

Numerical Simulation of Chloride Diffusion in RC Structures and the Implications of Chloride Binding Capacities and Concrete Mix

Ali H. Al-Gadhib

Abstract—The durability of reinforced concrete structures is influenced by the chloride penetration and susceptibility of the reinforcement to chloride-induced corrosion, when exposed to marine environment or deicing salts. The ingress of chloride in concrete depends on various factors including the degree of humidity, environmental conditions, and more importantly, the composition and the characteristics of the concrete itself. The latter factor is controlled by the chloride diffusivity of concrete. Of the diffusivity influence factors, the effects of concrete quality parameters such as water-binder ratio and binder content have been found to be crucial from a number of studies. Yet, there is lack of cohesive coverage of the problem with regard to concurrent impact or confluence of the influence factors operating under field conditions. This paper is therefore concerned with finite element formulation and modeling of the chloride transport in concrete considering the importance of the multivariate diffusivity function (MDF) in delaying or expediting the time for the initiation of corrosion. The formulation of the numerical model is implemented taking into account the chemophysical phenomena associated with various bounded-chloride functions and its influence on chloride diffusivity. Results from the analysis including the effect of bounded-chloride formulation on the diffusion behavior of chloride have been assessed and highlighted. Similar analysis has been performed using ANSYS based on thermal analogy technique. Feasibility of the results of this investigation to match with those of the experimental findings has been ascertained.

Index Terms—ANSYS, chloride diffusivity, chloride ingress, concrete durability, corrosion, FE modeling.

I. INTRODUCTION

THE durability of reinforced concrete structures is impacted by the chloride penetration and susceptibility of the reinforcement to chloride-induced corrosion, when exposed to marine environment or deicing salts. Once the chloride content at the reinforcement reaches a threshold value and enough oxygen and moisture are present, the reinforcement corrosion will be initiated.

Quality concrete is able to prevent the embedded

reinforcing steel from potential corrosion in many ways, including hydration products of cement which form high alkalinity where the passivated film covering the steel surface remains chemically stable enough to protect the reinforcing steel from corroding [1]. However, chloride penetration may result in the accumulation of chloride content at the reinforcement to such a level that the high alkaline environment is destroyed and then the passivated film on the steel surface is disrupted [2], [3].

The corrosion of steel in concrete induced by chloride ion contamination is a major problem [4]. The importance of chloride ions in reinforcement corrosion has led to the concept of a chloride threshold level, namely the chloride content at the depth of steel necessary to initiate corrosion-induced deterioration [5]. It is widely perceived that the chloride threshold for corrosion-induced deterioration in steel reinforced concrete is best expressed as the chloride to hydroxyl concentration ratio present in the electrolyte in the concrete pores [6], [7]. This implies that bound chloride presents a negligible corrosion risk and dissolved hydroxyl ions are the principal inhibitors in concrete [8], [9].

Most cases of deterioration in reinforced concrete structures under service conditions are related to corrosion of the reinforcement occurring as a consequence of chloride transport in concrete. Thus, by recognizing the widely accepted conceptual model for corrosion of steel in concrete attributed to concrete durability to resist chloride exposure loads in the field is observed to be significantly limited to the corrosion initiation time. In this regard, the notional measure of chloride-induced corrosion initiation time is very much dependent on the chloride diffusivity property of the concrete. The diffusivity itself exhibits characteristic behavior which in turn is controlled by a number of other factors external and internal to the concrete medium. Of the diffusivity influence factors internal to the concrete, the effects of concrete quality parameters such as water-binder ratio (w/b) and binder content (b) have been found to be crucial from a number of studies. Scheme of literature studies surveyed, however, is observed to have focused on the analysis of chloride diffusivity associated with disparate or individual effects of these factors. There is

therefore lack of cohesive coverage of the problem with regard to concurrent impact or confluence of the influence factors operating under field conditions.

This paper is therefore concerned with finite element formulation and modeling of the chloride transport in concrete considering the importance of the multivariate diffusivity function (MDF). Based on phenomenological behavior allied to experimental findings, discrete diffusivity influence functions (DIFs) are specifically described to account for the sheer effect of water-binder ratio (w/b), binder content (b), and curing regime (t_c) in concrete. A major feature of the finite element formulation is the consideration of the nonlinear control that both the chloride species and the influence functions exercise over the solution procedure to the problem. Results from the two-dimensional simulation of a concrete element subjected to the influence of the diffusivity influence functions confluence arising from the amalgamation of the three concrete quality parameters studied, are included as representative numerical examples. The results show that recourse to confluence rather than individual itinerary of the diffusivity factors is of greater practical significance to the proper understanding of durability performance and quantification of service life of concrete structures in the field.

The importance of chloride ions to concrete durability is reflected in the tremendous amount of literature devoted to its study in terms of its role in inducing corrosion of reinforcing steel in concrete. It is widely accepted that at the early age of the reinforced concrete, the high alkalinity results in the transformation of a surface layer of the embedded steel to a tightly adhering film comprising an inner dense spinel phase of gamma iron-III oxide in epitaxial orientation to the steel and an outer layer of alpha iron-I hydroxide [10]. As long as this film remains passive and is not disturbed, it will keep the steel passive and protected from active corrosion.

