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Analytical solution for chloride ions bilateral diffusion

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Abstract. An analytical solution for chloride ions bilateral diffusion within concrete was developed based on Fourier transform method, by taking into account the bilateral diffusion and time-dependent chloride diffusion coefficient. The accuracy and applicability of the proposed analytical solution were validated by the field data after 10 years. Analysis results show that the ERFC is not suitable for solving chloride ions bilateral diffusion within concrete slabs exposed to the natural submerged environment. The proposed solution is in good accuracy to simulate the chloride concentration distribution within concrete in field site.

1. Introduction

In marine environment, long term chloride penetration in concrete resulted in the corrosion of reinforcement[1]. It has been widely recognized that the chloride diffusion coefficient and surface chloride concentration are two important parameters for simulating the initial corrosion time. Therefore, abundant researchers have been done on analytical solution for chloride diffusion in concrete. Tang and Gulikers[2]developed an analytical solution for the time-dependent chloride diffusion coefficient by taking into account the age of concrete initially exposed to chloride environment. Yang and Li[3] developed an analytical solution for two-dimensional diffusion. Yang et al.[4] developed an analytical solution for dual time-dependent chloride diffusion, by taking into account of the time-dependent surface chloride concentration and time-dependent chloride diffusion coefficient. Yu et al.[5] developed an analytical solution, by chloride binding capacity and time-dependent chloride diffusion coefficient. However, these solutions above are not suitable for solving chloride ions bilateral diffusion. Therefore, it is desirable to develop an efficient analytical solution for chloride ions bilateral diffusion.

2. Analytical solution for chloride ions bilateral diffusion

According to reference [6], the time varying chloride diffusion coefficient can be described as

$$D(t) = D_0 \left(\frac{t_0}{t + t_0} \right)^n$$

(1)

where t_0 is the age of concrete initially exposed to chloride environment, t is the exposure time, D_0 is chloride diffusion coefficient at t_0.

$$\begin{cases} \dfrac{\partial C}{\partial t} = D(t)\dfrac{\partial^2 C}{\partial x^2} \\ C(0 \leq x < l, t = 0) = C_0 \\ C(x = 0, t) = C_L, C(x = l, t) = C_R \end{cases}$$

(2)

where C is the chloride concentration at diffusion depth x and exposure time t (% by weight of binder), C_0 is the initial chloride concentration, l is the thickness of concrete slab, C_L is the chloride concentration at left boundary of concrete slab, C_R is the chloride concentration at right boundary of concrete slab.

Let the first derivative of the T versus t is equal to equivalent diffusion coefficient D, then D can be defined as follows

$$D(t) = D_0 \frac{dT(t)}{dt}$$

(3)

By integrating the function D with respect to t from t_0 to t_0+t, one gets

$$T = \int_{t_0}^{t_0+t} \frac{D(t)}{D_0} dt = \frac{t_0^n}{1-n}\left[(t+t_0) - t_0^{1-n}\right]$$

(4)

By substituting Eq. (3) into Eq. (2), the differential equation can be rewritten as

$$\frac{\partial C}{\partial t} = \frac{\partial C}{\partial T}\frac{dT}{dt} = \frac{D(t)}{D_0}\frac{\partial C}{\partial T} = D(t)\frac{\partial^2 C}{\partial x^2}$$

(5)

Then, the governing equation for chloride diffusion, the boundary conditions and initial conditions can be transformed into

$$\begin{cases} \dfrac{\partial C}{\partial T} = D_0\dfrac{\partial^2 C}{\partial x^2} \\ C(0 \leq x < l, T = 0) = C_0 \\ C(x = 0, T) = C_L, C(x = l, T) = C_R \end{cases}$$

(6)

The analytical solution consist of general solution C_1 and particular solution C_2

$$C(x,T) = C_1(x,T) + C_2(x)$$

(7)

C_2 can be defined as

$$C_2(x) = C_L + \frac{x}{l}(C_R - C_L)$$

(8)

Eq. (8) is the particular solution of Eq. (6). The homogeneous partial differential equation can be expressed as

$$\begin{cases} \dfrac{\partial C_1}{\partial T} = D_0 \dfrac{\partial^2 C_1}{\partial x^2} \\ C_1\left(0 \le x < l, T = 0\right) = C_0 - C_2\left(x\right) \\ C_1\left(x = 0, T\right) = 0, C_2\left(x = l, T\right) = 0 \end{cases} \tag{9}$$

Based on the separation-of-variables method[7], C_1 can be expressed as

$$C_1\left(x, T\right) = X\left(x\right) \cdot F\left(T\right) \tag{10}$$

By substituting Eq. (10) into Eq. (9), one gets

$$\frac{F'\left(T\right)}{D_0 F\left(T\right)} = \frac{X''\left(x\right)}{X\left(x\right)} = -\alpha \tag{11}$$

The equivalent expression of Eq. (11) is as follow

$$\begin{cases} F'\left(T\right) + \alpha D_0 F\left(T\right) = 0 \\ X''\left(x\right) + \alpha X\left(x\right) = 0 \end{cases} \tag{12}$$

