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Modeling of chloride diffusion in concrete considering wedge-shaped single crack and steady-state condition

Keun-Hyeok Yang[1a], Ju Hyun Cheon[2b] and Seung-Jun Kwon[*3]

[1]*Plant Architectural Engineering, Kyonggi University, Suwon, 16227, South Korea*
[2]*High-Tech Construction Materials Center, Korea Conformity Laboratories, Seoul, 08503, South Korea*
[3]*Civil and Environmental Engineering, Hannam University, Daejeon, 34430, South Korea*

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Abstract. Crack on concrete surface allows more rapid penetration of chlorides. Crack width and depth are dominant parameters for chloride behavior, however their effects on chloride penetration are difficult to quantify. In the present work, the previous anisotropic (1-D) model on chloride diffusion in concrete with single crack is improved considering crack shape and roughness. In the previous model, parallel-piped shape was adopted for crack shape in steady-state condition. The previous model with single crack is improved considering wedge shape of crack profile and roughness. For verifying the proposed model, concrete samples for nuclear power plant are prepared and various crack widths are induced 0.0 to 1.2 mm. The chloride diffusion coefficients in steady-state condition are evaluated and compared with simulation results. The proposed model which can handle crack shape and roughness factor is evaluated to decrease chloride diffusion and can provide more reasonable results due to reduced area of crack profile. The roughness effect on diffusion is evaluated to be 10-20% of reduction in chloride diffusion.

Keywords: nuclear power plant concrete; crack width; diffusion coefficient; roughness; wedge shape

1. Introduction

Concrete is an attractive construction material with high durability, low cost of manufacturing, and stable supply system. The capillary pores in concrete can provide a room for evaporation and avoiding internal gas pressure to outside, however they can be the main routes of intrusion of harmful ions (Kwon *et al*. 2009, Park *et al*. 2012). For enhancement of concrete durability, several techniques can be considered in material, construction, and design stage. Durability enhancement through improvement of material properties is preferred since another expense due to altering design parameters and construction level can be saved. Many researches on durability enhancement in concrete with supplementary material have been carried out such as lower diffusion coefficient and larger absorption of chlorides (Thomas and Bamforth 1999, Saraswathy *et al*. 2003, Elfmarkova *et al*. 2015, Yoo and Kwon 2016, Song *et al*. 2016). It can be achieved by replacing OPC (Ordinary Portland Cement) with mineral admixtures like FA (Fly Ash), GGBFS (Ground Granulated Blast Furnace Slag), RHA (Rice Husk Ash), and SF (Silica Fume).

Crack in HPC (High Performance Concrete) containing a large unit content of binder easily occurs due to differential material behavior of such as hydration heat and drying shrinkage (Song *et al*. 2001, Park *et al*. 2012a). The cracks on concrete surface can be additional path of chloride ion intrusion, so that local corrosion in steel starts more rapidly (Win *et al*. 2004). The enlarged chlorides through existing crack width also accelerates wider crack opening due to swelling of corrosion rust. The previous models with crack effect on chloride diffusion have almost similar parameters considering crack width. The rectangular (parallel-piped) shape of crack in anisotropic and isotropic was proposed for modeling on diffusion in cracked concrete (JSCE 2007, Gerard and Marchand 2000), however they disregarded crack patterns and surface roughness, which showed overestimation for test results.

REV (Representative Element Volume) theory has been adopted for modeling on chloride behavior in heterogeneous like concrete with cracks. It explains that total ion flow is the same as the summation of ion flow in crack width and sound concrete (Jacobsen *et al*. 1996, Gerard and Marchand 2000, Kwon *et al*. 2009, Park *et al*. 2012a). If steady-state condition is assumed, the chloride diffusion mechanism in REV can be applied to carbonation behavior (Song *et al*. 2006) and permeation behavior (Park *et al*. 2012b). Field investigation or survey on crack effect also gives valuable results. The more deteriorating state due to crack occurrence can be found in the previous researches (Yokozeki *et al*. 1998, Kwon *et al*. 2009, Pang and Li 2016). Numerical techniques based on the models covering early-aged concrete behavior such as porosity development and hydration have been proposed, where chloride behavior in non-steady state condition with complicated binding capacity of chloride ion can be considered (Ishida *et al*.