Normally, the free chloride refers to the water-soluble chloride in concrete and the bound chloride means the total chloride minus the free one. The total chloride refers to the acid-soluble chloride in concrete.

The chloride binding capacity of concrete may influence the durability of concrete in chloride containing environment [11]–[14]. It is known that mineral admixtures, such as fly ash, slag, silica fume, etc., may increase the chloride binding capacity or decrease the chloride diffusivity in concrete. It is supposed that only the free chloride is capable of initiating the corrosion of reinforcement. The bound chloride should be harmless. This point of view is still controversial, not only on the definition of “free” and “bound,” but also on the release of the bound chloride.

A concrete structure is often exposed to chloride sources comprising deicing salts, salt splashes, salt spray, seawater, or chloride contaminated concrete making constituents. The amount of salt introduced by mixing and curing waters may be generally small, but in arid areas where amount of desalinated water is scarce, concrete is often mixed and cured with brackish water. Chloride ions from these sources will slowly penetrate into the concrete through the pores of the hydrated

cement paste in the concrete and will eventually reach the steel. When the penetrated chloride at the face of the steel accumulates beyond a certain threshold concentration level, the protective film is destroyed leaving the steel to corrode in as much as oxygen and moisture are present at the steel-concrete interface. In this regard, chloride ions have been identified as the unique and specific destroyer of passivity of the reinforcing steel [11], [15], [16].

The main objective of this paper is to establish a numerical model based on a nonlinear finite element method to predict the diffusion of chloride into concrete structures. The formulation of the numerical model is implemented considering the chemo-physical phenomena associated with various bounded chloride functions and its influence on chloride diffusivity. Results from the analysis including the effect of bounded-chloride formulation on the diffusion behavior of chloride have been assessed and highlighted. Similar analysis has been performed using ANSYS based on thermal analogy technique. Feasibility of the results of this investigation to match with those of the experimental findings has been ascertained.

II. CHLORIDE TRANSFER AND FIELD EQUATIONS

The transport of chloride from the environment to concrete is governed generally by two phenomena: one is diffusion and the other is convection. While the former takes place when concrete is saturated, the latter happens when concrete is partially saturated. The mechanism of chloride diffusion (mass diffusion) within the cementitious medium is governed by a law analogous to Fourier’s law, which can be stated as:

“The rate of mass transport within a cementitious medium by means of diffusion is proportional to the moisture gradient in the direction of flow”:

$$\vec{j}(x_k, t) = -D\rho\vec{\nabla} Cl + \rho Cl\vec{V} \quad (1)$$

where \vec{j} is the maximum flux in unit of [kg/cm² (sec)], D is the diffusivity in unit of cm²/day, $\vec{\nabla}$ is del operator, Cl is mass fraction of chloride, ρ is density of chloride, and \vec{V} is the bulk motion of the fluid via which chloride is moving (in this case $\vec{V} = 0$, because of other fluid media).

The general continuity equation (conservation of mass) can be expressed for mass transfer as follows:

$$-\vec{\nabla} \cdot \rho D \vec{\nabla} Cl + \vec{\nabla} \cdot \rho Cl \vec{V} + \frac{\partial(\rho Cl)}{\partial t} - r_A = 0 \quad (2)$$

where the term r_A is denoting the rate of chemical reaction and has units of reaction mass per unit volume-unit time (kg/cm³·s).

Mass Flux:

$$\vec{j}(x_k, t) = -D(x_k) \vec{\nabla} Cl(x_k, t) \quad (3)$$

Continuity Equation:

$$-\vec{\nabla} \cdot (D \vec{\nabla} Cl) + \frac{\partial Cl(x_k, t)}{\partial t} = 0 \quad (4)$$

In order to determine whether a unique solution is proper, initial and boundary conditions must be specified which are compatible with the physical conditions of a particular problem. The initial condition is defined by prescribing the initial chloride content throughout the domain at time $t = 0$. As the differential equation is first order in time, one initial condition is required.

$$Cl(x_k, t) = Cl_0 \quad @ t = 0 \quad k = 1, 2 \quad \text{for 2-D} \quad (5)$$

The boundary conditions may be defined by specifying the existing surface chloride on a portion of the boundary of the body as

$$Cl(x_k, t) = Cl_1(x_k, t) \quad x_k \in \Gamma_c \quad (6)$$

The chloride content may be either constant or a function of time. This boundary condition is the easiest to work with. A prescribed chloride flow boundary condition can be expressed as

$$D(Cl) \frac{\partial Cl(x_k, t)}{\partial x_i} n_i = j_i(x_k, t) \quad x_k \in \Gamma_j \quad (7)$$

where n_i is the outward normal at the boundary and j_i is the specified amount of chloride flow @ x_k on j of the boundary where the normal derivative of the chloride is prescribed. Yet, for the case of free convection of chloride, the rate of chloride transfer across the boundary layer, (7) is written as

$$D(Cl) \frac{\partial Cl(x_k, t)}{\partial x_i} n_i = h_f (Cl_e - Cl_s) \quad x_i \in \Gamma_f \quad (8)$$

where h_f is the surface chloride transfer coefficient, Cl_e is the chloride concentration of the external environment, Cl_s is the chloride content on the surface of the solid, and $\frac{\partial Cl(x_k, t)}{\partial x_i} n_i$ is the chloride flux normal to the exposed surface.

