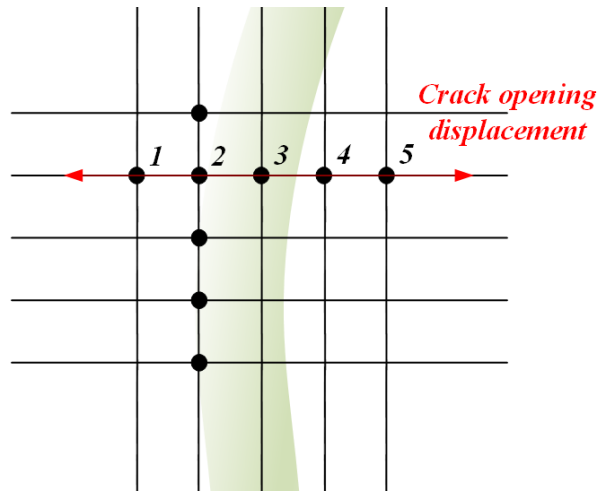


Figure 3 Semi-elliptical non-uniform corrosion model [40, 46].



(a)



(b)

Figure 4 Determination of crack width: (a) A 1D bar to demonstrate the crack extension and (b) the way of estimation of the crack opening displacement in a 2D mesh.

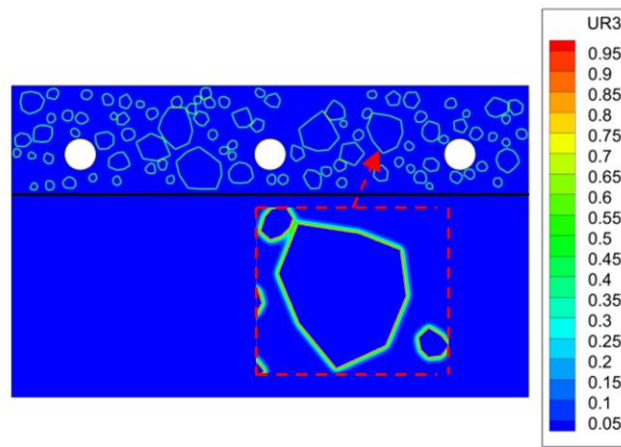
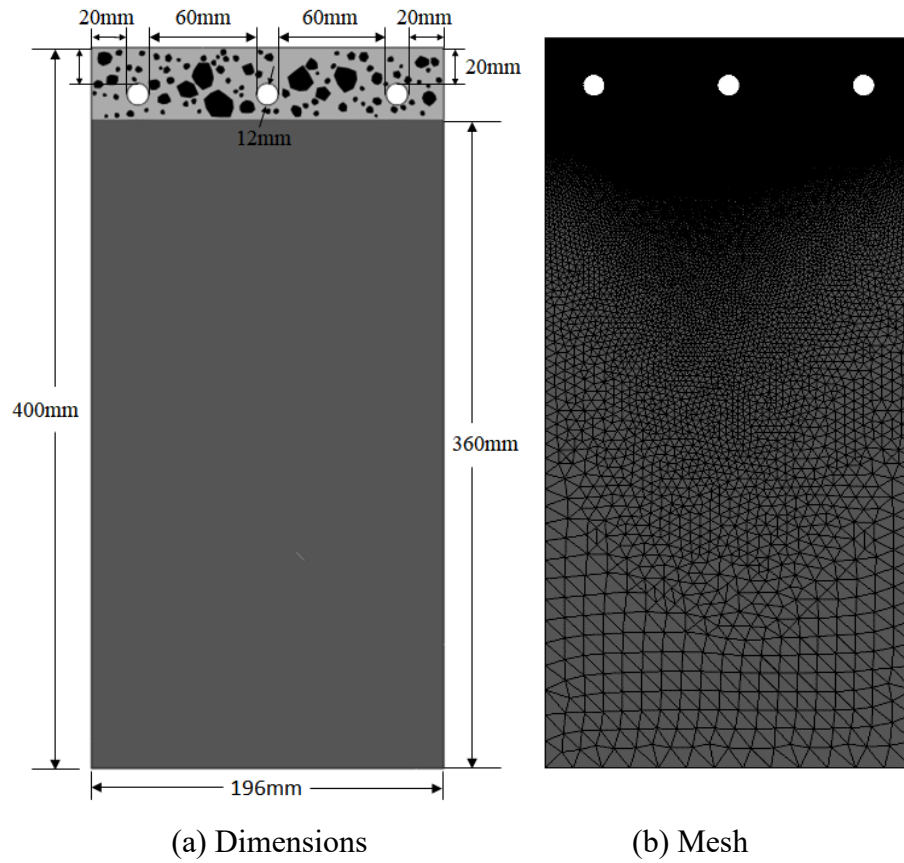


