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6	Influence of cracks on chloride diffusivity in concrete: a five-phase
7	mesoscale model approach
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13	Abstract: This paper presents a mesoscale numerical approach to investigate the chloride diffusivity in
14	cracked concrete. Concrete is treated as a five-phase material, including cement paste, aggregate, interfacial
15	transition zone (ITZ), crack, and damaged zone (DZ), for its heterogeneity. In the mesoscale model, the
16	randomly distributed aggregates were treated as impermeable, whereas all other phases are assumed
17	permeable but with different diffusion coefficients. It is assumed that the crack is located in the middle of
18	the DZ, and there is a liner relationship of the chloride diffusion coefficients between the DZ and the crack.
19	The developed mesoscale model is validated by comparing the simulation results with the experimental
20	data. Finally, the influence of the DZ, such as the chloride diffusion coefficient, the width and length of the
21	DZ, the width and length of the crack, on the penetration of chlorides in cracked concrete is examined and
22	discussed.
23	Keywords: Concrete, Crack, Chloride diffusion, Mesoscale model, Numerical simulation, Multi-phase

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27 **1. Introduction**

Corrosion of reinforcing bars caused by chloride ions is a major cause of reducing or shortening the 28 service life of reinforced concrete (RC) structures [1-6]. Corroded RC structures are easy to be cracked by 29 30 the effect of the loading. Cracks provide easy paths for chloride ions penetration in concrete. In recent years, efforts were made to investigate the influence of cracks on chloride diffusivity in cracked concrete. 31 Rodriguez and Hooton [7] conducted an experiment of chloride diffusion in specimens with parallel-wall 32 33 cracks with widths ranging from 0.10 to 0.68 mm. Win et al. [8] conducted an experimental study on chloride diffusion in cracked reinforced beams exposed to NaCl solution and found that when the water-to-34 35 cement ratio is 0.45 and 0.65, there is no significant difference between the chloride ion penetration depth from the surface of the cracked concrete and that from the exposed surface in specimens. Jang et al. [9] 36 37 reported that chloride diffusion coefficient of the crack will not increase when its width reached to the " threshold crack width " which is found to be around 55-80 um. Li et al. [10] investigated chloride ion 38 39 transport in cracked concrete specimens with crack widths of 0.05 mm, 0.08 mm, 0.1 mm and 0.2 mm by 40 using the rapid chloride migration (RCM) test. In their experiment, they found that the accelerated chloride 41 migration takes place at the crack width ranging from 0.08 mm to 0.1 mm. When the crack width is less than 0.05 mm, the influence of the cracks is ignorable, and when the crack width exceeds 0.1 mm, the 42 chloride transport is similar to that in liquid. Ismail et al. [11] conducted an experimental study on five 43 cracked specimens which were exposed to a chloride solution for 10 hours with the crack width in the range 44 of 21 to 128 µm. They found that there was an impediment of the capacity of chloride diffusion in the crack 45 when its width was less than 53 µm. Further, Ismail et al. [12] found from a test of chloride diffusion in 46 47 cracks with width ranging from 6 to 325 µm that cracks with width of 30 µm or less have no significant effect on chloride diffusion. These works can help us to realize the influence of cracks on chloride diffusivity in cracked concrete. However, it should be noted that the above-mentioned conclusions are not generalizable, since a lot of other factors which will also affect the chloride diffusivity in cracked concrete, such as cement types, the crack length, the crack form, etc. were not examined.

52 With the development of computer technology, more and more researchers focus on the use of 53 numerical simulations to investigate chloride diffusivity in cracked concrete. This kind of simulations is 54 efficient and requires less time than that needed in the process of the experimental study. In some works 55 [13-16] the concrete was treated as a homogeneous material when they carried out a simulation of chloride 56 diffusivity in cracked concrete. However, this kind of simulations, which neglect the heterogeneity of concrete, could result in inaccuracy of simulation results. Thus, recent efforts in the simulation of chloride 57 58 diffusivity in cracked concrete have taken into account this influence. Wang et al. [17] proposed a 2-D mesoscale lattice model considering the mortar, aggregates and ITZ, which was validated by using the 59 60 experimental data, to investigate chloride and water transport in cracked-unsaturated concrete with a single crack. They found that drying-wetting action, crack width and length within concrete are crucial for chloride 61 62 transport in unsaturated cracked concrete. Du et al. [18] developed a four-phase mesoscale model consisting of the cement paste, aggregates, ITZ and cracks to study the effect of the artificial cracks and the tortuous 63 cracks on chloride ions diffusion in cracked concrete, and found that the chloride diffusivity in cracked 64 concrete was affected by the depth and width of the crack. Liu et al. [19] carried out a numerical study on 65 the migration of chloride ions in cracked concrete, in which the concrete was treated as a homogeneous and 66 heterogeneous material considering ionic interactions between different species. In their work, the damaged 67 68 zone was considered to be homogenous in which the aggregate effect is deliberately not considered on the

69 diffusion pattern of chlorides in cracked zone. Note that, the modeling of chloride diffusivity in cracked concrete should consider the effect of aggregate distribution as it can influence the chloride penetration 70 paths, particularly in the region between the crack/damage zone and the aggregate. Generally, according to 71 72 the above-mentioned studies, it can be concluded that the inhomogeneous effect of concrete on chloride 73 diffusivity should be considered in the research on chloride diffusivity in cracked concrete. However, few 74 studies have investigated the chloride diffusivity in cracked concrete by considering the effect of both the 75 crack and the damage zone (DZ) around the crack at the mesoscale levels. Jones et al. (Jones, et al., 2015) proposed a two-dimensional model, which consisted of the cement paste, the DZ, and the crack, to 76 77 investigate chloride diffusion in cracked concrete. However, aggregates and the ITZs were not taken into 78 account in their study.

In this study, a five-phase mesoscale model consisting of the cement paste, aggregates, ITZs, crack, and the DZ, is developed to investigate the chloride diffusivity in cracked concrete. In the mesoscale model, the randomly distributed aggregates were treated as impermeable, whereas all other phases are assumed permeable but with different diffusion coefficients. The model is validated using experimental data. The influence of the DZ, such as the chloride diffusion coefficient of the DZ, the width and length of the DZ, and the crack, such as the width and length of the crack and the crack pattern, on the penetration of chloride ions in cracked concrete is also examined and discussed.