The nonzero solution of $X''\left(x\right) + \alpha X\left(x\right) = 0$ can be found, when the value of α is positive. And the corresponding solution is

$$X\left(x\right) = a\cos\left(\sqrt{\alpha}x\right) + b\sin\left(\sqrt{\alpha}x\right) \tag{13}$$

According to the boundary conditions, one gets

$$X\left(0\right) = 0, X\left(l\right) = 0 \tag{14}$$

By substituting Eq. (14) into Eq. (13), one gets

$$a = 0, b\sin\left(\sqrt{\alpha}l\right) = 0 \tag{15}$$

The nonzero solution of Eq. (13) can be found, when $\sqrt{\alpha}l$ is equal to $n\pi$. Then, α can be expressed as

$$\alpha = \left(\frac{n\pi}{l}\right)^2, n = 1, 2, \cdots \tag{16}$$

The solution of Eq. (12) is as follow

$$X_n\left(x\right) = b_n \sin\left(\frac{n\pi}{l}x\right) \quad n = 1, 2, \cdots \tag{17}$$

$$F_n\left(T\right) = a_n \exp\left(-\left(\frac{n\pi}{l}\right)^2 D_0 T\right) \tag{18}$$

According to Eq. (17) and Eq. (18), one gets

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$$C_{1n}(x,T) = a_n b_n \sin\left(\frac{n\pi}{l}x\right) \cdot \exp\left(-\left(\frac{n\pi}{l}\right)^2 D_0 T\right) \tag{19}$$

Based on the method of superposition, Eq. (19) can be transformed into

$$C_1(x,T) = \sum_{n=1}^{\infty} C_{1n}(x,T) = \sum_{n=1}^{\infty} a_n b_n \sin\left(\frac{n\pi}{l}x\right) \cdot \exp\left(-\left(\frac{n\pi}{l}\right)^2 D_0 T\right) \tag{20}$$

Let A_n is equal to $a_n b_n$. By substituting Eq. (20) into Eq. (9), we get

$$C_0 - C_2(x) = \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi}{l}x\right) \tag{21}$$

According to the orthogonal properties of trigonometric functions, we multiply both sides of Eq. (20) by $\sin\left(\frac{m\pi}{l}x\right)$, and then get

$$A_n = \frac{2}{l} \int_0^l \left(C_0 - C_2(x)\right) \sin\left(\frac{n\pi}{l}x\right) dx \tag{22}$$

By substituting Eq. (8) into Eq. (22), and solving the combined Eq. (7) and Eq. (20), we get

$$C(x,t) = C_L - \frac{(C_L - C_R)x}{l} + \sum_{n=1}^{\infty} \left\{ \frac{2}{n^2\pi^2} \exp\left[-\left(\frac{n\pi}{l}\right)^2 D_0 T\right] \right.$$
$$\left. \sin\left(\frac{n\pi x}{l}\right) \left[(C_L - C_R)\sin(n\pi) + (C_R - C_0)n\pi\cos(n\pi) - (C_L - C_0)n\pi \right] \right\} \tag{23}$$

By substituting Eq. (8) into Eq. (13), one gets

$$C(x,t) = C_L - \frac{(C_L - C_R)x}{l} + \sum_{n=1}^{\infty} \left\{ \frac{2}{n^2\pi^2} \exp\left[-\left(\frac{n\pi}{l}\right)^2 \frac{D_0 t_0^n}{1-n}\left[(t+t_0) - t_0^{1-n}\right]\right] \right.$$
$$\left. \sin\left(\frac{n\pi x}{l}\right) \left[(C_L - C_R)\sin(n\pi) + (C_R - C_0)n\pi\cos(n\pi) - (C_L - C_0)n\pi \right] \right\} \tag{24}$$

3. Validation and analysis

Field data of chloride concentration distribution within concrete specimens exposed to the natural submerged environment presented by Tang [8] were collected to validate the accuracy and applicability. The water-to-cement ratio of concrete is 0.40. The compressive strength of concrete is 58 MPa at the age of 28 days. The size of concrete slabs is 100×100×100 mm. After 14 days moist curing, the concrete slabs were transported to field site. The annual average temperature of seawater is 11℃. The chloride concentration of seawater varies from 10 to 18 g Cl per litre. The specimens with the size of 100×100×100 mm were cut away from each slab in submerged zone, when the exposure time is 10 years. And then the cores were drilled in each specimen. The powder samples of each core were collected by means of dry grinding with a diamond tool, successively from the exposed surface to a certain depth. The acid chloride content of each sample was determined in accordance with AASHTO T260. Finally, the chloride concentration distribution within concrete can be obtained, as is shown in Fig. 1. It is noted that the left is correspond to bottom side of concrete in casting, and the right is corresponding to topside of concrete in casting. Due to the segregation, the volume of

aggregate in bottom side is greater than the topside, and the surface chloride concentration of topside is greater than the bottom side.

Table 1. The fitting parameters for ERFC.