Figure 5 Worked example for RC beam with three reinforcements: (a) dimensions; (b) mesh; (c) the auxiliary phase field's distribution.

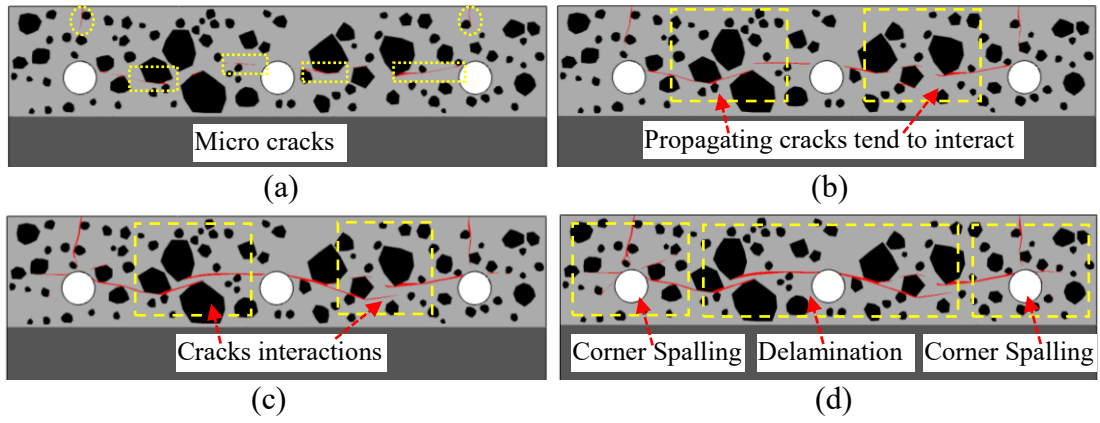


Figure 6 Crack development in concrete when corrosion degree reaches (a) 0.37%; (b) 0.51%; (c) 0.73%; (d) 0.81%.

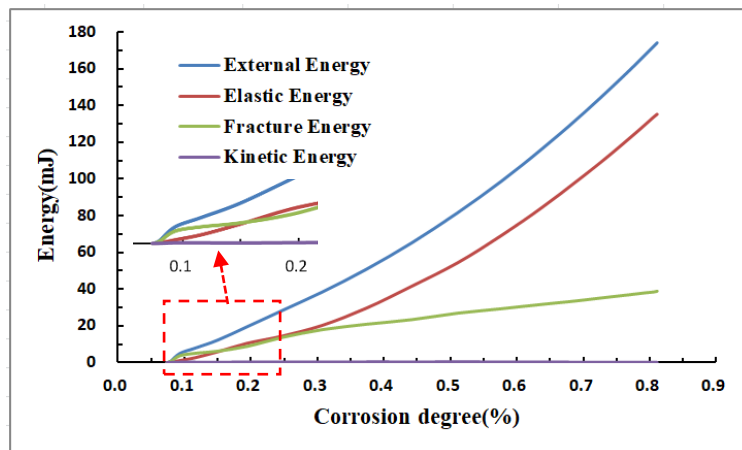


Figure 7 Energy evolutions as a function of corrosion degree.