∗Corresponding author, Ph.D.
E-mail: jjuni98@hannam.ac.kr
[a]Professor
E-mail: yangkh@kgu.ac.kr
[b]E-mail: jhcheon@kcl.re.kr

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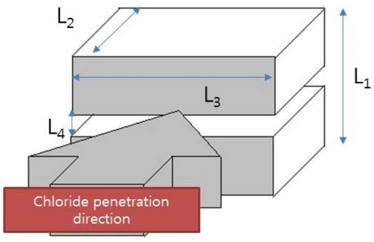


Fig. 1 Chloride diffusion in steady state condition (Anisotropic model)

2009, Iqbal *et al*. 2009, Ishida *et al*. 2011, Chen *et al*. 2016).

In the present work, a simplistic modeling on diffusion in cracked concrete is proposed considering steady-state condition and 1-dimensional intrusion of chlorides (anisotropic model). For the work, crack shape and roughness are newly considered, and the results are compared with test results. For evaluation of roughness and crack effect, mix proportions for nuclear power plant concrete are prepared and RCPT (Rapid Chloride Penetration Test) are performed in steady-state condition.

2. Previous modeling on chloride diffusivity in concrete with single crack-anisotropic model

In the previous research, REV theory is adopted for isotropic and anisotropic conditions like Fig. 1. It requires the condition of constant temperature without physical/chemical interaction of ions, which means steady-state condition. In Fig. 1 schematic diagram is shown for anisotropic and isotropic diffusion model. In the precious research, crack spacing factor (f) which is based on average crack spacing and average crack width is assumed as Eq. (1)

$$f_1 = \frac{L_1}{L_4} \tag{1}$$

Where L_1 and L_4 are average crack spacing and average crack width.

In steady-state and anisotropic condition, flux keeps constant so that total flow (F_t) consists of flow via crack width (F_c) and sound concrete (F_s), which yields Eq. (2).

$$F_t = F_c + F_s \tag{2}$$

Assuming steady-state condition, equivalent flux (J_t) in REV can be calculated as Eq. (3) where each area and flux for crack and sound concrete are considered, respectively.

$$J_t = [J_c A_c + J_s A_s]/[A_c + A_s] \tag{3}$$

Regarding Eq. (3), diffusion coefficient (D_0) in sound concrete (reference diffusion coefficient) and diffusion coefficient in crack (D_1) are considered. The equivalent diffusion coefficient ($\overline{D}$) in REV can be written as Eq. (4) considering area ratio parameter ($S=A_s/A_c$).

$$\overline{D} = [D_1 A_c + D_0 A_s]/[A_c + A_s] = D_0[(D_1/D_0 + S)/(1+S)] \tag{4}$$

Considering area ratio parameter as Eq. (5), equivalent diffusion coefficient in anisotropic condition ($\overline{D}$) can be finally obtained as Eq. (6).

$$S = A_s/A_c = (L_1 - L_4)/L_4 = f - 1 \tag{5}$$

$$\overline{D} = D_0[(D_1/D_0 f) + 1] \tag{6}$$

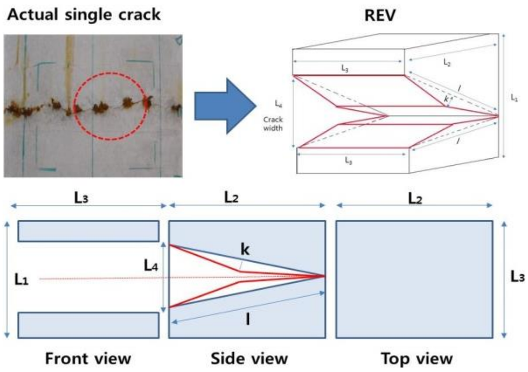


Fig. 2 Modified REV with crack and roughness (isotropic condition)

