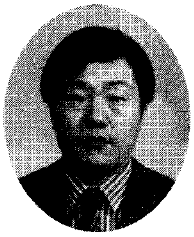
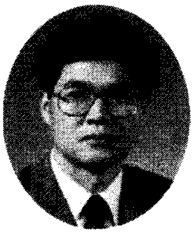
Finite Element Analysis of Chloride Ion Intrusion into Coastal Concrete Structure





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ABSTRACT

In order to predict the onset of the corrosion of steel bars in concrete, a mathematical model was presented to observe the diffusion of chloride ion in aqueous phase of pores, the adsorption and desorption of chloride ions to and from the surface of solid phase of concrete, and the chemical reaction of chloride ions with solid phase. The finite element method was employed to carry out the numerical analysis.

The chlorides penetrating through the wall of the concrete structure from the external environment and the chlorides contained in the concrete admixture were confirmed to be two important factors to determine the onset of the corrosion of steel bars.

Keywords : concrete, corrosion of steel bar, chloride ion, diffusion, reaction, mathematical model

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1. INTRODUCTION

Properly constituted, placed and cured concrete has a long service life under most natural and industrial environments. However premature failures of concrete structures may occur due to various physical and chemical effects(1). Especially, concrete carbonation and chlorination are the two main physicochemical processes which limit the useful lifetime of reinforced concrete structures. Steel bar in reinforced concrete are protected from corrosion in the presence of moisture and oxygen by a microscopic oxide layer which forms on their surface due to the high alkalinity ($pH \approx 13$) *of the surrounding concrete.* Protection from corrosion ends, if this passive layer disappears due to the reaction of its $Ca(OH)_2$ with atmosphere CO_2 and the subsequent drop of the pH value below 11.5. When the concentration of chloride ions in the pore water in the vicinity of the bars exceeds a threshold value, of the order of 0.05% by weight in concrete, it is reported that the protective film may be destroyed even at pH values considerably above 11.5(2). The transformation of metallic iron to rust is accompanied by an increase in volume which, depending on the state of oxidation, may be as large as 600 percent of the original metal. This volume increase is believed to be the principal cause of concrete expansion and cracking. The onset of cracks due to reinforcement corrosion enhances the intrusion of moisture, oxygen and chlorides ions and, therefore, accelerates the deterioration of concrete structure(3),(4).

Recently, premature reinforcement corrosion in concrete structures exposed to chloride containing environments has an important problem. This is due to an increasing use of deicing agents in cold-weather area and marine aggregate of chloride containing admixture at the mixing stage as well as due to an increase of concrete construction in marine environments(5).

In this study, the behavior of chloride ions introduced into concrete from concrete surface by a marine environment and contained in admixture at the mixing stage was modeled. The physicochemical processes including the diffusion of chloride ion in aqueous phase of pores, the adsorption and desorption of chloride *ions to and from the surface of solid* phase of concrete, and the chemical reaction of chloride ion with solid phase were analyzed by using the finite element method. The results of this study may be used to predict the onset of reinforcement corrosion, to identify the maximum limit of chloride ions contained in admixtures, and to decide a repair method for reinforced concrete damaged by chloride ion attack.

2. MODEL FORMULATION

A schematic of the problem domain(i.e. the cross section of a corner of concrete structure) is shown in Fig.1(a). The dimensions of the domain are shown in Fig.1(b). The change of the chloride ion concentration is traced at three locations A, B and C where steel bars embedded.

The chloride ions dissolved in pore water of concrete, $Cl^-(aq)$, are adsorbed by calcium silicate hydrate (C-S-H) and by the other constituents of hardened

Fig.1(a) Problem domain and boundaries and

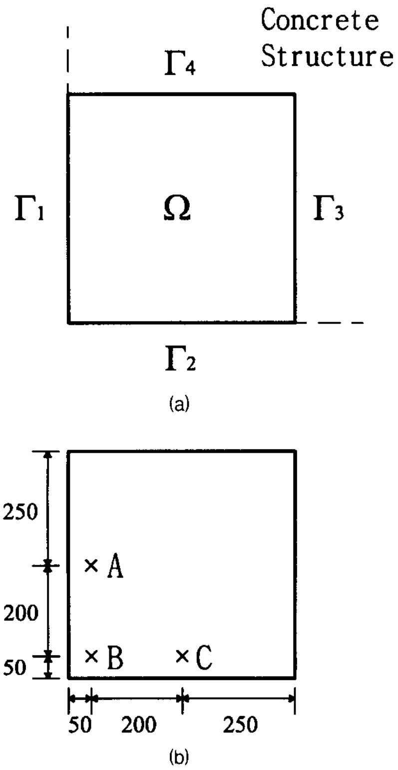

Fig.1(a) Problem domain and boundaries and (b) dimensions of problem domain.