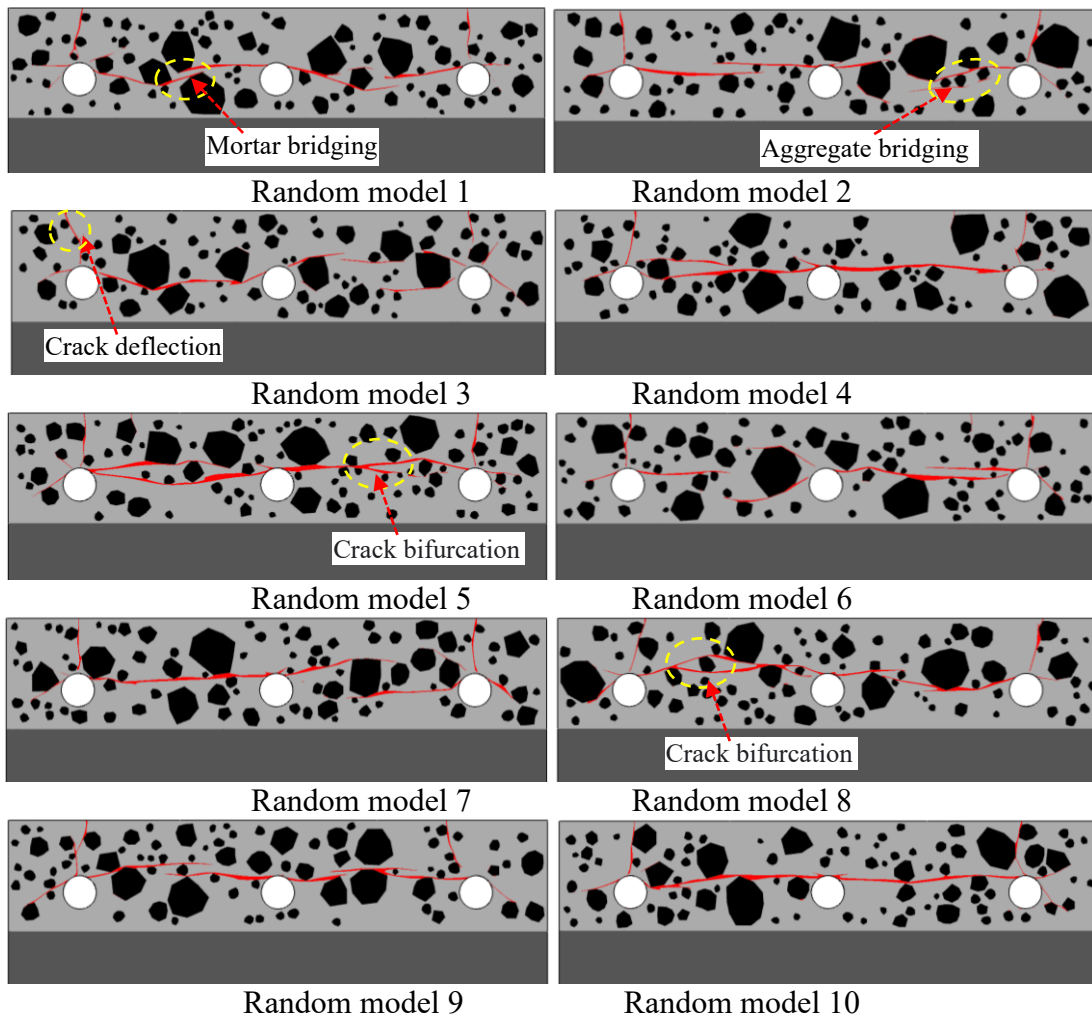


Figure 8 Crack patterns of 10 random meso-scale models.