3. Modeling on chloride diffusion coefficient in isotropic condition

3.1 Consideration of wedged shape of crack profile with roughness factor

The previous models considered a parallel-piped crack profile without torturity but crack opening on concrete surface decreases to concrete depth. Furthermore, the surface of cracked section is not smooth or even and it impedes ion intrusion to the steel, so called roughness or torturity effect (Maekawa *et al*. 2003, 2009). In the present model, crack profile is assumed to have wedge shape with roughness like Fig. 2. The cracked section has very complicated surface inside but bi-linear shape along to concrete depth direction is assumed for simplicity of modeling.

In Fig. 2, k is roughness height from middle of the length (l).

3.1 Formulation of diffusion

Considering REV with unit depth, Eq. (4) can be written as Eq. (7) considering sound (V_s) and crack volume (V_c), respectively. They can be determined as Eq. (8) and Eq. (9).

$$\overline{D} = D_0\left[\frac{D_1/D_0 + V}{1+V}\right],\quad V = \frac{V_u}{V_c} \tag{7}$$

$$V_s = (L_1 - L_4)L_2L_3 \tag{8}$$

$$V_c = \frac{1}{2}(L_2L_3L_4) - lkL_3 \tag{9}$$

Table 1 Mix proportions for concrete samples

Grade (MPa)	w/c (%)	S/a (%)	Slump (mm)	G_{max} (mm)	Unit weight (kg/m^3)					Chemical Ad (kg/m^3)	
					Water	Cement	Fly ash	Sand	Gravel	AE*	WRA**
27	50	46.7	150	19	162.8	260.6	64.9	822.0	938.8	2.08	20.83

*Air Entrainer, **Water Reducing Agent

In the wedge shape of crack profile in Fig. 2, L_4 is much lower than L_2, so that l can be assumed as Eq. (10).

$$l = \sqrt{(L_4/2)^2 + L_2^2} \approx L_2 \quad (10)$$

Considering f>>1, the volume ratio of V can be formulated to Eq. (11) and the equivalent diffusion coefficient in anisotropic condition can be obtained in Eq. (12).

$$V = \frac{2(L_1 - L_4)L_2L_3}{(L_2L_3L_4) - lkL_3} = \frac{2(L_1 - L_4)}{L_4 - 2pL_4} = \frac{2(f-1)}{1-p} \approx \frac{2f}{1-2p} \quad (11)$$

$$\overline{D} = D_0\left[\frac{D_1(1-2p)}{2fD_0} + 1\right] \quad (12)$$

Where the parameter of $p(=k/L_4)$ is determined as the ratio of k to crack width (L_4).

4. Verification of the model

4.1 Experimental program

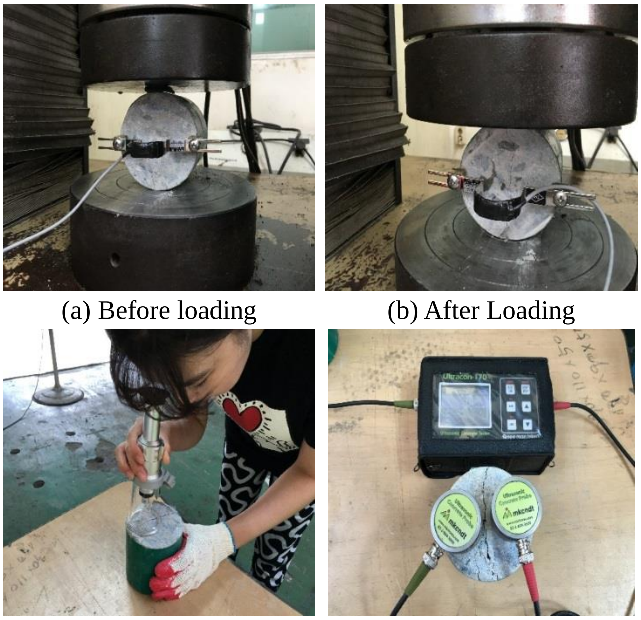
4.1.1 Concrete samples with single crack