cement paste. They also chemically react with C_3A and C_4AF constituents of cement and producing the so-called Friedel's salt. Some of the adsorbed chloride ion, $Cl^-(s)$, is desorbed and the process tends to equilibrium between $Cl^-(aq)$ and $Cl^-(s)$. Therefore, the net rate of binding Cl^- in the solid phase, r, is given by(Pereira and Hegedus 1984)

$$r = k_a \varepsilon f[Cl^-(aq)]\{[Cl^-(s)]_{sat} - [Cl^-(s)]\} - \frac{k_a}{K_{eq}}[Cl^-(s)] \qquad (1)$$

where k_a and K_{eq} are kinetic constant of a desorption and equilibrium constant, respectively, ε is the concrete porosity, f is the fraction of pore volume filled with water, and $Cl^-(aq)$ and $Cl^-(s)$ are the concentrations of Cl^- in aqueous and solid phases, respectively.

The mass balance equations of $Cl^-(aq)$ and $Cl^-(s)$ are expressed as (Papadakis et al. 1996) :

$$\frac{\partial(\varepsilon f[Cl^-(aq)])}{\partial t} = \nabla^2(D_{e,Cl^-}[Cl^-(aq)]) - r \quad \text{in } \Omega \qquad (2)$$

$$\frac{\partial([Cl^-(s)])}{\partial t} = r \quad \text{in } \Omega \qquad (3)$$

where D_{e,Cl^-} is the effective diffusivity of Cl^- in concrete, t is the time, and Ω is the problem domain shown in Fig.1(a).

The boundary and initial conditions applied are

$$[Cl^-(aq)] = [Cl^-(aq)]_1 \quad at\ \Gamma_1 \qquad (4)$$

$$[Cl^-(aq)] = [Cl^-(aq)]_2 \quad at\ \Gamma_2 \qquad (5)$$

$$\frac{\partial[Cl^-(aq)]}{\partial n} = 0 \quad at\ \Gamma_3 \text{ and } \Gamma_4 \qquad (6)$$

$$\frac{\partial[Cl^-(s)]}{\partial n} = 0 \quad at\ \Gamma_1,\ \Gamma_2,\ \Gamma_3 \text{ and } \Gamma_4 \qquad (7)$$

$$[Cl^-(aq)] = [Cl^-(aq))]_{in} \quad \text{in } \Omega \quad \text{at } t=0 \qquad (8)$$

$$[Cl^-(s)] = [Cl^-(s)]_{in} \quad \text{in } \Omega \quad \text{at } t=0 \qquad (9)$$

Boundary conditions (4) and (5) imply that the concentrations of $Cl^-(aq)$ at Γ_1 and Γ_2 have fixed values, which are dependent on the external environment of concrete structure. Boundary condition (6) implies that $Cl^-(aq)$ does not penetrate to the normal direction of Γ_3 and Γ_4. Boundary condition (7) implies that $Cl^-(s)$ does not move through the boundaries. $[Cl^-(aq)]_{in}$ of Eq.(8) and $[Cl^-(s)]_{in}$ of Eq.(9) denote the initial concentrations of Cl^- in aqueous and solid phases, respectively.

3. FINITE ELEMENT FORMULATION

The functional spaces of Sobolev type employed as follows :

$$H^1(\Omega) = \{ W | W \in L^2(\Omega),\ \frac{\partial w}{\partial x} \in L^2(\Omega),\ \frac{\partial w}{\partial y} \in L^2(\Omega) \} \qquad (10)$$

$$V(\Omega) = \{ W | W \in H^1(\Omega),\ W = 0 \text{ on } \Gamma_1 \,\&\, \Gamma_2 \} \qquad (11)$$

$$S(\Omega) = \{ W | W \in H^1(\Omega),\ W = [Cl^-(aq)]_1 \text{ on } \Gamma_1,\ W = [Cl^-(aq)]_2 \text{ on } \Gamma_2 \} \qquad (12)$$

where, $L^2(\Omega) = \{ w \,|\, \int_\Omega W^2 d\Omega < +\infty \}$ (13)

The variational form of the problem can be stated as follows:

Find $\Phi^1 \in S$, $\Phi^2 \in H^1$ such that

$$\int_\Omega W^1 (\varepsilon f \frac{\partial \Phi^1}{\partial t}) d\Omega + \int_\Omega \nabla W^1 \cdot (D_{e,Cl^-} \nabla \Phi^1) d\Omega + \int_\Omega W^1 r d\Omega = 0,\ \forall W^1 \in V \qquad (14)$$

$$\int_\Omega W^2 \frac{\partial \Phi^2}{\partial t} d\Omega + \int_\Omega W^2 r d\Omega = 0,\ \forall W^2 \in H^1 \qquad (15)$$

where r is a nonlinear function of Φ^1 and Φ^2.