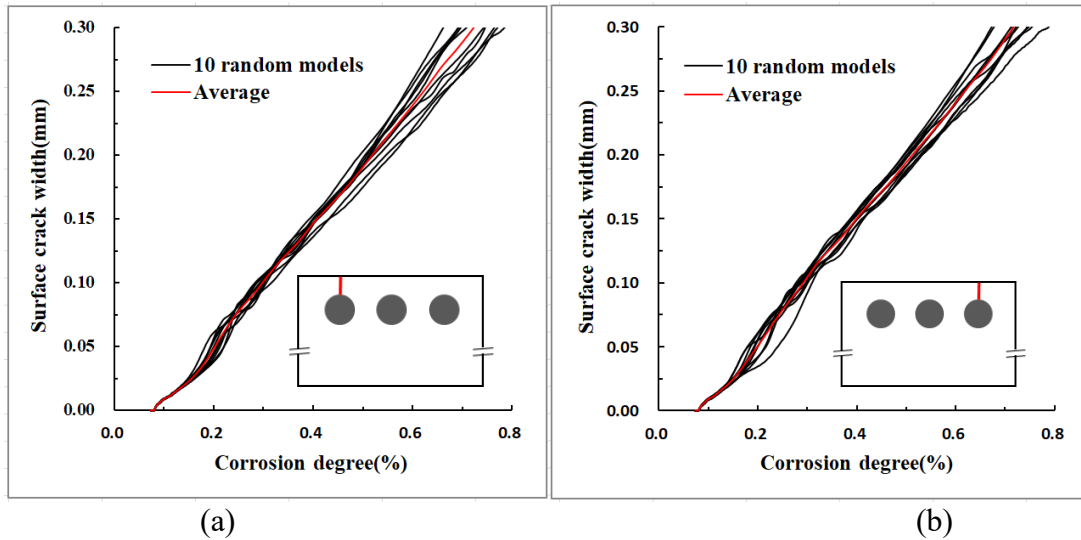


Figure 9 Crack width as a function of corrosion expansion displacement for 10 random models: (a) left top surface (b) right top surface.

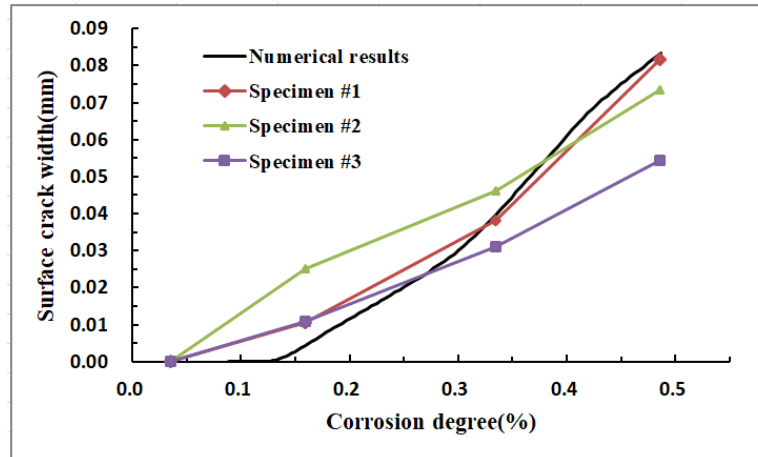


Figure 10 Comparison of surface crack width from numerical and experimental results [38].

The differences at the initial stage may be caused by the measurement error from a binocular lens with a precision of 0.01 mm.

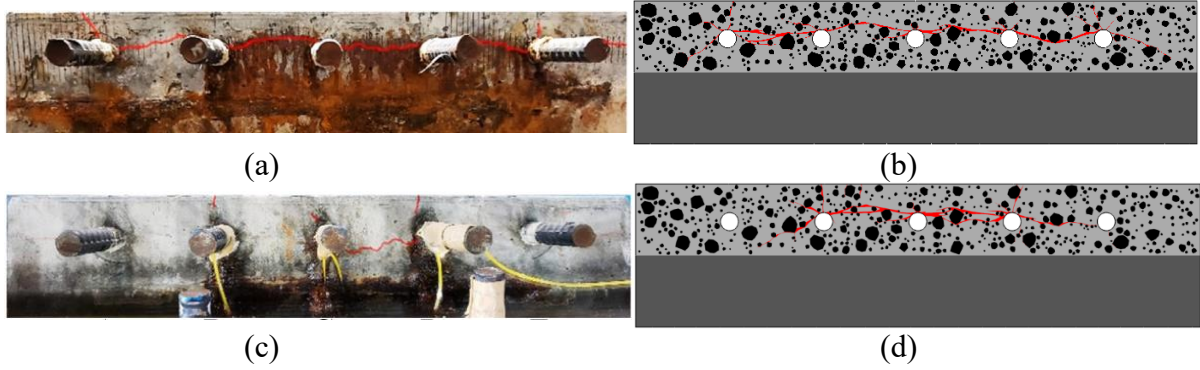


Figure 11 Comparison of crack patterns from numerical and experimental results [49]. (a) and (b) show the experimental and numerical results for all five reinforcement corrosion, respectively. (c) and (d) show the experimental and numerical results for the middle three reinforcement corrosion.