86 2. Mesoscale model of cracked concrete

In this paper, a two-dimensional mesoscale model is developed to simulate the concrete on the basis of COMSOL software, in which concrete is treated as a five-phase composite material. Each phase has an independent diffusivity property related to its micro-structure. The aggregate phase is considered as

90	impermeable, and other four phases are treated as permeable with different diffusion coefficients. Fig.1
91	shows a schematic of the cracked concrete, in which the crack is modeled as an equilateral triangle within
92	the DZ and the DZ is modeled as a rectangle shape as shown by the gray color in Fig.1. It should be noted
93	herein that, the crack modelled in the present study has been simplified. In reality the crack would not be
94	perfectly straight as the form of cracks will be affected by surrounding aggregates. Nevertheless, as the
95	crack is relatively short the effect of its tortuosity on the transport of chlorides would be rather small. The
96	dash line is for measured position and the distance between the crack and the measured position is 2 mm.
97	The crack is assumed to be located in the middle of the damaged zone. In Fig.1, w_{cr} and w_{DZ} are the width
98	of the crack and the DZ, respectively, and, d_{cr} and d_{DZ} are the length of the crack and the DZ, respectively.
99	This type of the crack can be commonly found in concrete beams subjected to bending.

101

Fig. 1. Schematic of the cracked concrete

One of the key problems is to generate random aggregates for the mesoscale analysis. If the volume 102 fraction and sizes of aggregates are provided, the distribution of aggregates can be obtained according to 103 the Walraven function [20]. Fig.2 shows a typical two-dimensional mesoscale model of the cracked 104 105 concrete, in which the circular areas represent aggregates with the diameter ranging from 7 mm to 20 mm 106 and the dash line represents the measured position for chloride concentration profiles. The shapes of aggregates in real concrete are unlikely to be perfectly spherical. However, some works have demonstrated 107 that the effect of the shape of aggregates on the chloride diffusivity in concrete is not significant [21, 22]; 108 109 whereas in some cases (such as 3-D dimensions, migration process, recycled aggregates) its effect may be important [10, 23-26]. For each aggregate there is an ITZ surrounding it, and the thickness of the ITZ is 110 assumed to be identical. As known, the ITZ has a higher porosity than the cement paste which leads to a 111

112	higher chloride diffusivity [27-29]. The real thickness of the ITZ in concrete is in the range of 10-50 μ m
113	[30-33], and herein the thickness of the ITZ is set as 30 μ m in the mesoscale model. Fig.3 shows the finite
114	element meshes of the mesoscale model with triangular meshes, and the total number of meshed triangular
115	elements is 610,724.
116	
117 118 119	Fig. 2. Two-dimensional mesoscale model of the cracked concrete with dimensions of 100×100 mm
120	Fig. 3. Finite element meshes of the two-dimensional mesoscale model of the cracked concrete
121	3. Diffusion coefficient
122	3.1 Chloride diffusion coefficient in cement paste and ITZ
123	Zheng and Zhou [34] proposed an analytical solution, which was derived on the basis of the general
124	effective medium theory, to determine chloride diffusion coefficient of the cement paste, D_{cp} , which can
125	consider the effect of gel and capillary pores and the solid part of the cement, as
126	$D_{cp} = \frac{2.14 \times 10^{-10} V_{p}^{2.75}}{V_{p}^{1.75} (3 - V_{p}) + 14.44 (1 - V_{p})^{2.75}} $ (1)
127	where V _p is the porosity of cement paste, and its expression is given by
128	$V_{p} = \frac{w/c - 0.17\alpha}{w/c + 0.32} $ (2)
129	Where w/c is the water-to-cement ratio, α denotes the degree of hydration and its expression is given by
130	[35]
131	$\alpha = 1 - 3.15 \exp(w/c) \tag{3}$
132	It is worth noting that Garboczi and Bentz [36] pointed out that the w/c redistribution will take place
133	for a high w/c of 0.5. Therefore, the w/c ratio is preferably selected to be less than 0.5 in this approach.

134 Pan et al. [37] studied the relationship between D_{ITZ}/D_{cp} and t_{ITZ} based on existing experimental data, and then obtained an empirical formula by fitting the data. The expression is written as 135 $D_{TTZ} = D_{cp} (139.434/t_{TTZ} + 1.0)$ 136 (4)where t_{ITZ} is the thickness of the ITZ. D_{ITZ} and D_{cp} are the diffusion coefficient of ions in the ITZ and in 137 the cement paste, respectively. 138 In this study, concrete is considered fully saturated and the transport of ions is driven by the gradient 139 of the concentration, and thus Fick's second law is adopted to determine the chloride concentration 140 $\frac{\partial C_k}{\partial t} - \mathbf{D}_{k,x} \frac{\partial^2 C_k}{\partial x^2} - \mathbf{D}_{k,y} \frac{\partial^2 C_k}{\partial y^2} = 0$ 141 (5)where C_k is the chloride concentration, D_k is the chloride diffusion coefficient in phase k (k=1~5), namely 142 143 the cement paste, aggregates, ITZs, crack, and the DZ, and D,x and D,y are the chloride diffusion coefficient in x and y directions, respectively. 144 3.2 Diffusion coefficient of ions in cracks 145 As mentioned above, the crack can significantly accelerate chloride penetration in concrete, and thus 146 it is critical to determine the chloride diffusion coefficient of the crack in the mesoscale model. There are a 147 lot of liner relationships between crack widths and chloride diffusion coefficients which were derived on 148 149 the basis of the experimental data. In the work of [18], the relationship between the crack width and chloride 150 diffusion coefficient was obtained by taking an average of the two equations, which were fitted to the test 151 data of chloride diffusion into cracked ordinary concrete, respectively. However, one of the shortcomings 152 in their work is to ignore the influence of threshold value of the crack. Hence, the expression proposed by Djerbi et al. [38] is introduced into this study, which was also employed by Šavija, et al. [39] in the lattice 153 model of the cracked concrete, which demonstrated that the simulation results matched experimental data 154

155 well. The expression is given as

156
$$\begin{aligned} D_{cr} &= 2 \times 10^{-11} w_{cr} - 4 \times 10^{-10} & 30 \mu \text{m} \le w_{cr} \le 80 \mu \text{m} \\ D_{cr} &= 14 \times 10^{-10} & w_{cr} \ge 80 \mu \text{m} \end{aligned}$$
 (6)

157 where w_{cr} in μ m represents the crack width.