The total flow of chlorides into partially-saturated concrete can be obtained by combining the flow of chlorides due to diffusion and the flow of chlorides due to convection. Establishing chloride mass conservation results in:

$$\frac{\partial C_{tc}}{\partial t} = - \underbrace{\frac{\partial J_{cy}}{\partial x} - \frac{\partial J_{cy}}{\partial y}}_{\text{diffusion}} - \underbrace{\frac{\partial J'_{cx}}{\partial x} - \frac{\partial J'_{cy}}{\partial y}}_{\text{convection}} \quad [\text{kg}/(\text{m}^3 \cdot \text{s})] \quad (9)$$

where J'_{cx} is flux of chloride ions due to convection in the x -direction ($\text{kg}/\text{m}^2 \cdot \text{s}$) and J'_{cy} is flux of chloride ions due to convection in the y -direction ($\text{kg}/\text{m}^2 \cdot \text{s}$).

By considering chloride binding in the diffusion process and substituting the mass flux equation into (9), the following modified Fick's 2nd law equation applicable to partially-saturated concrete results:

$$\begin{aligned} \frac{\partial C_{tc}}{\partial t} = & \underbrace{\frac{\partial}{\partial x} \left(D_c^* \frac{\partial C_{fc}}{\partial x} \right) + \frac{\partial}{\partial y} \left(D_c^* \frac{\partial C_{fc}}{\partial y} \right)}_{\text{diffusion}} \\ & - \underbrace{\frac{\partial}{\partial x} (w_c \cdot C_{fc} \cdot J_{mx}) - \frac{\partial}{\partial y} (w_e \cdot C_{fc} \cdot J_{my})}_{\text{convection}} \quad [\text{kg}/(\text{m}^3 \cdot \text{s})] \end{aligned} \quad (10)$$

where J_{mx} and J_{my} are the moisture fluxes along the x and y directions, respectively. Equation (10) is the governing equation of chloride ingress into partially-saturated concrete. Note that it is written in terms of the free chloride concentration C_{fc} (kg/m^3 of pore solution). Once the binding isotherm that characterizes the specific concrete cementitious system is known and the concentration of free chlorides is determined, the total amount of chlorides in concrete is calculated as

$$C_{tc} = C_{bc} + w_e C_{fc} \quad (11)$$

Which upon taking its derivative and substituting into (10), one has

$$\begin{aligned} \frac{\partial C_{fc}}{\partial t} = & \frac{\partial}{\partial x} \left(D_c^* \frac{\partial C_{fc}}{\partial x} \right) + \frac{\partial}{\partial y} \left(D_c^* \frac{\partial C_{fc}}{\partial y} \right) \\ & + \frac{\partial}{\partial x} \left(C_{fc} \frac{\partial h}{\partial x} D_h^* \right) + \frac{\partial}{\partial y} \left(C_{fc} \frac{\partial h}{\partial y} D_h^* \right) \end{aligned} \quad (12)$$

where

$$D_c^* = D_c / \left[1 + \frac{1}{w_e} \frac{\partial C_{bc}}{\partial C_{fc}} \right] \quad (13a)$$

$$D_h^* = D_h / \left[1 + \frac{1}{w_e} \frac{\partial C_{bc}}{\partial C_{fc}} \right] \quad (13b)$$

Equations (11) and (12) can be solved once the relationship between the bounded chloride and the free chloride is specified.

There are many forms of the chloride binding capacities, from which the bounded chloride and thus the total chloride

will be calculated. For example, consider the following various forms of chloride binding capacities:

No binding: $C_{bc} = 0$, which gives $D_c^* = D_c$ (14a)

Linear isotherm $C_{bc} = \alpha C_{fc}$, which gives $D_c^* = \frac{D_c}{1 + \frac{\alpha}{w_e}}$ (14b)

Langmuir isotherm $C_{bc} = \frac{\alpha C_{fc}}{1 + \beta C_{fc}}$, which gives

$$D_c^* = \frac{D_c}{1 + \frac{\alpha}{w_e(1 + \beta C_{fc})^2}} \quad (14c)$$

Freundlich isotherm $C_{bc} = \alpha C_{fc}^\beta$, which gives

$$D_c^* = \frac{D_c}{1 + \frac{1}{w_e} \alpha \beta C_{fc}^{\beta-1}} \quad (14d)$$

Although the system may look complicated, it can be degenerated for any special case. Such as the case of one-dimensional chloride transport with only constant D_c , (12) reduces to

$$\frac{\partial C_{fc}}{\partial x} = D_c \frac{\partial^2 C_{fc}}{\partial x^2}$$

and with the initial and boundary conditions:

$$C_{fc}(x, t) = C_{fc}(x, 0) = 0$$

$$C_{fc}(0, t) = C_s = \text{constant}$$

The solution gives the following:

$$C_{fc}(x, t) = C_s \left[1 - \text{erf} \left(\frac{x}{2\sqrt{D_c t}} \right) \right] \quad [\text{kg/m}^3] \quad (15)$$

where $C_{fc}(x, t)$ is the concentration of free chlorides at depth x after time t (kg/m^3 of pore solution), C_s is the chloride concentration at the surface $x = 0$ (kg/m^3 of solution), and erf is the error function. This is diffusion of chloride **without** reaction and **constant diffusivity** parameter and **fixed** chloride exposure for **saturated concrete**.