For concrete with single crack, cylindrical concrete samples are prepared. After 56 days curing in submerged condition, they are cut into disk samples with 100 mm of diameter and 100 mm of thickness. For crack inducing, LVDT is installed on the concrete surface perpendicular to loading direction. The crack width increases during loading process and after unloading, crack width slightly decreases. The finally measured crack widths are considered for the chloride diffusion test. It is very difficult to obtain the designed crack width so that various crack widths are grouped with 0.1 mm interval. The concrete mix proportions are listed in Table 1. The concrete mix proportions are for nuclear power plant with fly ash.

The test result for compressive strength at 56 days is evaluated to be 39.7 MPa.

4.1.2 Test for chloride diffusion coefficient in steady state condition

In order to evaluate the equivalent diffusion in concrete with crack, accelerated migration test in steady-state condition are adopted, so called Andrade method, based on the previous research (Andrade 1993). The effective diffusion coefficient (D_{eff}) in cracked concrete can be obtained as Eq. (13) and it is compared with equivalent diffusion coefficient in cracked REV in Eq. (12). For the test, NaCl solution of 0.5 M and NaOH solution of 0.1 M



(a) Before loading (b) After Loading

(c) Crack width measurement (d) Crack depth measurement

Fig. 3 Photo for crack including and crack measurement

(a) Sample preparation after cutting (b) Test set-up

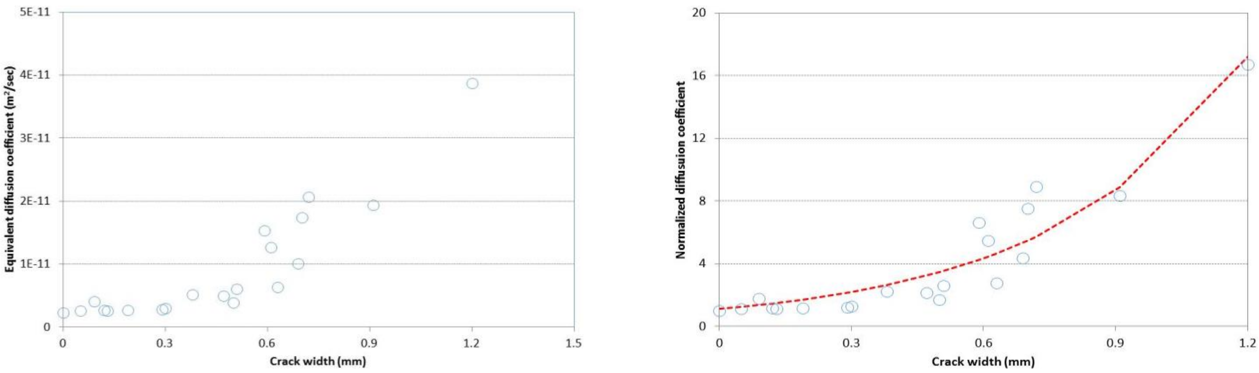
Fig. 4 Photos for test setup of diffusion cell in steady state condition

$$D_{eff} = \frac{RTit_{cl}l}{nF^2 \Delta EAC_{cl}Z} \quad (13)$$

are used for the catholyte and anolyte in a migration cell, respectively (Andrade 1993).

Where n is 1.0, ΔE is applied potential (30 V), i is current (A), t_{cl} transference number, A is cross section of concrete sample (m^2), Z is ion valence C_{cl} is the concentration of chloride ion in diffusion cell (mol/l). The current varies at initial period and keeps almost constant after 1-2 days. The results of diffusion coefficient are compared with the proposed model for anisotropic condition. The photos for crack including and measurement are shown in Fig. 3, and the diffusion test set-up is shown in Fig. 4, respectively.