158 **4. Validation of the mesoscale model**

159 In order to verify the developed mesoscale model, experimental data published in [40], which is for 160 concrete beams with water-to-cement ratio (w/c) of 0.485 and having the exposed time of 30 days, are utilized. In the experiment of [40], the reinforced concrete beam specimens were cracked with different 161 widths by bending. In this study, six cracks, which are obtained from the experiment, are divided into two 162 163 groups. The first group, which has three cracks with the crack width of 0 µm, 29.4 µm, and 102.9 µm, and corresponding length of 0 mm, 18.7 mm, and 36.6 mm, respectively, are used to determine the magnitude 164 of D_{DZ}/D_{cp} (D_{DZ} is the diffusion coefficient in the damaged zone). At present, few investigations were made 165 on the quantitative relationship of chloride diffusion coefficients in the DZ and that in the cement paste, 166 and thus one of the key problems is to determine the magnitude of D_{DZ}/D_{cp}. In this study, the width of the 167 DZ is assumed to be the same as 2 mm, the length of the DZ is 10 mm longer than the corresponding crack's 168 length, and the surface chloride concentration is 0.51%. It should be pointed out that, the surface chloride 169 170 concentration used in the model refers to the chloride concentration of the NaCl solution which will not 171 change with time, and the chloride diffusion into concrete is in non-steady-state condition. Herein, three magnitudes of D_{DZ}/D_{cp} are selected as 15, 20 and 25 in the present mesoscale model to investigate which 172 173 will yield in good agreement with the test data. A comparative analysis between simulation results with different magnitudes of D_{DZ}/D_{cp} and the test data is carried out, as presented in Fig.4. It is concluded that 174 when the magnitude of D_{DZ}/D_{cp} is selected as 20, the simulation results match the experimental data well 175

by using the statistical method. Hence, the magnitude of D_{DZ}/D_{cp} in this study is recommended to be 20, which is similar to the works of [13, 19].

Fig. 4. Comparison of simulation results and the test data with different magnitudes of the D_{DZ}/Dcp 178 179 The second group of cracks used herein, which also has three cracks with the crack width of 49 µm, 210.7 µm, and 283 µm, and corresponding length of 28.1 mm, 47.3 mm, and 63.2 mm, respectively, is to 180 validate the developed model, as presented in Fig.5. It can be seen from Fig.5 that, in general, the simulation 181 results can match the test data well. However, there is still a slight difference for the chloride diffusion close 182 183 to the two-dimensional diffusion when the crack width is larger than 210 µm. Therefore, it can be concluded that the developed mesoscale model in this paper has a good accuracy in predicting the chloride diffusivity 184 in cracked concrete when the crack width is less than 210 µm, and there are some works needed to 185 186 investigate the influence of large cracks on chloride diffusion in cracked concrete.

Fig. 5. Comparison of the simulation results and the test data of [40]

188

Fig. 6. Comparison of the simulation results and the test data of [41]

Moreover, ZHANG et al. [41] carried out an experiment to investigate the influence of cracks on 189 190 chloride diffusivity, in which the w/c ratio is 0.6 and each specimen only contains a parallel crack. The surface chloride concentration is 5% (by weight of cement), and the time of exposure is 30 days. In this 191 paper, the group B test data is selected to validate the proposed model, in which the crack width is 0.2 mm 192 and 0.3 mm, but the crack length is the same, both are 100 mm. Fig. 6 shows the comparison of the 193 simulation results and the test data. It can be indicated from Fig. 6 that, when the penetration depth is deeper 194 than 10 mm, the simulation results are in good agreement with the test data. In addition, it is noted from 195 196 Fig. 5 and Fig. 6 that, in order to obtain more accurately simulated results, it is crucial to determine the real 197 chloride diffusion coefficient when the crack width is larger than 200 µm. Overall, the five-phase mesoscale 198 model proposed in this study can be used to predict chloride diffusivity in cracked concrete with good 199 accuracy.

200 5. Analysis with/without considering the influence of the DZ

201 To obtain a better understanding of the influence of the DZ on chloride diffusivity in cracked concrete, a sensitivity analysis is carried out. In the analysis, the crack width, length, and the time of exposure are 202 taken as 100 µm, 30 mm, and 365 days, respectively; whereas the width and length of the DZ are taken as 203 2 mm and 40 mm, respectively. Chloride concentration distributions at 365 days of exposure obtained from 204 the present mesoscale model with and without considering the influence of the DZ are shown in Fig.7. It 205 can be noted from Fig.7 that the crack has a significant influence on the chloride diffusivity in cracked 206 207 concrete, and the chloride penetration depth with considering the influence of the DZ is much deeper than that without considering it. A comparison of chloride concentration profiles between the mesoscale models 208 209 with considering the influence of the DZ and that without considering it is performed, as presented in Fig.8. 210 It can be seen from Fig.8 that the DZ has a significant influence on chloride diffusivity in cracked concrete 211 for it can accelerate chloride penetration in concrete. This is because the chloride concentration calculated by the mesoscale model with considering the influence of the DZ is much higher than that without 212 considering it, and the reason for this is that the DZ has higher porosity when compared with the cement 213 paste. In addition, one can obviously see from Fig.8 that the chloride concentration profile in the region 214 near the top of the damaged zone varies evidently, indicating that the length of the DZ is a turning point of 215 the chloride concentration profile along the depth. 216