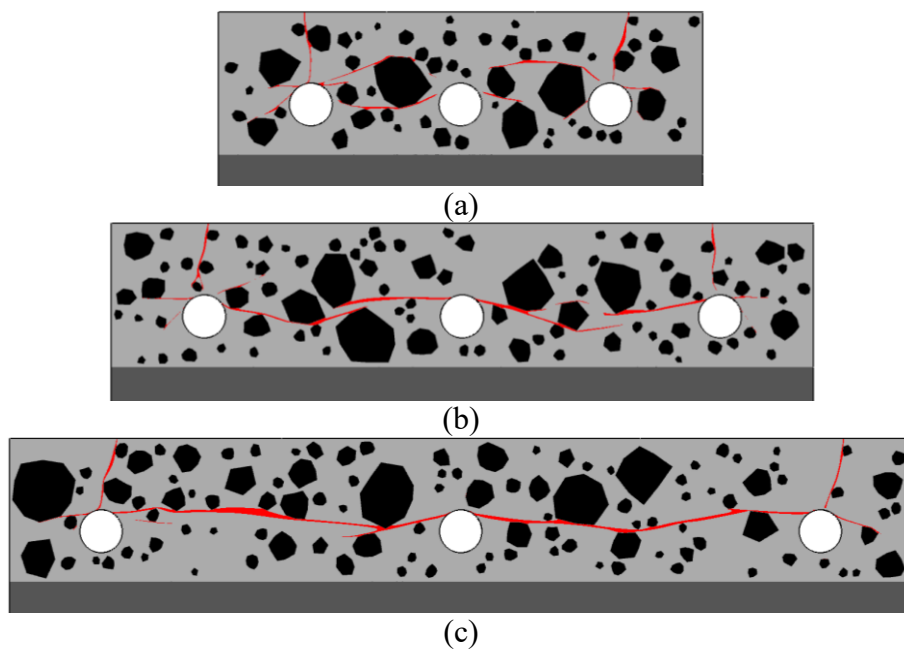


Figure 12 Crack patterns for different clearing spaces of reinforcements: (a) 30 mm; (b) 60 mm; (c) 90 mm.

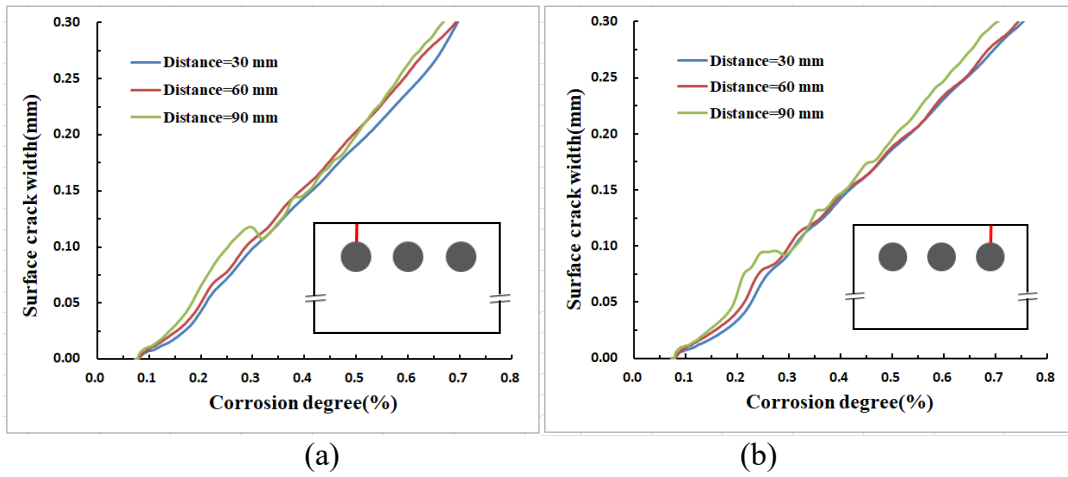


Figure 13 The crack width developments affected by the clear spacing of reinforcement: (a) left top surface (b) right top surface. A sudden drop of top surface crack width occurs when a through crack forms for the clear spacing 90 mm.