The results are listed in Table 2 where equivalent diffusion coefficient increases by about 2.0-2.5 times when crack width reaches around 0.4 mm. The normalized results to sound concrete are shown in Fig. 5. The regression analysis result is obtained as Eq. (14) regarding crack width (w)



(a) Equivalent diffusion coefficient (b) Normalized diffusion coefficient

Fig. 5 Diffusion coefficients with increasing crack width (steady-state condition)

Table 2 Equivalent diffusion coefficient in cracked REV

Crack width (mm)	Chloride diffusion coefficient (m^2/sec)	Crack width (mm)	Chloride diffusion coefficient (m^2/sec)
0.00	2.316E-12	0.50	3.912E-12
0.05	2.621E-12	0.51	6.023E-12
0.09	4.126E-12	0.59	1.540E-11
0.12	2.731E-12	0.61	1.272E-11
0.13	2.610E-12	0.63	6.381E-12
0.19	2.670E-12	0.69	1.018E-11
0.29	2.809E-12	0.70	1.748E-11
0.30	3.011E-12	0.72	2.071E-11
0.38	5.161E-12	0.91	1.942E-11
0.47	4.983E-12	1.20	3.870E-11

$$D_{eff}(w) = 1.105 D_0 e^{2.287w}, \quad R^2 = 0.883 \tag{14}$$

Where $D_{eff}(w)$ is equivalent chloride diffusion coefficient in concrete with crack.

4.2 Simulation with varying parameters

4.2.1 Roughness and crack density effect

In the section, normalized chloride diffusion coefficient is simulated with varying *p* and *f*. D_0 is the reference diffusion coefficient in sound concrete and it usually within the range of 1.0E-11-10E-12 m^2/sec. For the simulation, the reference diffusion coefficient (D_0) is set as 2.32E-12 m^2/s based on the test results and the equivalent diffusion coefficients are simulated with varying *p* and *f*.

The simulated results are shown in Fig. 6. With increasing *f*, the equivalent diffusion ratio significantly decreases to 1.0 since the effect of diffusion in the reference is dominant.

When *f* has a range from 25 to 800 without the effect of *f*, the equivalent diffusion ratio decreases from 21 to 1.625. The enlarged *p* means more hindrance of chloride diffusion with reducing of chloride intrusion area. When *p* goes to 0.4 and *f* increases to 800, the equivalent diffusion coefficient decreases to 7.74%-22.5%.

4.2.2 Reference diffusion coefficient effect

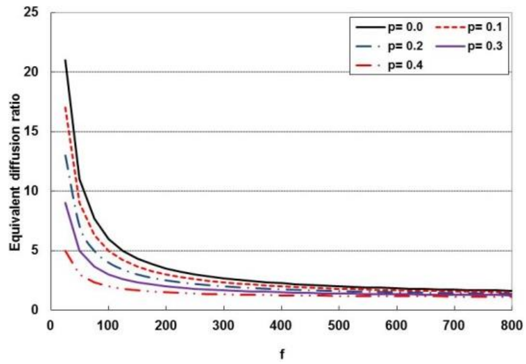


Fig. 6 Simulation results with varying roughness

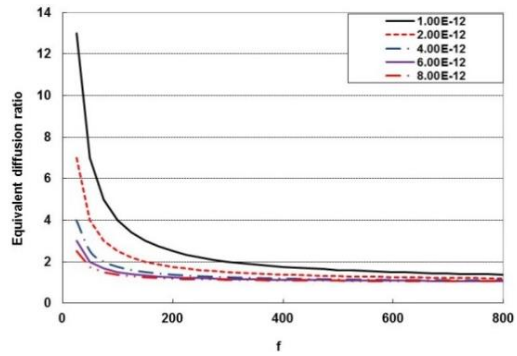
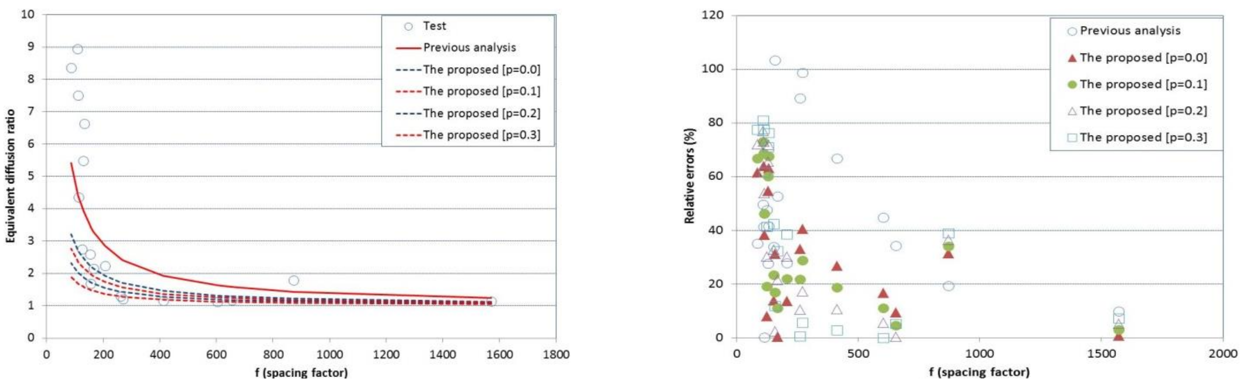