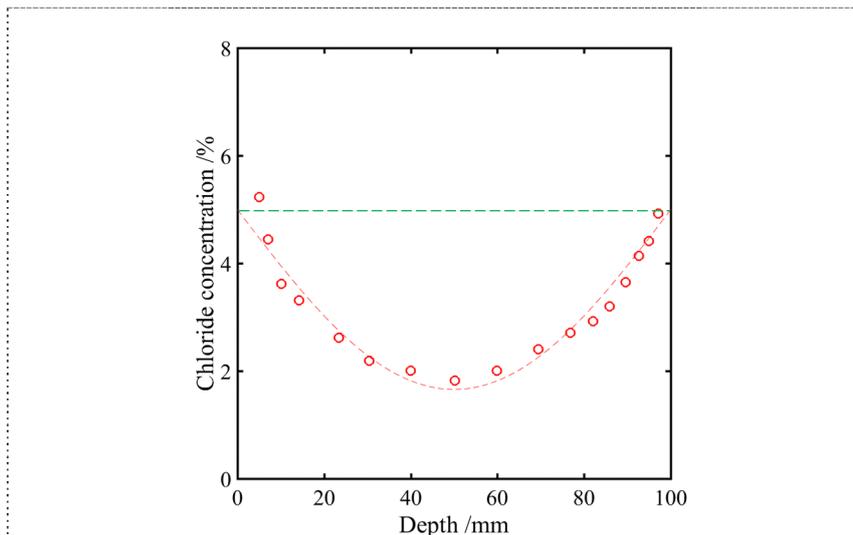|	C_L(%)	C_R(%)	D_a(×10⁻¹²m²/s)	R^2
ERFC	5.0	5.0	2.06	0.93

Figure 1. Comparison between experimental data and predicted results of the ERFC when exposure time is 10a.

Table 2. The fitting parameters for the proposed solution.

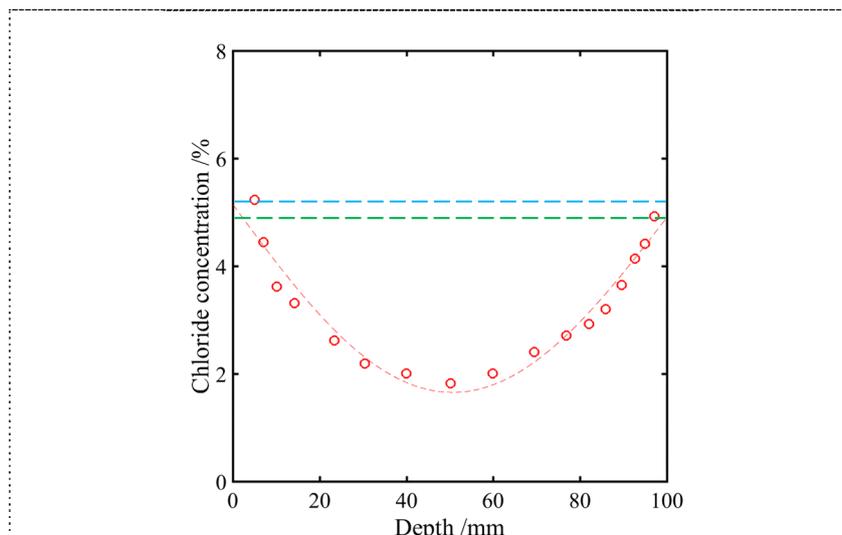|	C_L(%)	C_R(%)	D_0(×10⁻¹²m²/s)	n	R^2
Proposed solution	5.1	4.9	2.06	0.26	0.94

Figure 2. Comparison between experimental data and predicted results of the proposed solution when exposure time is 10a.

Generally, the apparent surface chloride concentration was obtained by nonlinear curve fitting analysis in terms of the error function solution, which is denoted by ERFC hereinafter. The

corresponding results of nonlinear curve fitting analysis are listed in Tab.1. As shown in Fig.1, the fitted curve of chloride concentration distribution is visibly different from tested curve on the left. It is due to the fact that the ERFC is not suitable for solving chloride ions bilateral diffusion. In contrast, the chloride concentration at left boundary C_L and the chloride concentration at right boundary C_R were obtained by nonlinear curve fitting analysis in terms of Eq. (24). The corresponding results of nonlinear curve fitting analysis are listed in Tab.2. As shown in Fig.2, the fitted curve of chloride concentration distribution agree well with tested curve on the left, which indicates that the accuracy of the proposed analytical solution for chloride ions bilateral diffusion.

4. Conclusions

An analytical solution for chloride ions bilateral diffusion within concrete was developed based on Fourier transform method, by taking into account the bilateral diffusion and time-dependent chloride diffusion coefficient. Following conclusions can be drawn:

  1. The proposed analytical solution for chloride ions bilateral diffusion is applicable for predicting the chloride concentration distribution within concrete slabs exposed to the natural submerged environment.

  2. The ERFC is not suitable for solving chloride ions bilateral diffusion.

Acknowledgments

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