However, for partially saturated concrete, the role of moisture content and moisture diffusion has to be included and coupled with that of chloride transport. The moisture diffusion equation in 2-D can be expressed as:

$$\frac{\partial w_e}{\partial h} \frac{\partial h}{\partial t} = \frac{\partial}{\partial x} \left(D_h \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(D_h \frac{\partial h}{\partial y} \right) \quad (16)$$

where w_e is the evaporable water content at depths x and y (m^3 of water/ m^3 of concrete), D_h is the humidity diffusion coefficient (m^2/s), and h is the pore relative humidity at depths x and y .

III. FINITE ELEMENT FORMULATION

To solve chloride diffusion for partially saturated concrete, humidity and moisture transport need to be considered as they affect not only the transport of chloride but also the diffusivity problem. So, we have two systems of equations simultaneously: one that governs the transport of free chloride and the other one is the diffusion of moisture:

$$[1] \quad \frac{\partial C_{fc}}{\partial t} = \frac{\partial}{\partial x} \left(D_c^* \frac{\partial C_{fc}}{\partial x} \right) + \frac{\partial}{\partial y} \left(D_c^* \frac{\partial C_{fc}}{\partial y} \right) + \frac{\partial}{\partial x} \left(D_h^* C_{fc} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(D_h^* C_{fc} \frac{\partial h}{\partial y} \right) \quad (17)$$

$$[2] \quad \frac{\partial h}{\partial t} \left(\frac{\partial w_e}{\partial h} \right) = \frac{\partial}{\partial x} \left(D_h \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(D_h \frac{\partial h}{\partial y} \right) \quad (18)$$

Both of these systems can be expressed in general by

$$k \frac{\partial \phi}{\partial t} + \underbrace{\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y}}_{\text{diffusion}} + \underbrace{\frac{\partial J'_x}{\partial x} + \frac{\partial J'_y}{\partial y}}_{\text{convection}} = 0 \quad (19)$$

in which ϕ could be C_{fc} or h

$$- D \left(\frac{\partial \phi}{\partial x} \cos \gamma + \frac{\partial \phi}{\partial y} \sin \gamma \right) = L \phi_b - M \quad (20)$$

in which $M = h_f * Cl$ and $L = h_f$, upon comparison with (8).

Using Galerkin method in which the GDE is weighted by the shape function and equating the error to zero yields:

$$[C] \{\dot{\Phi}\} = [K] \{\Phi\} - \{F\} = 0 \quad (21)$$

Using finite difference for the time derivative, one may have

$$([C] + \theta \Delta t [K]) \{\Phi\}^{t+\Delta t} = ([C] - (1-\theta) \Delta t [K]) \{\Phi\}^t + \Delta t \left((1-\theta) \{F\}^t + \theta \{F\}^{t+\Delta t} \right) \quad (22)$$

where θ is a parameter ranging from 0 to 1 and Δt denotes a time increment.

For $\theta = 1$, and divide throughout by Δt , we have the following form:

$$[K] \{\phi\}_{t+\Delta t} = \{F\} \quad (23)$$

in which

$$[K] = \frac{1}{\Delta t} [C] + [k_1] + [k_2]$$

and

$$\{F\} = \frac{1}{\Delta t} [C] \{\phi\}_t + \{f\}_{t+\Delta t}$$

Along with

$$[C] = \int_A k [N]^T [N] dA$$

$$[k_2] = \oint L [N]^T [N] ds$$

$$[k_1] = \int_A D [B]^T [B] dA$$

$$\{f\}_{t+\Delta t} = \oint_s M [N]^T ds$$

To ensure unconditional stability in all the computations performed in this paper, we have fixed $\theta = 1$, resulting in a fully implicit scheme. The above FE equation is implemented in FORTRAN 95 in a code modeled according to the program structure described in [17]. The FE based computer program has been developed to predict the chloride progression in concrete structures and given the name **CPICS** (Chloride Profile In Concrete Structures). This program is mainly an extension of the work done by the authors on moisture diffusion on concrete which has been documented in a number of publications [18]–[22].

A combined experimental-finite element based approach is used for calibrating the chloride diffusivity using the experimental results of measured diffusivity based on variable w/c ratio and the binder ratio. The calibrated diffusivity parameter is then used in the program to predict the chloride movement front into concrete and estimate the time to initiate corrosion as this is the longest period for the safety of the structure.

IV. CHLORIDE INGRESS SIMULATION

Influence of Binder and W/C Ratio on Chloride Front Movement

At saturation level, the total chloride ingressed into concrete will be assumed to be equal to that of free chloride as the diffusion mechanism is the one to take place. To predict and assess the chloride transport and to bring about the effect of water/cement ratio and the binder content, experimental results from [23] have been employed in the developed computer program. The regressed form found in [23] depicting the influence of w/c ratio and the cement content (cc) normalized by 350, the controlling test is given in the

following form:

$$D_0 * 10^8 = 82.74 - 425.9 (w/c) + 568.42 (w/c)^2 + 9.26 (cc)^{-6} \quad (24)$$

Although here we have a single value for the chloride diffusivity, yet a multivaried diffusivity function [14] could be used in such form:

$$D = D_0 * F(w/c) * F(cc) * F(t_e) \quad (25)$$

And D_0 itself is a function of the chloride level which may take various specific forms.