Fig. 7. Chloride concentration distributions without / with considering influence of the DZ
 Fig. 8. Comparisons of chloride concentration profiles between the mesoscale models

with / without considering the DZ

220	As mentioned above, the DZ has a pronounced influence on chloride diffusivity in cracked concrete,
221	and in order to effectively distinguish this influence, three magnitudes of D_{DZ}/D_{cp} , i.e., 10, 20 and 30, are
222	selected to investigate the influence of the D _{DZ} on chloride diffusivity in cracked concrete, as presented in
223	Fig.9. It can be seen from Fig.9 that the larger the value of the D_{DZ} , the deeper the penetration depth. Fig.10
224	shows a comparison of chloride concentration profiles between different models with different values of
225	the D_{DZ} . In Fig.10, it can be seen that different magnitudes of the D_{DZ}/D_{cp} lead to significant difference in
226	chloride concentration, especially in the region from the surface to the length of the DZ, the difference
227	between the profiles of the chloride concentration increases gradually. However, when the penetrated depth
228	exceeds the length of the DZ, the difference narrows.
229	Fig. 9. Chloride concentration distributions with different magnitudes of DZ
230	Fig. 10. Comparisons of chloride concentration profiles between different models
231	with different values of D _{DZ}
231 232	with different values of D_{DZ} The influence of geometric parameters of the damaged zone, i.e., the width and length of the DZ, on
232	The influence of geometric parameters of the damaged zone, i.e., the width and length of the DZ, on
232 233	The influence of geometric parameters of the damaged zone, i.e., the width and length of the DZ, on chloride diffusivity in cracked concrete is also examined numerically herein. First, three lengths of the DZ,
232 233 234	The influence of geometric parameters of the damaged zone, i.e., the width and length of the DZ, on chloride diffusivity in cracked concrete is also examined numerically herein. First, three lengths of the DZ, i.e., 30 mm, 35 mm, and 40 mm, are accounted for in the mesoscale model, but the width of the DZ is
232233234235	The influence of geometric parameters of the damaged zone, i.e., the width and length of the DZ, on chloride diffusivity in cracked concrete is also examined numerically herein. First, three lengths of the DZ, i.e., 30 mm, 35 mm, and 40 mm, are accounted for in the mesoscale model, but the width of the DZ is assumed to be the same as 2 mm. Fig.11 shows the chloride concentration distributions simulated by using
 232 233 234 235 236 	The influence of geometric parameters of the damaged zone, i.e., the width and length of the DZ, on chloride diffusivity in cracked concrete is also examined numerically herein. First, three lengths of the DZ, i.e., 30 mm, 35 mm, and 40 mm, are accounted for in the mesoscale model, but the width of the DZ is assumed to be the same as 2 mm. Fig.11 shows the chloride concentration distributions simulated by using the mesoscale model with different lengths of the DZ. It can be obviously seen from Fig.11 that the chloride
 232 233 234 235 236 237 	The influence of geometric parameters of the damaged zone, i.e., the width and length of the DZ, on chloride diffusivity in cracked concrete is also examined numerically herein. First, three lengths of the DZ, i.e., 30 mm, 35 mm, and 40 mm, are accounted for in the mesoscale model, but the width of the DZ is assumed to be the same as 2 mm. Fig.11 shows the chloride concentration distributions simulated by using the mesoscale model with different lengths of the DZ. It can be obviously seen from Fig.11 that the chloride penetration depth increases with the increase of the length of the DZ. In order to clearly reveal the difference
 232 233 234 235 236 237 238 	The influence of geometric parameters of the damaged zone, i.e., the width and length of the DZ, on chloride diffusivity in cracked concrete is also examined numerically herein. First, three lengths of the DZ, i.e., 30 mm, 35 mm, and 40 mm, are accounted for in the mesoscale model, but the width of the DZ is assumed to be the same as 2 mm. Fig.11 shows the chloride concentration distributions simulated by using the mesoscale model with different lengths of the DZ. It can be obviously seen from Fig.11 that the chloride penetration depth increases with the increase of the length of the DZ. In order to clearly reveal the difference of chloride concentrations between the mesoscale models, a comparison of chloride concentration profiles

reason for this is that chloride diffusion rate is markedly influenced by the length of the DZ. When the region is close to the surface, owing to the different chloride diffusion rate, the chloride concentration in the region with shorter length DZ is higher than that with higher length DZ. However, when the penetration depth is deeper than the length of the intersection, the situation becomes opposite. This is because the penetration depth of chlorides is positively related to the length of the DZ.

Fig. 11. Chloride concentration distributions with different lengths of the damaged zone
 Fig. 12. Comparisons of chloride concentration profiles between three models (different lengths of the DZ)

Similarly, three widths of the DZ, i.e., 1.5 mm, 2.0 mm, and 3.0 mm, are selected in the mesoscale model to investigate its influence on chloride diffusivity in cracked concrete. Fig.13 shows the chloride concentration distributions simulated by mesoscale models with different widths of the DZ, in which the length of the DZ is kept as a constant (40 mm). It can be seen from Fig.13 that the chloride penetration depth increases with the increase of the width of the DZ. Also, a comparison of chloride concentration profiles between three models with different widths of the DZ is presented in Fig.14, showing that the width of the DZ has a pronounced influence on chloride diffusivity in cracked concrete.

Fig. 13. Chloride concentration distributions with different widths of the damaged zone
 Fig. 14. Comparisons of chloride concentration profiles between three models (different widths of the DZ)
 As a result, either the width or the length of DZ is not a negligible influencing factor in the mesoscale
 analysis for chloride diffusivity in cracked concrete. Therefore, how to accurately determine the width,

length, and the area of the DZ is an important and meaningful work in the future.

13

263 6. Parametric analysis

264 6.1 Influence of crack width

To investigate the influence of the width of cracks on chloride diffusivity in cracked concrete, five 265 crack widths of 30, 50, 70, 100, and 300 µm, are utilized; while the crack length remains unchanged (30 266 mm) in the simulations. The width and length of the damaged zone are set as 2 mm and 40 mm, respectively. 267 Note that, in general, the larger width of the crack leads to the larger length, that is to say, the crack length 268 should also change when the crack width varies. However, as this is a parametric study it is more convenient 269 to investigate each individual parameter separately. In the mesoscale model, the surface chloride 270 concentration is 0.50% and the time of exposure is 365 days. Fig.15 shows the chloride concentration 271 distributions calculated by the models with different crack widths. Fig.16 shows the comparisons of 272 273 chloride concentration profiles along the depth between different models. It can be seen from Fig 16 that the width of the crack has a significant influence on chloride diffusion in cracked concrete, and the bigger 274 275 difference takes place at the region from the surface to the length of the DZ.