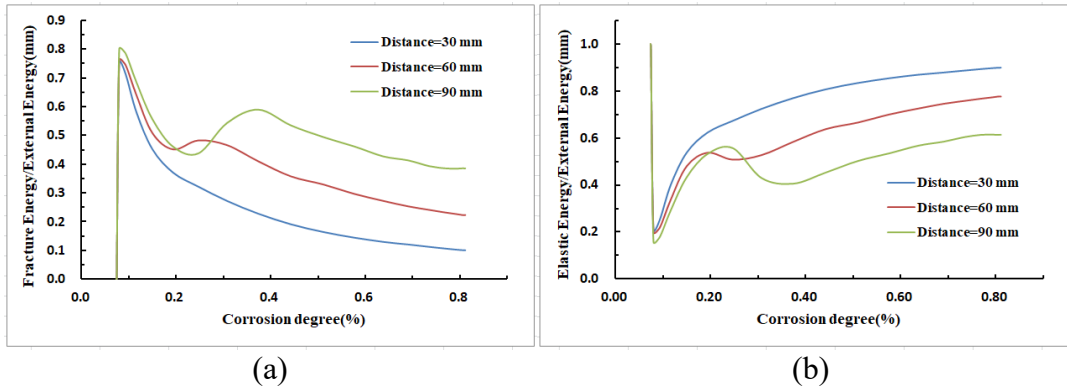


Figure 14 The energy ratio developments for different reinforcement spacing: (a) fracture energy to external energy; (b) elastic energy to external energy. More external energy caused by corrosion is transferred to elastic energy for the RC structures with a smaller reinforcement clearing space.

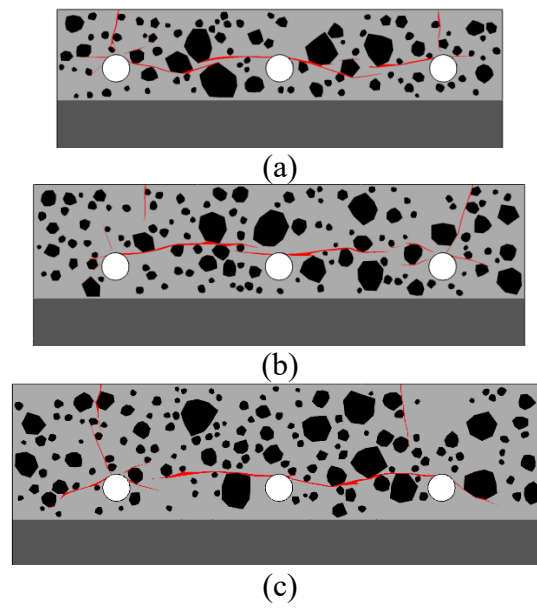


Figure 15 Crack patterns for different thicknesses of concrete cover: (a) 20 mm; (b) 30 mm; (c) 40 mm.

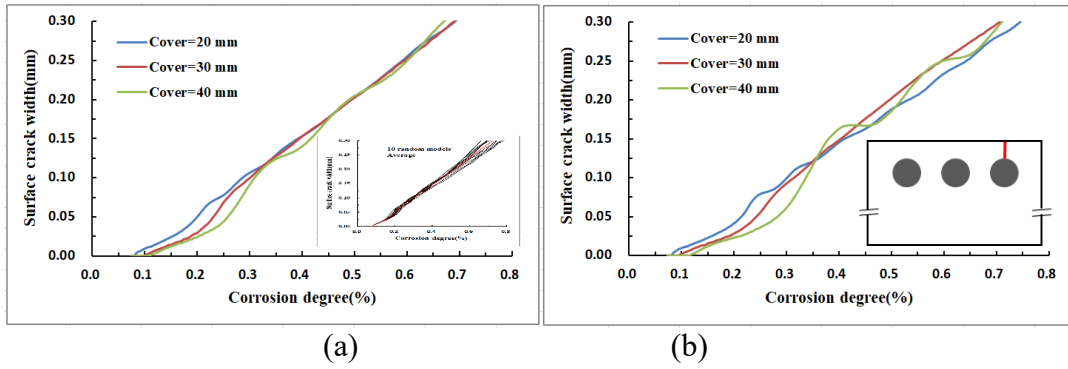


Figure 16 The crack width developments for different thicknesses of concrete cover: (a) left top surface (b) right top surface.