V. PROBLEM STATEMENT

A reinforced concrete beam sample of width 7.5 cm with a reinforcing bar placed at the center such that the cover is 3.75 cm, is immersed in a chloride content of 17 kg/m³ of pore solution. It is required to assess how long it will take for the chloride level to reach the given concentration throughout the width of the beam and thus reach the reinforcement. Also, it is required to plot the chloride movement front into concrete as a function of w/c ratio and the cement content.

This problem has been solved using the computer program in which a concrete sample of dimension 100 mm * 100 mm * B (B = 75 mm) is used and subjected to chloride environment from both sides. The sample has been discretized to 100 elements, each of which has 9 nodes as shown in Fig. 1. Due to the symmetry of the problem, only half of the sample will be considered.

VI. RESULTS AND DISCUSSION

Three types of concrete have been used with different w/c and cement content with three diffusivities. For cement content of 350 kg/m³ with three w/c = 0.4, 0.55, and 0.7, the corresponding calculated chloride diffusivities are 8.28E-8, 28.10E-8, and 67.4E-8, respectively, from (24). In Fig. 2, the plot of chloride profile for various water-cement ratios with cc = 350 kg/m³ is shown in which series 1 through series 3 representing the order of increasing w/c ratio with constant cc = 350 kg/m³. Of course, as expected, the higher the w/c ratio, the higher is the diffusivity and thus the faster the movement of the chloride front.

For w/c = 0.4 and with cc = 300 kg, 350 kg, and 400 kg, the chloride profile is shown in Fig. 3 where a similar trend of the influence of w/c ratio and that of cement content is shown in the Figure. The higher the cement content, the lower is the diffusivity and thus it takes longer time for chloride to reach the same level as that for the lower cement content. It is clear that diffusivity plays a role in improving concrete durability and prolonging the service life of concrete structures.

Influence of Binding Capacity on Chloride Diffusion

In order to assess and predict the ingress of chloride into the concrete structures, two methods have been adopted using the previous problem of the beam sample subjected to chloride solution of 17 kg/m^3 . The first method was based on the nonlinear finite element method in which the in-house software CPICS was used to predict the effect of chloride binding capacity where the chloride diffusivities have been modified to incorporate the chemical reaction. The second method was using the ANSYS package to run the same problem, adopting the thermal analogy as they have the same governing field equations.

Three forms of chloride diffusivity functions have been investigated. First, is the constant diffusivity in which the binding chloride is neglected and thus the free chloride is the total chloride, (14a), in which the diffusivity of $8.64\text{E-}4 \text{ m}^2/\text{s}$ is adopted. The second is where the binding chloride is considered to be linearly related to the free chloride, (14b), in which $\alpha = 0.07$. The third is the Freundlich isotherm, (14d), in which $\alpha = 1.05$ and $\beta = 0.36$. Different exposure duration was investigated including 1–25 years, and the behavior of free chloride ingress was captured along with the associated binding chloride. The exposure condition is a chloride intensity of 17 kg/m^3 of pore solution.

In Fig. 4, the progressive buildup of chloride within the concrete cover is shown up to 25 years. Of course, such trend could be altered with another form of diffusivity function. As the unit of free chloride is different from that of binding chloride, percentage of both of them with respect to the weight of cement has been calculated and subsequently the total chloride is calculated. Fig. 5 shows the total chloride for two cases, one in which the reaction is not included and the other in which the linear form for binding chloride is used. It is readily seen that the total chloride prediction for these two cases is almost double. For the second case in which reaction is included, the total chloride and its associated components, the free and binding chloride, are shown in Fig. 6.

It is recognized that the magnitude of chloride diffusivity in concrete not only can reflect the permeability of concrete, but also can be used to predict the service life of concrete as the model is predicting the concentration of chloride at the location of steel reinforcement [24]. It has been shown that the total chloride diffusivity is near 3.0 times the free chloride diffusivity [25]. That is to say, the bound chloride content is about two times the free chloride.

The prediction of free chloride based on ANSYS thermal analogy for different diffusivity functions including constant, linear and power law is shown in Fig. 7. It is clear how the diffusivity function influences not only the amount of the predicted free chloride but also the amount of the binding chloride. After 25 years, the constant diffusivity predicted that the free chloride at a depth of 4 cm is 11.4. Marked difference is noticed in the rate at which the chloride front is moving among three different chloride binding capacities.

VII. CONCLUSIONS

This paper focuses on the influence of w/c ratio and cement content and its impact on chloride ingress in concrete. It has been noticed from the numerical model and from the experiments that the lower the water cement ratio, the lower is the chloride diffusivity and therefore the longer it will take for chloride to move forward into concrete. A similar trend was obtained for varying cement content in which the higher the cement content, the lower is the diffusivity.