Fig. 15. Chloride concentration distributions with different widths of the crack

Fig. 16. Comparisons of chloride concentration profiles between different models (different widths of the

278

crack)

279 6.2 Influence of the crack length

Similar to the crack width, three crack lengths, i.e., 10 mm, 20 mm, and 30 mm, were selected in this section to investigate the influence of the crack length on chloride diffusivity in cracked concrete, while the crack width is kept unchanged ($100 \mu m$). The width of the DZ is set as 2 mm, and the length of the DZ is assumed to be 10 mm longer than the length of the corresponding crack. In the mesoscale model, the surface 284 chloride concentration and days of exposure is 0.50% and 365 days, respectively. Fig.17 shows the chloride concentration distributions calculated by models with different lengths of the crack. Fig.18 shows the 285 comparisons of chloride concentration profiles along the depth between different models, and it can be seen 286 from Fig. 18 that the influence of the crack length on chloride diffusivity in cracked concrete is significant. 287 Similar to the above study of influence of the length of the DZ on chloride diffusivity, there is an intersection 288 between the chloride concentration profiles. When the penetration depth is deeper than the length of the 289 intersection, the longer the length of the crack, the higher the chloride concentration in front of the DZ. 290 291 However, when the penetration depth is less than the depth of the intersection, the shorter the length of the crack, the higher the chloride concentration. The reason for this is similar to the aforementioned analysis 292 of the influence of the DZ, but owing to the influence of the crack, the profiles of chloride concentration 293 294 change significantly when compared with that shown in Fig. 14.

Fig. 17. Chloride concentration distributions with different crack lengths

Fig. 18. Comparison of chloride concentration profiles between different models (different crack lengths) As a result, it can be concluded that both the crack width and length can influence the chloride diffusivity in cracked concrete. If there is a crack and there is a DZ around it, when the influence of the crack is considered in the mesoscale model, the influence of the DZ should be also taken into account.

300 6.3 Influence of the crack pattern

In the above study, it can be found that the type of crack is considered to be tapered crack. However, in reality the form of cracks could vary. To investigate the influence of the form of the crack on chloride diffusivity, three forms of the cracks, i.e., tapered, tortuous and parallel-wall are taken into account. Whereas the length and width of cracks are kept the same for the three different crack types used in the

305	mesoscale model. Note that the tortuous crack is connected by straight lines, and there are two turning
306	points in the middle of the crack. The surface chloride concentration is 0.5% and the time of exposure is
307	365 days. Fig. 19 shows the chloride concentration distributions with different forms of the cracks. Fig 20
308	shows a comparison of chloride concentration profiles between different models. It can be noted from Fig
309	20 that the crack shape can affect the chloride diffusivity in cracked concrete. Moreover, the chloride
310	concentration calculated by Parallel-wall crack is higher that calculated by the tapered and tortuous crack,
311	respectively. Specifically, it can be concluded that the biggest influence on chloride diffusion is the tapered
312	crack, the second is the tortuous crack, and the smallest is the parallel-wall crack.
313	Fig. 19. Chloride concentration distributions with different forms of the crack
314	Fig. 20. Comparison of chloride concentration profiles between different models (different crack patterns)
315	7. Conclusions
515	
316	By treating concrete as a five-phase material, i.e., the cement paste, aggregates, ITZs, crack, and
316	By treating concrete as a five-phase material, i.e., the cement paste, aggregates, ITZs, crack, and
316 317	By treating concrete as a five-phase material, i.e., the cement paste, aggregates, ITZs, crack, and damage zone, the mesoscale model with consideration of the influence of the heterogeneous concrete has
316317318	By treating concrete as a five-phase material, i.e., the cement paste, aggregates, ITZs, crack, and damage zone, the mesoscale model with consideration of the influence of the heterogeneous concrete has been developed to investigate chloride ions diffusion in cracked concrete. In the mesoscale model, the
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 316 317 318 319 320 	By treating concrete as a five-phase material, i.e., the cement paste, aggregates, ITZs, crack, and damage zone, the mesoscale model with consideration of the influence of the heterogeneous concrete has been developed to investigate chloride ions diffusion in cracked concrete. In the mesoscale model, the randomly distributed aggregates were considered impermeable, whereas the other four phases were treated as permeable materials but with different chloride diffusion coefficients. It was assumed that the crack was
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326	(1) The magnitude of D_{DZ}/D_{cp} is recommended to be 20 in the mesoscale model in which the simulation
327	results were in good agreement with the experimental data for the chloride diffusion process is a steady
328	state.

329	(2) The influence of the DZ cannot be ignored in the mesoscale analysis for chloride diffusivity in
330	cracked concrete, and the chloride concentration profiles changed sharply at the length of DZ.

(3) The shape of the crack can affect the chloride diffusivity in cracked concrete, however the
 difference of the chloride concentration profiles between the tortuous and the parallel-wall crack is not
 significant.

(4) Both the extent of the DZ and the diffusion coefficient in the DZ are the important parameters in
the present five-phase model. Therefore, experimental studies are required to determine the extent of the
DZ around the crack, and to obtain a quantitative relationship between the diffusion coefficient of the DZ
and that of the cement paste.

