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Time dependent models of apparent diffusion coefficient and surface chloride for chloride transport in fly ash concrete

Aruz Petcherdchoo *

Department of Civil Engineering, Faculty of Engineering, King Mongkut's University of Technology North Bangkok, 1518 Pibulsongkram Road, Bangsue, Bangkok 10800, Thailand

HIGHLIGHTS

- ▸ The inconsistency in diffusion coefficient and surface chloride models is shown.
- ▸ A consistent chloride transport model for fly ash concrete is developed.
- ▸ The sensitivity analysis of the developed model coefficients is performed.
- ▸ Remarks on the diffusion coefficient and surface chloride are shown.

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ABSTRACT

This paper presents a Fick-based chloride transport model, which is mathematically consistent with time dependent apparent diffusion coefficient and surface chloride for fly ash concrete. In the paper, the inconsistency in a simple close-formed solution used to predict chloride penetration through fly ash concrete in a previous study of other researchers is pointed out. The inconsistency can be seen by comparing chloride profiles calculated by the simple close-formed solution to those calculated by a finite difference program. The inconsistency is caused by the use of simplified diffusion coefficient and mathematically incompatible surface chloride models. To avoid the inconsistency, a chloride transport model is developed in this study. In developing the model, regression analysis to fit coefficients of the developed model is compared to the regression analysis results obtained from the experiment of the researchers. In the experiment of the researchers, the effect of water to binder ratio and the amount of fly ash replacement in concrete is considered. Furthermore, the chloride transport calculated from the developed model is validated by comparing to other experimental results. Finally, the sensitivity analysis of the model coefficients and some remarks on the developed model are presented.

1. Introduction

For many years, concrete structures have been known as one of the main materials in construction industry. After a period of exposure time, the concrete structures, especially marine structures, inevitably deteriorate. The deterioration of concrete structures can be considered in different terms, for example, concrete deterioration, reinforcement corrosion, or a combination of them. Chloride attack is considered as one of the important factors in these deterioration mechanisms. Whenever the threshold amount of chloride ions at the surface of reinforcement is reached, reinforcement corrosion and concrete cracking may occur resulting in decreasing the bond strength between concrete and reinforcement, and subsequently reducing the flexural or shear strength of the structure. As a result, the corrosion of reinforcement adversely affects the safety and serviceability of concrete structures, and hence shortens their service life [1]. To avoid these, there are two main approaches; producing durable concrete [2–4], or applying appropriate maintenance plans [5,6], e.g., preventive maintenance, essential maintenance, or a combination of them. For the first approach, several researchers studied and recommended durable and sustainable materials, such as fly ash [7–9]. It is evident that the use of fly ash increased the chloride binding capacity in concrete. This binding capacity caused reduction of free chloride ions which were found to be related to corrosion of reinforced steel in concrete located in marine environment [9]. For the second approach, the maintenance plans will of course affect the allocation of the reasonable amount of funds in the administration level. According to these two approaches, the development of a model to predict the corrosion initiation time of concrete structures with durable and sustainable materials, e.g., fly ash, and the application time of maintenance is of importance. In many occasions, the corrosion initiation time and the maintenance application time are defined as service life.

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* Tel.: +66 82 555 2000x8637.
E-mail address: aruzp@kmutnb.ac.th

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Table 1
Value of β and C_S for $W/B = 0.65$[22].

Mix no.	β				C_S			
	2-yr exp.	3-yr exp.	4-yr exp.	5-yr exp.	2-yr exp.	3-yr exp.	4-yr exp.	5-yr exp.
I65	0.71	0.71	0.71	0.75	4.0	5.2	5.6	6.2
I65FA15	0.79	0.78	0.78	0.77	5.3	6.5	6.9	7.3
I65FA25	0.81	0.805	0.80	0.78	5.5	6.0	6.3	7.0
I65FA35	0.83	0.83	0.82	0.81	4.8	5.4	5.7	6.3
I65FA50	0.84	0.84	0.83	0.82	4.8	5.4	5.5	6.2

In studying the service life of chloride exposed concrete structures, a quantitative assessment is preferable [10]. The diffusion theory based on the Fick's second law can be used for predicting the chloride penetration through concrete structures. In the study of researchers [11–14], if the surface chloride and the diffusion coefficient were assumed constant, one-dimensional partial differential equation (1-D PDE) of the Fick's second law could be analytically solved, and a simple close-formed solution can be obtained. However, from many studies [15–19], it was found that both surface chloride and diffusion coefficient were not constant but time dependent. If this is the case, the simple close-formed solution is inapplicable.