The influence of binding chloride and its impact on the way chloride front moves within concrete through the key parameter, the chloride diffusivity has been demonstrated. An in-house developed software CCICS, based on nonlinear finite element method, predicts well the movement of chloride front through concrete. The role of the specific form of the binding chloride has been captured, where marked difference in predicting the free chloride and its associated binding chloride and, thus, ultimately the total chloride was found. The results predicted by the software have been cross-checked by an independent source of software, namely ANSYS, where close agreement has been ascertained. It is clear that a low value of chloride diffusivity parameter plays an important role on improving concrete durability and, thus, prolonging the service life of concrete structures. The following points may be stated with regard to conclusions:

- Chloride transport prediction based on one or another form of chloride binding formulation may be quite different. Hence, the relevance of binding in terms of its type of representations by isotherm models is critical to permit a more accurate prediction of chloride transport models.
- Available binding measurements represented in a form of empirical equations must faithfully describe the underlying observed chloride binding behavior. Hence, measurement or acquisition of binding data relevant to the underlying binding behavior of the material being evaluated is not an exercise in futility but an unavoidable endeavor for modeling of the chloride binding in its most fundamental manner.
- Chloride transport predicated on null binding and/or constant diffusivity assumptions is misleading and can lead to erroneous conclusions.

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Ali H. Al-Gadhib was born in Saudi Arabia on February 12, 1956 and graduated from King Fahd University of Petroleum & Minerals (KFUPM), Dhahran, Saudi Arabia with a BS and MS in civil engineering (structures) in 1980 and 1982, respectively. He obtained his PhD from NCSU, Raleigh, USA in December 1988 in civil engineering.

Currently, he is working as an associate professor in the Department of Civil Engineering at KFUPM. He earned the British Council research awards for two consecutive summers of 1994 and 1995 to conduct research at the University of Sheffield, U.K., sponsored by the British Aerospace of Saudi Arabia. He is the co-editor of the International Conference on Construction and Building Technology, held in Kuala Lumpur, Malaysia on 11-20 June, 2008. Some of his recent publications include:

- A. H. Al-Gadhib, M. H. Baluch, and M. K. Rahman, "Repair and retrofitting of deteriorated and distressed concrete structures – three case studies," *J. Int. Assoc. Concr. Technol.*, vol. 1, no. 2, pp. 153–160, Dec. 2003.
- M. A. Shazali, M. H. Baluch, and A. H. Al-Gadhib, "Predicting residual strength in unsaturated concrete exposed to sulfate attack," *J. Mater. Civ. Eng.*, ASCE, vol. 18, no. 3, pp. 343–354, May/June 2006.
- A. R. Khan, A. H. Al-Gadhib, and M. H. Baluch, "Experimental and computational modeling of low cycle fatigue damage of CFRP strengthened reinforced concrete beams," *Int. J. Damage Mech.*, March 10, 2010.

His research area includes computational modeling of reinforced concrete structures, computational concrete durability, plasticity, and damage mechanics.

Dr. Al-Gadhib is a member of several professional societies including ICBO and ACI, and he is a board member of the ASCE-Saudi Arabia section. He served as the president of ASCE (Saudi Arabian Section) for the year 1997.

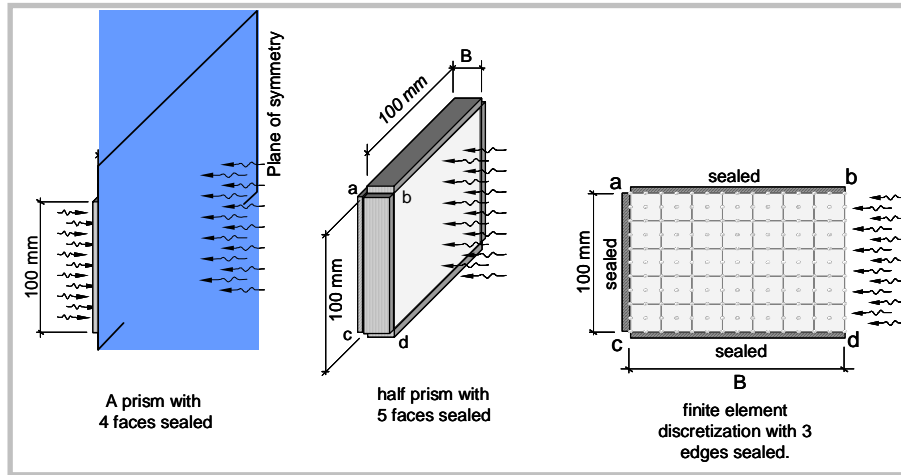


Fig. 1. Modeling and discretization of the concrete sample.