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347 **References**

- 348 [1] Y. Ma, F. Xu, L. Wang, J. Zhang, X. Zhang, Influence of corrosion-induced cracking on structural
- behavior of reinforced concrete arch ribs, Engineering Structures 117 (2016) 184-194.
- 350 [2] Y. Ma, Z. Guo, L. Wang, J. Zhang, Experimental investigation of corrosion effect on bond behavior
- between reinforcing bar and concrete, Construction and Building Materials 152 (2017) 240-249.
- 352 [3] D.V. Val, P.A. Trapper, Probabilistic evaluation of initiation time of chloride-induced corrosion,
- Reliability Engineering & System Safety 93(3) (2008) 364-372.
- 354 [4] M.K. Kassir, M. Ghosn, Chloride-induced corrosion of reinforced concrete bridge decks, Cement
- 355 and Concrete Research 32(1) (2002) 139-143.
- 356 [5] Y. Yang, J. Peng, J. Zhang, C. Cai, A new method for estimating the scale of fluctuation in reliability
- assessment of reinforced concrete structures considering spatial variability, Advances in Structural
 Engineering (2018) 1369433218760891.
- [6] S. Hu, J. Peng, J. Zhang, C. Cai, Influences of Time, Temperature, and Humidity on Chloride
 Diffusivity: Mesoscopic Numerical Research, Journal of Materials in Civil Engineering 29(11) (2017)
 04017223.
- [7] O.G. Rodriguez, R.D. Hooton, Influence of cracks on chloride ingress into concrete, Aci Materials
 Journal 100(2) (2003) 120-126.
- [8] P.P. Win, M. Watanabe, A. Machida, Penetration profile of chloride ion in cracked reinforced
 concrete, Cement and Concrete Research 34(7) (2004) 1073-1079.
- 366 [9] S.Y. Jang, B.S. Kim, B.H. Oh, Effect of crack width on chloride diffusion coefficients of concrete
- 367 by steady-state migration tests, Cement and Concrete Research 41(1) (2011) 9-19.

368	[10] Y. Li, X. Chen, L. Jin, R. Zhang, Experimental and numerical study on chloride transmission in
369	cracked concrete, Construction and Building Materials 127 (2016) 425-435.
370	[11] M. Ismail, A. Toumi, R. François, R. Gagné, Effect of crack opening on the local diffusion of
371	chloride in inert materials, Cement and Concrete Research 34(4) (2004) 711-716.
372	[12] M. Ismail, A. Toumi, R. François, R. Gagné, Effect of crack opening on the local diffusion of
373	chloride in cracked mortar samples, Cement and Concrete Research 38(8-9) (2008) 1106-1111.
374	[13] D.P. Bentz, E.J. Garboczi, Y. Lu, N. Martys, A.R. Sakulich, W.J. Weiss, Modeling of the influence
375	of transverse cracking on chloride penetration into concrete, Cement and Concrete Composites 38 (2013)
376	65-74.
377	[14] L. Marsavina, K. Audenaert, G. De Schutter, N. Faur, D. Marsavina, Experimental and numerical
378	determination of the chloride penetration in cracked concrete, Construction and Building Materials 23(1)
379	(2009) 264-274.
380	[15] XY. Wang, LN. Zhang, Simulation of Chloride Diffusion in Cracked Concrete with Different
381	Crack Patterns, Advances in Materials Science and Engineering 2016 (2016) 1-11.
382	[16] S. Jones, N. Martys, Y. Lu, D. Bentz, Simulation studies of methods to delay corrosion and
383	increase service life for cracked concrete exposed to chlorides, Cement and Concrete Composites 58 (2015)
384	59-69.
385	[17] L. Wang, J. Bao, T. Ueda, Prediction of mass transport in cracked-unsaturated concrete by
386	mesoscale lattice model, Ocean Engineering 127 (2016) 144-157.
387	[18] X. Du, L. Jin, R. Zhang, Y. Li, Effect of cracks on concrete diffusivity: A meso-scale numerical
388	study, Ocean Engineering 108 (2015) 539-551.

389	[19] Qf. Liu, J. Yang, J. Xia, D. Easterbrook, Ly. Li, XY. Lu, A numerical study on chloride
390	migration in cracked concrete using multi-component ionic transport models, Computational Materials
391	Science 99 (2015) 396-416.
392	[20] J.C. Walranen, Reinhardt H W, Theory and Experiments on the Mechanical Behaviour of Cracks
393	in Plain and Reinforced Concrete Subjected to Shear Loading, HERON 26(1A) (1981) 26-35.
394	[21] X. Du, L. Jin, G. Ma, A meso-scale numerical method for the simulation of chloride diffusivity
395	in concrete, Finite Elements in Analysis and Design 85 (2014) 87-100.
396	[22] LY. Li, J. Xia, SS. Lin, A multi-phase model for predicting the effective diffusion coefficient
397	of chlorides in concrete, Construction and Building Materials 26(1) (2012) 295-301.
398	[23] Z. Hu, Lx. Mao, J. Xia, Jb. Liu, J. Gao, J. Yang, Qf. Liu, Five-phase modelling for effective
399	diffusion coefficient of chlorides in recycled concrete, Magazine of Concrete Research (2017) 1-12.
400	[24] Qf. Liu, D. Easterbrook, Ly. Li, D. Li, Prediction of chloride diffusion coefficients using multi-
401	phase models, Magazine of Concrete Research 69(3) (2016) 134-144.
402	[25] Qf. Liu, Gl. Feng, J. Xia, J. Yang, Ly. Li, Ionic transport features in concrete composites
403	containing various shaped aggregates: a numerical study, Composite Structures 183 (2018) 371-380.
404	[26] S.D. Abyaneh, H. Wong, N. Buenfeld, Modelling the diffusivity of mortar and concrete using a
405	three-dimensional mesostructure with several aggregate shapes, Computational Materials Science 78 (2013)
406	63-73.
407	[27] W. Li, J. Xiao, Z. Sun, S. Kawashima, S.P. Shah, Interfacial transition zones in recycled aggregate
408	concrete with different mixing approaches, Construction and Building Materials 35 (2012) 1045-1055.
409	[28] J. Xiao, W. Li, D.J. Corr, S.P. Shah, Simulation study on the stress distribution in modeled

410	recycled aggregate concrete under uniaxial compression, Journal of materials in civil engineering 25(4
411	(2012) 504-518.