In the study of Tang and Gulikers [20], the apparent time dependent diffusion coefficient for concrete was proposed so that it could directly be input into the simple close-formed solution. In 2009, Ann et al. [21] compared chloride ingress in concrete by using different forms of time dependent surface chlorides. However, they assumed constant diffusion coefficients in addition to a set of assumed data for study. Subsequently, Chalee et al. [22] proposed a chloride transport model including the time dependent diffusion coefficient and surface chloride, and validated their models with their experimental results. However, their model contained simplified diffusion coefficient and mathematically incompatible surface chloride leading to the inconsistency in predicting chloride transport as indicated in the next section. As a result, in order to bridge the gap, a chloride transport model, which is mathematically consistent with the time dependent surface chloride and diffusion coefficient, is required.

2. Statement of problems and observations

2.1. Fundamental of chloride transport models

The fundamental one-dimensional partial differential equation (1-D PDE) for chloride diffusion through concrete structures [23,24] can be written as

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} D \frac{\partial C}{\partial x} \tag{1}$$

where C is the chloride content as a function of position x and time t, and D is the chloride diffusion coefficient of concrete. If the initial condition (initial chloride content), boundary condition (surface chloride) and material property (chloride diffusion coefficient) are assumed to be zero, constant C_S, and constant D, respectively, the simple closed-form solution for Eq. (1) can be shown as

$$C(x,t) = C_S\left[1 - erf\left(\frac{x}{2\sqrt{Dt}}\right)\right] \tag{2}$$

where $erf(\cdot)$ is an error function.

2.2. Time dependency of diffusion coefficient and surface chloride

In 2009, Chalee et al. [22] proposed a chloride transport model for fly ash concrete in seawater, and validated the model with their experimental data. For model formulation, they employed the time dependent diffusion coefficient $D(t)$, which is based on the simplified model of Magnat and Limbachiya [25], as follows

$$D(t) = \left(\frac{1}{t}\right)^{\beta} \tag{3}$$

where β is an empirical coefficient, and t is concrete exposure time (s). Hence, the PDE for the Fick's second law was written as

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} D(t) \frac{\partial C}{\partial x} \tag{4a}$$

$$\frac{\partial C}{\partial t} = \left(\frac{1}{t}\right)^{\beta} \frac{\partial^2 C}{\partial x^2} \tag{4b}$$

in which its close-formed solution was expressed as

$$C(x,t) = C_S\left[1 - erf\left(\frac{x}{2\sqrt{\frac{t^{(1-\beta)}}{1-\beta}}}\right)\right] \tag{5}$$

where $C(x, t)$ is the total chloride content (% by weight of binder) at the position x (mm) and the exposure time t (s), C_S is the chloride content at the concrete surface (% by weight of binder).

By the regression analysis with their experimental data, they computed the values of β and C_S for each test, e.g., for $W/B = 0.65$ as shown in Table 1.

By data analysis, they further proposed the equation for the coefficient β and the time dependent surface chloride C_S as follows

$$\beta = [-0.0015\,(W/B) + 0.0034]\,[F] + [-0.175\,(W/B) + 0.840] \tag{6}$$

where W/B and F are the water to binder ratio and the amount of fly ash replacement (%), respectively, and

$$C_S(t) = [-0.379(W/B) + 2.064]\ln(t) + [4.078(W/B) + 1.011] \tag{7}$$

where $C_S(t)$ is the time dependent surface chloride.

For comparing the chloride profiles based on the model using Eqs. (5)–(7) to those based on a Crank–Nicolson based finite difference method (FDM), we can approximate Eq. (4a) as

$$\frac{c_{i,j+1} - c_{i,j}}{\Delta t} = \frac{1}{2}\left(\frac{D_{,j+1}(c_{i+1,j+1} - 2c_{i,j+1} - c_{i-1,j+1})}{(\Delta x)^2} + \frac{D_{,j}(c_{i+1,j} - 2c_{i,j} - c_{i-1,j})}{(\Delta x)^2}\right) \tag{8}$$

where $c_{x,t}$, in a general form, is the chloride content at a mesh point x and time t, and $D_{,t}$ is the diffusion coefficient at time t. In addition, Δx and Δt are the size of the mesh point and the incremental time step, respectively. In computation, they are chosen as 1 mm and 1 week, respectively. It is noted that for the finite difference program, the time dependent diffusion coefficient in Eq. (3) can directly be input. However, for the close-formed solution in Eq. (5), the time dependent diffusion coefficient in Eq. (3) must be integrated over time to have a constant or apparent diffusion coefficient before replacing into Eq. (2) to get Eq. (5). In addition, the time dependent surface chloride in Eq. (7) can directly be input into the finite difference program and the close-formed solution of Eq. (5).