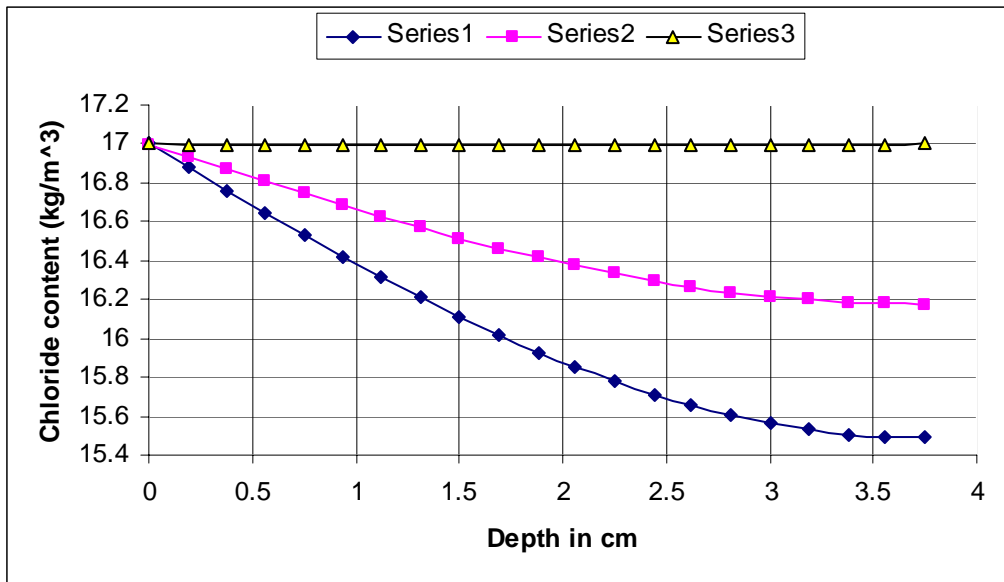


Fig. 2. The behavior of chloride ingress as a function of w/c ratio.

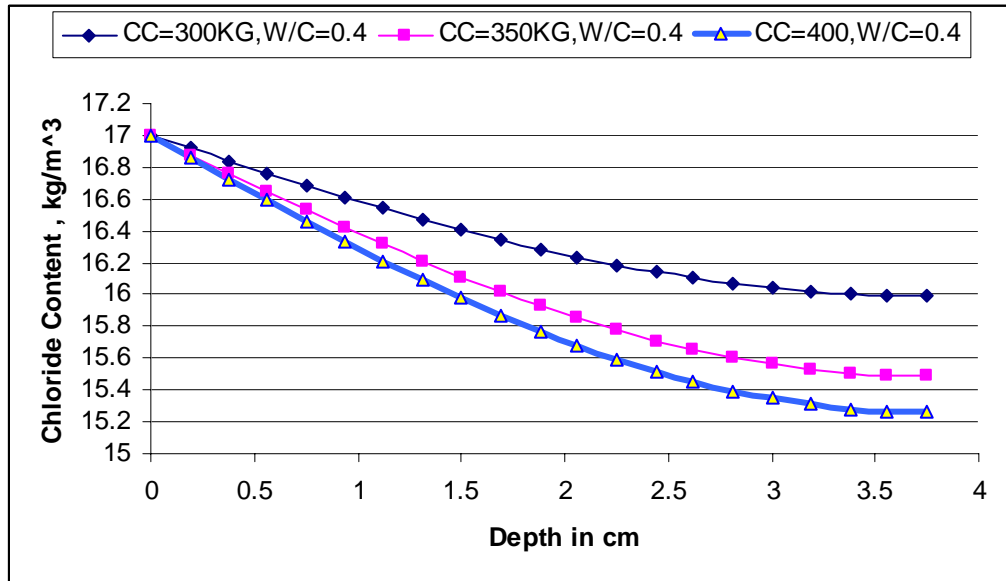


Fig. 3. The influence of cement content on chloride profile.

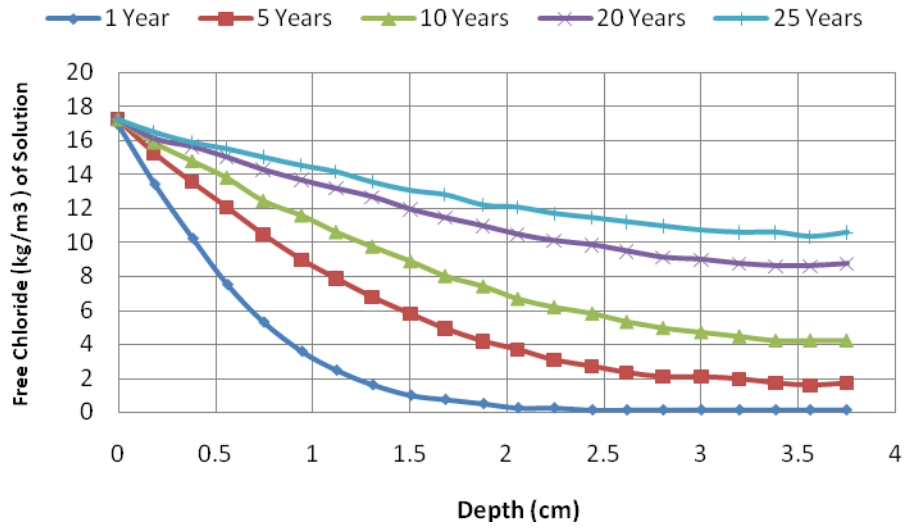


Fig. 4. Prediction of free chloride movement front with time.