A finite element spatial discretization of Eq.(14) and Eq.(15) leads to a set of nonlinear ordinary differential equations :

$$M\dot{d} + N(d) = F \qquad (16)$$

$$d(0) = d_0 \qquad (17)$$

where d is the vector of nodal values of unknowns, $\dot{d}$ is its time derivative, M is the mass matrix, N is the nonlinear vector function of d. F is the right-hand side constant vector and d_0 is a given vector corresponding to the initial conditions (8) and (9). These equations are solved by a predictor/multicorrector temporal integration scheme(Heghes et al. 1979)$^{(6)}$.

The finite element mesh used is shown in Fig.2. The element mesh was made denser where steeper concentration gradients are expected. 1024 bilinear quadrilateral elements (and 1089 nodes) were used for the mesh. Calculations were performed on HP 715/50 workstation. CPU time required for one time step was 3 seconds.

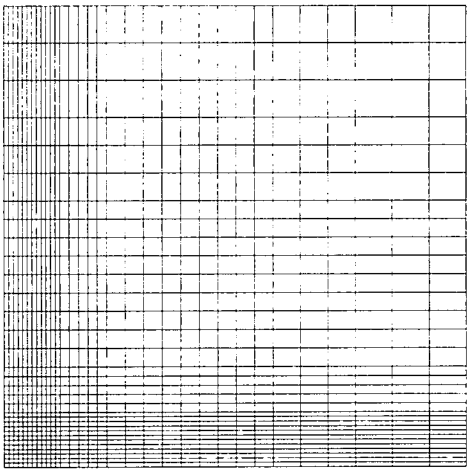

Fig.2 Finite element mesh used

4. RESULTS AND DISCUSSION

In this study, the values of $[Cl^-(aq)]_1$ and $[Cl^-(aq)]_2$ are fixed as 0.22wt% and 0.10wt% of concrete. As initial conditions, two cases with and without initial presence of Cl^- in the admixture are considered. The value of Cl^- is 0.3wt% for the case when chloride ion is introduced at the mixing stage by using marine aggregate. Parameter values used for the analysis are the same as those of Papadakis(1996) and summarized in Table 1.

Table 1 Parameters Used in Calculations.

Parameter	Value
ε	0.20
f	0.7
D_e	2.0×10^{-12} m^2/s
k_a	1×10^{-5} m^3/mol s
$[Cl^-(s)]_{sat}$	214 mol/m^3
K_{eq}	1.64×10^{-2} m^3/mol

Fig.3 shows the variation of chloride ion concentrations of aqueous and solid phase with time for the case without initial presence of chloride ion at three locations A, B and C where steel bars are embedded. In this case, there exist only external sources of chloride ion penetrating through the surface of concrete. The threshold concentration of chloride ion in aqueous phase for the onset of corrosion of steel bars was set as 0.05wt% of concrete. It takes 2.5 years for the value of $[Cl^-(aq)]$ at B to reach this threshold value and it takes 3 years for the case of A. However, even after 20 years, this threshold value has not been reached at C. Therefore, one can conclude that the chloride ion from the external environment is an important factor to determine the onset of corrosion of steel bars. Fig.4 and Fig.5 shows the concentration distributions of chloride ions in aqueous and solid phases, respectively, after 20 years under the same conditions as in Fig.3. From Fig.4, it can be predicted that the corrosion of steel bars near the boundary Γ_1 is in progress, since the value of $[Cl^-(aq)]$ exceeds 0.05wt% of concrete. Fig.5 indicates that a large fraction of chloride ions are bound in solid phase. Hence, without the consideration of binding of chloride ions in solid phase, calculation