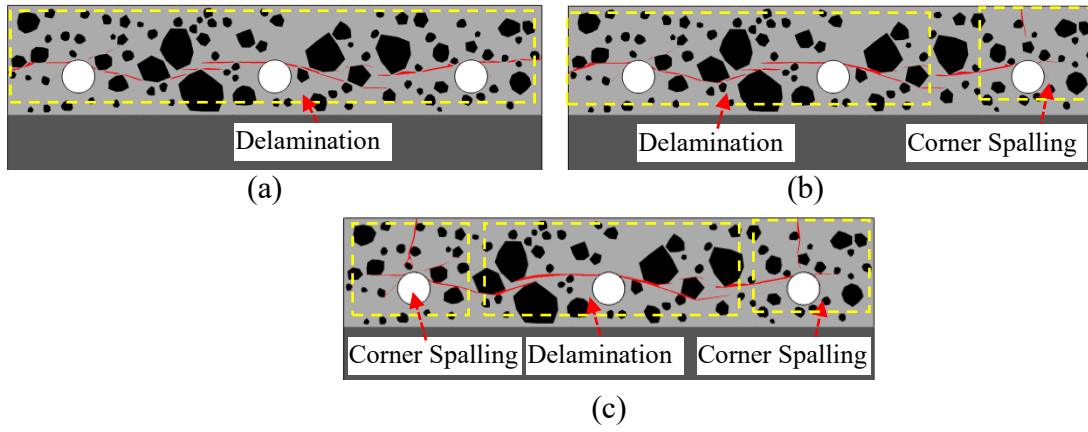


Figure 17 Crack patterns for different strengths of ITZ: (a) 0.1 MPa; (b) 0.25 MPa; (c) 1 MPa.

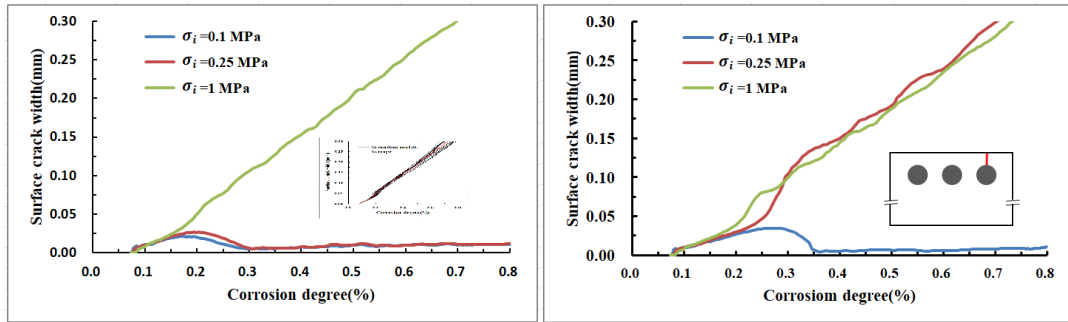


Figure 18 The crack width developments for different strengths of ITZ: (a) left top surface (b) right top surface.

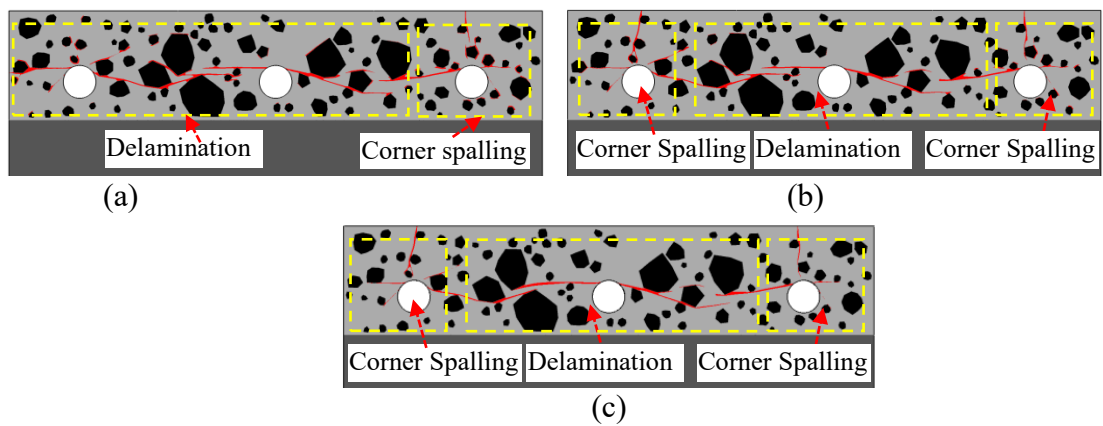


Figure 19 Crack patterns of concrete for different fracture energies of ITZ: (a) 0.00525 N/mm (b) 0.0105 N/mm; (c) 0.021 N/mm.