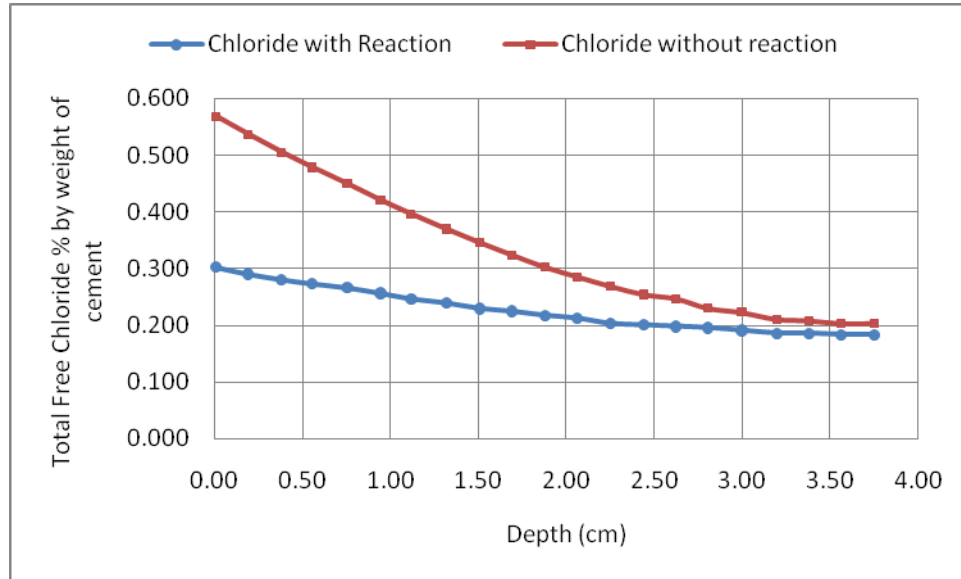


Fig. 5. Prediction of total free chloride with and without reaction.

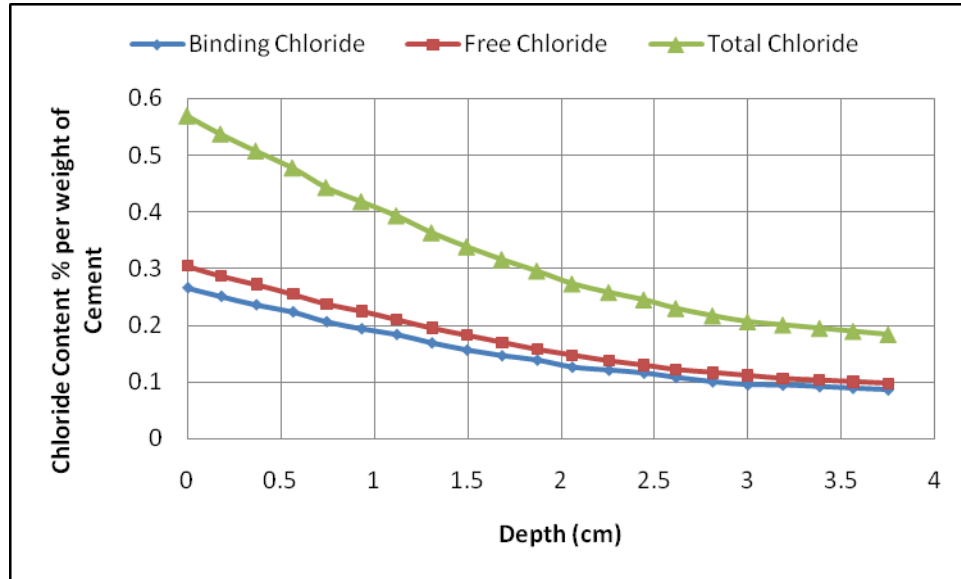


Fig. 6. The decomposition of the total chloride to its components with linear binding capacity.

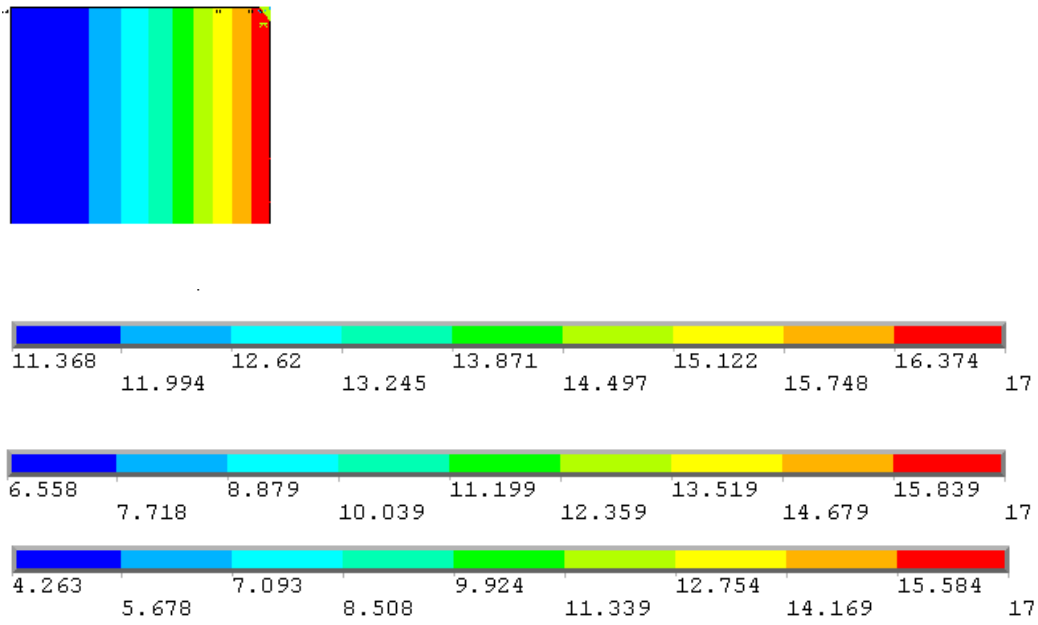


Fig. 7. Prediction of ANSYS using three different binding capacities: no reaction, linear and Freundlich