Fig. 9 Simulation results with varying reference diffusion coefficient

The increase in reference diffusion coefficient can cause variation of equivalent diffusion coefficient. The lower diffusion coefficient means the diffusion coefficient in concrete with low *w*/*c* ratio and high strength. In the given condition of *p*=0.2, equivalent diffusion coefficient is simulated with varying D_0 from 1.0E-12 to 8.0E-12. The results are shown in Fig. 7.

With decreasing diffusion coefficient in high strength concrete, the changes in equivalent diffusion ratio significantly increases. It shows that crack effect on diffusion affects high strength concrete more severely. The crack effect on deterioration is relatively remarkable in concrete with high strength since the ingress of harmful ion is very limitedly penetrated without crack. The trends can be found in previous researches on chloride attack (Park *et al*. 2012a) and carbonation (Song *et al*. 2005, 2006).



(a) Equivalent diffusion coefficient with *f*

(b) Relative errors with *f*

Fig. 11 Equivalent diffusion coefficient and relative errors in anisotropic condition

When *f* increases to 800 in the anisotropic condition, the equivalent diffusion significantly decreases to 10.57% for 1.00E-12 m^2/sec of reference diffusion coefficient (high strength concrete) but it decreases to 41.88% for 8.00E-12 m^2/sec of reference diffusion coefficient (low strength concrete).

4.3 Verification of the proposed model

The concrete area in the chloride diffusion test is different from REV model in Fig. 2 since concrete area under diffusion test has circular section containing 100 mm of diameter. The height of concrete REV (L_1) is considered as $100\pi/4$ (mm) for the same equivalent exposure area for diffusion. It is important to assume the diffusion coefficient in cracked area which is free water condition in the electrical field. The verification results for anisotropic condition are shown in Fig. 10 which shows that the proposed diffusion models with wedge shape containing 0.1-0.2 of roughness factor (p) are well matched with the test results.

The averaged relative errors within 0.05-0.91 mm of crack width 45.8% (previous parallel shape model), 32.1% (wedge model). 33.2% (wedge model with 0.1 of p), 34.3% wedge model with 0.2 of p), and 44.2% (wedge model with 0.3 of p), respectively.

This verifies that wedge shape of crack with suitable roughness can reasonably evaluate the reduced diffusion of chloride in concrete with crack.

5. Conclusions

In the present work, chloride diffusion in cracked REV is modeled considering anisotropic condition which is concrete with single crack. In the previous model, parallel-piped section of crack profile is assumed but it is improved through considering wedged-crack shape and roughness. In the verification test in steady-state condition, the equivalent diffusion coefficient slowly increases with crack width. When crack width reaches over 0.4 mm, the increasing ratio of diffusion coefficient is 2.0-2.5 to sound concrete. Over 0.6 mm of crack width, it rapidly increases more than 10 times compared with concrete without crack. The proposed model is verified to have reasonable applicability when crack has wedge shape and 0.1-0.2 of roughness.

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