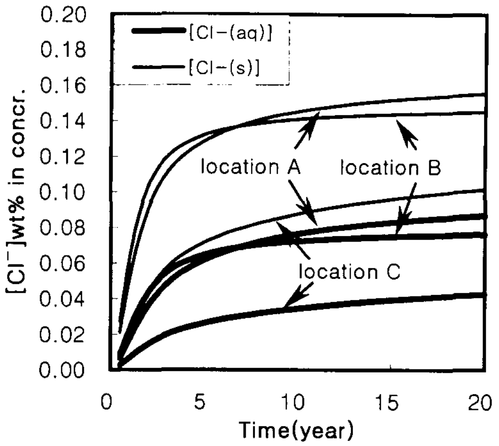

Fig.3 Variation of Cl^- concentration with time for the case without initial presence of Cl^-

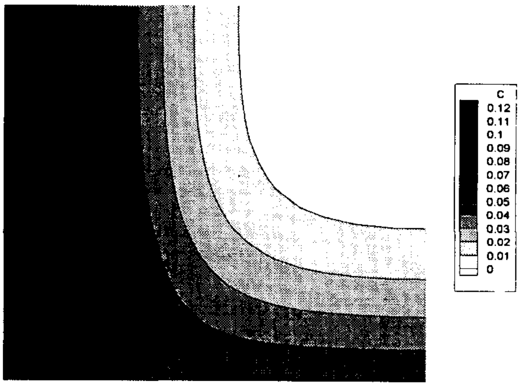

Fig.4 Contour plot of Cl− concentration in aqueous phase after 20 years. Conditions were as in Fig.3.

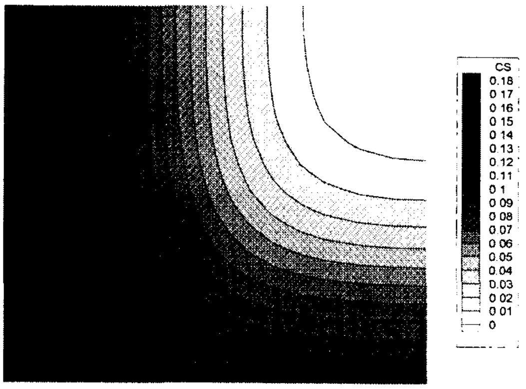

Fig.5 Contour plot of Cl− concentration in solid phase after 20 years. Conditions were as in Fig.3.

results can be erroneous.

Fig.6 illustrates the variation of chloride ion concentrations with time for the case with 0.3wt% of chloride ion introduced by using marine aggregate. As compared with the case of Fig.3, it takes less time (approximately 2 years) for the value of $[Cl^{-}(aq)]$ at A and B to reach 0.05wt%. For the case of C, after 20 years, this threshold value of $[Cl^{-}(aq)]$ has been exceeded. This result indicates that the use of marine aggregate accelerates the corrosion of steel bars.

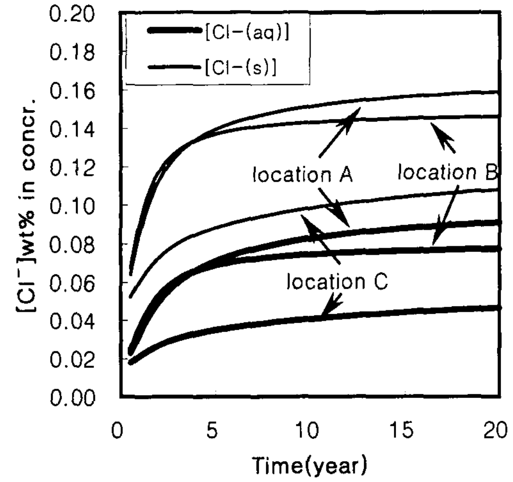

Fig.6 Variation of Cl^- concentration with time for the case with initial presence of Cl^-

5. CONCLUSIONS

A mathematical model including the diffusion of chloride ion in aqueous phase of pores, the adsorption and desorption of chloride ions to and from the surface of solid phase of concrete, and the chemical reaction of chloride ions with solid phase was presented to analyze the intrusion of chloride ion into concrete structures.

Two cases with and without initial presence of chloride ions in the admixture at the mixing stage were studied based on the finite element method. The concentration of chloride ion at the wall of concrete structure and the amount of chloride ion contained in the admixture were identified as the main factors to determine the onset of the corrosion of steel bars. It was confirmed that a considerable fraction of chloride ions is bound in solid phase of concrete. Therefore, the binding of chloride ions in solid phase must be considered in order to describe the behavior of chloride ions penetrating into concrete structure correctly.

The results of this study may be useful for the prediction of the onset of reinforcement corrosion and the identification of maximum limit of permissible amount of chloride ions contained in admixture.

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