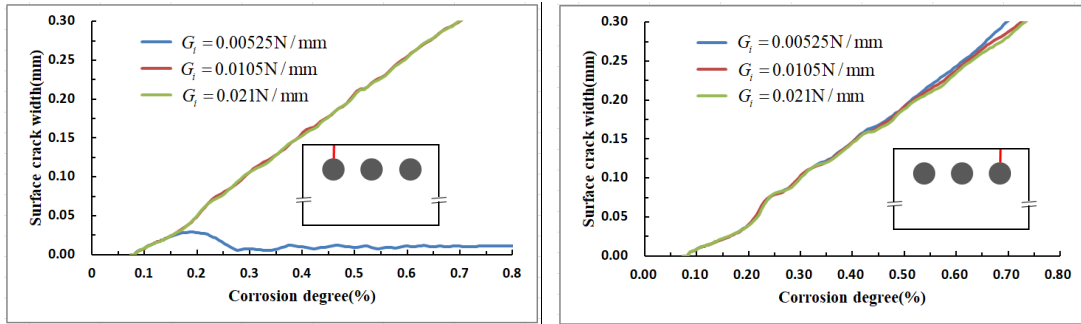
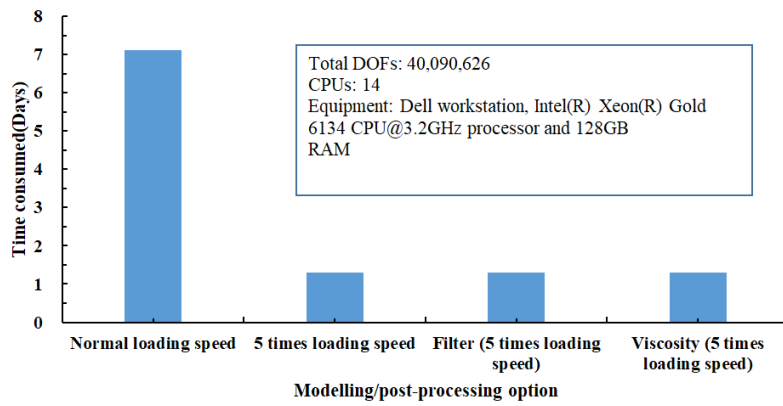
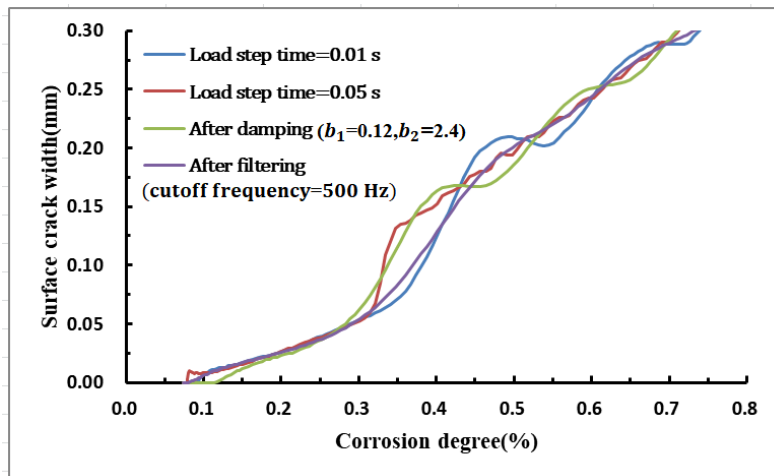


Figure 20 The crack width developments for different fracture energies of ITZ: (a) left top surface (b) right top surface.



(a)



(b)

Figure 21 Expensed time (a) and the modelling results (b) with different modelling approaches.