- 412 [29] J. Xiao, W. Li, Z. Sun, D.A. Lange, S.P. Shah, Properties of interfacial transition zones in recycled
- 413 aggregate concrete tested by nanoindentation, Cement and Concrete Composites 37 (2013) 276-292.
- [30] Z. Jiang, Q. Huang, Y. Xi, X. Gu, W. Zhang, Experimental Study of Diffusivity of the Interfacial
 Transition Zone between Cement Paste and Aggregate, Journal of Materials in Civil Engineering (2016)
 04016109.
- 417 [31] K.L. Scrivener, A.K. Crumbie, P. Laugesen, The Interfacial Transition Zone (ITZ) Between
- 418 Cement Paste and Aggregate in Concrete, Interface Science 12(4) (2004) 411-421.
- [32] A. Elsharief, M.D. Cohen, J. Olek, Influence of aggregate size, water cement ratio and age on the
 microstructure of the interfacial transition zone, Cement & Concrete Research 33(11) (2003) 1837-1849.
- 421 [33] Y. Gao, G.D. Schutter, G. Ye, Micro- and meso-scale pore structure in mortar in relation to 422 aggregate content, Cement & Concrete Research 52(10) (2013) 149-160.
- 423 [34] J. Zheng, X. Zhou, Analytical Solution for the Chloride Diffusivity of Hardened Cement Paste,
- 424 Journal of Materials in Civil Engineering 20(5) (2008) 384-391.
- 425 [35] B.H. Oh, S.Y. Jang, Prediction of diffusivity of concrete based on simple analytic equations,
- 426 Cement and Concrete Research 34(3) (2004) 463-480.
- 427 [36] E.J. Garboczi, D.P. Bentz, The Effect of the Interfacial Transition Zone on Concrete Properties:
- 428 The Dilute Limit, in: C. KP (Ed.) Materials for the New Millenium, 1996, pp. 1228-1237.
- 429 [37] Z. Pan, A. Chen, X. Ruan, Spatial variability of chloride and its influence on thickness of concrete
- 430 cover: A two-dimensional mesoscopic numerical research, Engineering Structures 95 (2015) 154-169.

431	[38] A. Djerbi, S. Bonnet, A. Khelidj, V. Baroghel-bouny, Influence of traversing crack on chloride
432	diffusion into concrete, Cement and Concrete Research 38(6) (2008) 877-883.

- 433 [39] B. Šavija, J. Pacheco, E. Schlangen, Lattice modeling of chloride diffusion in sound and cracked
- 434 concrete, Cement and Concrete Composites 42 (2013) 30-40.
- 435 [40] M. Şahmaran, Effect of flexure induced transverse crack and self-healing on chloride diffusivity
- 436 of reinforced mortar, Journal of Materials Science 42(22) (2007) 9131-9136.
- 437 [41] J. Zhang, Y. Liu, Z. Shi, Diffusion of Chloride Ions in Cracked Concrete, Journal of Building
- 438 Materials (2017).

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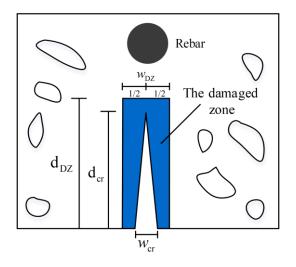


Fig. 1. Schematic of the cracked concrete

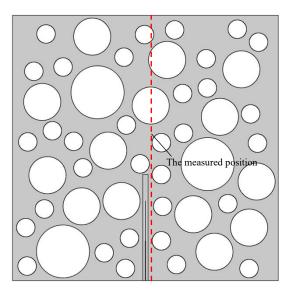


Fig. 2. Two-dimensional mesoscale model of the cracked concrete with dimensions of 100×100 mm

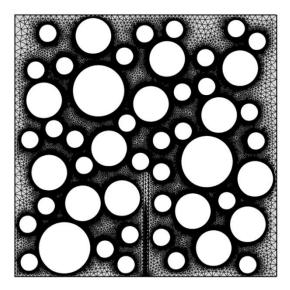


Fig. 3. Finite element meshes of the two-dimensional mesoscale model of the cracked concrete

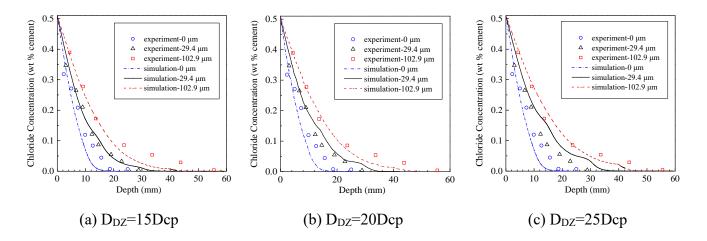


Fig. 4. Comparison of the simulation results and the test data with different magnitudes of the

D_{DZ}/Dcp

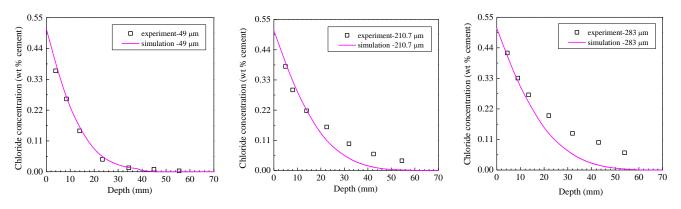


Fig. 5. Comparison of the simulation results and the test data of [40]

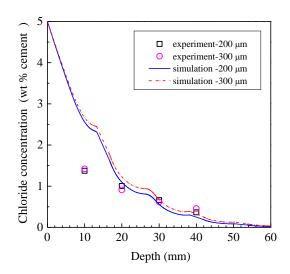
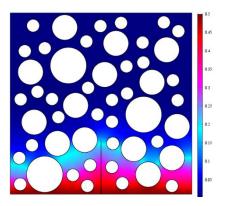
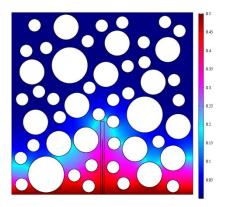


Fig. 6. Comparison of the simulation results and the test data of [41]



(a) Model without considering influence of the



(b) Model with considering influence of the DZ

DZ

Fig. 7. Chloride concentration distributions without / with considering influence of the DZ

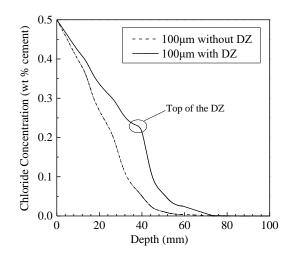


Fig. 8. Comparisons of chloride concentration profiles between the mesoscale models with / without

considering of the DZ

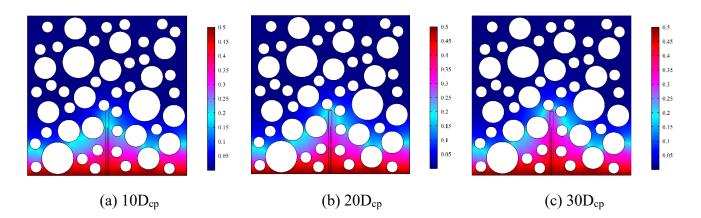


Fig. 9. Chloride concentration distributions with different magnitudes of DZ

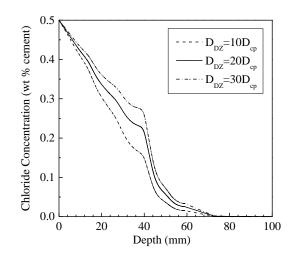
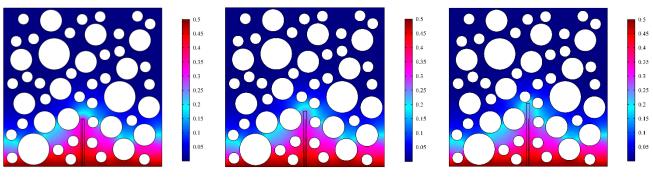


Fig. 10. Comparisons of chloride concentration profiles between different models with different values of

D_{DZ}



(a) 30 mm

(b) 35 mm

(c) 40 mm

Fig. 11. Chloride concentration distributions with different lengths of the damaged zone

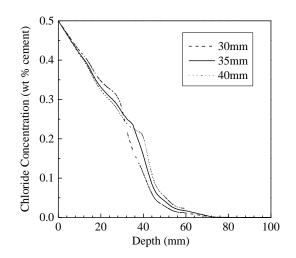
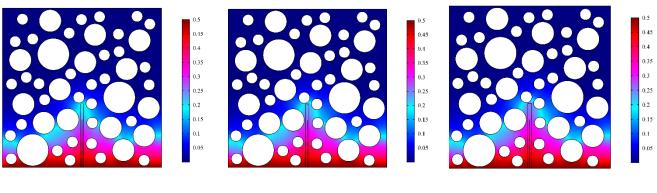


Fig. 12. Comparisons of chloride concentration profiles between three models (different lengths of the DZ)



(a) 1.5 mm

(b) 2.0 mm

(c) 2.5 mm

Fig. 13. Chloride concentration distributions with different widths of the damaged zone

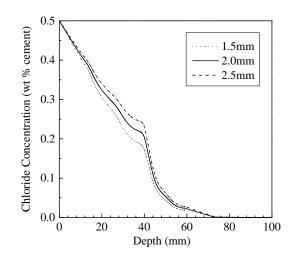


Fig. 14. Comparisons of chloride concentration profiles between three models (different widths of the DZ)

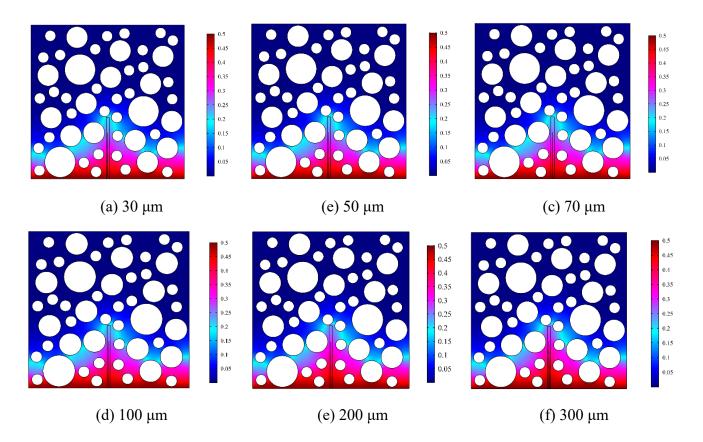


Fig. 15. Chloride concentration distributions with different widths of the crack

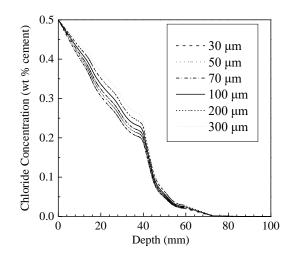


Fig. 16. Comparisons of chloride concentration profiles between different models (different widths of the

crack)

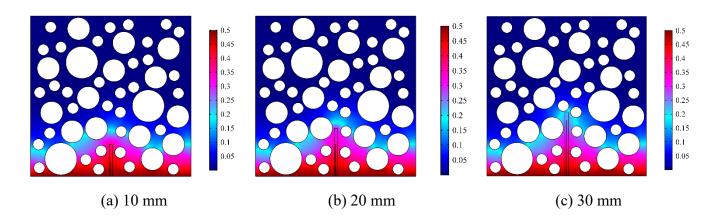


Fig. 17. Chloride concentration distributions with different crack lengths

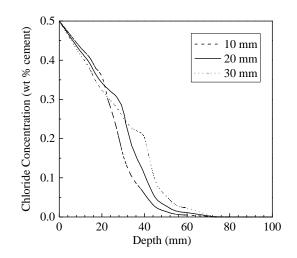
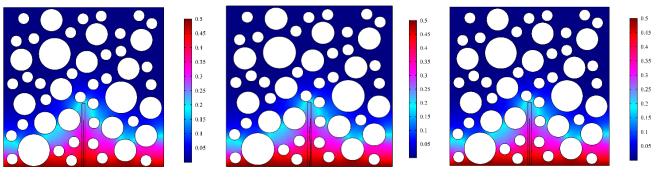


Fig. 18. Comparison of chloride concentration profiles between different models (different crack lengths)



(a) Tapered crack

(b) Tortuous crack

(c) Parallel-wall crack

Fig. 19. Chloride concentration distributions with different forms of the crack

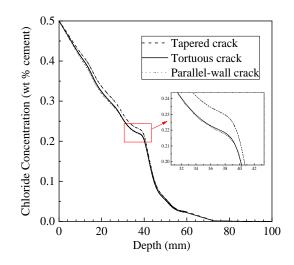


Fig. 20. Comparison of chloride concentration profiles between different models (different crack

patterns)