V－211 SIMULATION OF CHLORIDE PENETRATION INTO CONCRETE (CONDENSATION OF CHLORIDE DUE TO CARBONATION)

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1. INTRODUCTION

This paper introduces a 1-D model for simulating movement of chloride in concrete based on diffusion theory, taking into account chloride condensation due to carbonation. The condensation occurrence was simulated by introducing a simple idea for computing free chloride concentration. The condensation occurrence can then be simulated and the computational results were compared with the test results from Kobayashi, et.al[1]. The model will be useful for the prediction of time when critical amount of dissolved chloride to initiate steel corrosion presents in the concrete.

2. CHLORIDE AND ITS STATUS IN CONCRETE

Total chloride in hardened concrete (C) can be categorized mainly into 2 kinds namely free chloride (dissolved status) which can diffuse when there is free chloride concentration gradient and fixed chloride (non-dissolved status) which is stationary, then

$$C = Cfix + Cfr \qquad (1)$$

where Cfix and Cfr are concentration of fixed and free chloride, respectively. It is known that chloride formed in Friedel's salt is fixed chloride, however, report by Nagataki, et.al[2] says that Friedel's is just one kind of fixed chloride and then there should be mechanism other than Friedel's for the quantification of fixed chloride. According to their report, the amount of fixed chloride in normal condition, such as in case of no carbonation onset, is in the range of 64% to 78% of the total chloride . In this paper, the amount of free chloride was assumed to be an average of 70% of total chloride for simplicity as

$$Cfix = 0.7 \cdot C \qquad (2)$$

3. COMPUTATIONAL MODEL

The movement of free chloride in concrete was considered to obey Fick's law of diffusion which can be written in mathematical form as

$$F(x,t) = D(x,t) \cdot \frac{\partial Cfr(x,t)}{\partial x} \qquad (3)$$

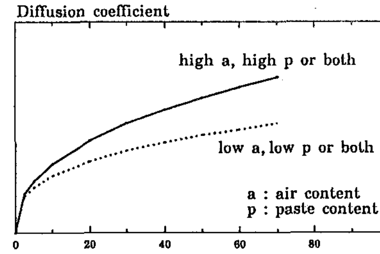

Fig.1 Assumed curve for diffusion coefficient

where F(x,t)is flow or flux of free chloride, D(x,t) is diffusion coefficient of free chloride in concrete, Cfr(x,t) is free chloride concentration, x is spatial coordinate in the flow direction and t is time.

By applying finite difference numerical method, the diffusion equation can be solved easily. The problem is to determine the diffusion coefficient for Eq.(3). The diffusion coefficient was considered to vary with pore volume, pore size distribution and humidity of the pore in the hardened concrete (to be studied quantitatively). However, it is difficult to derive the pore volume and pore size distribution without conducting measurement on concrete specimen. Here, the utilized function for obtaining diffusion coefficient, D, was assumed in order to obtain qualitative analytical result as shown in Fig.1.

Though the diffusion coefficient which reflects material properties of the concrete is determined, it is still not sufficient for accurate prediction of chloride movement in concrete. This is because the mechanisms of chloride penetration into concrete can be affected not only by the material properties but also by various environmental conditions, for example, the mechanisms of water loss and gain near the concrete surface (to be quantitatively investigated) and also the onset of carbonation as well. Since this paper was aimed to simulate the condensation of chloride by carbonation, the mechanism of water loss and water gain were not presented and the condition of concrete was assumed to be 100% saturated for non-carbonated area and 50% for carbonated portion for qualitative analysis.

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4. CARBONATION EFFECT

The effect of carbonation was considered as to dissolve fixed chloride (increase free chloride) of the carbonated portion. Free chloride amount released by carbonation (Ccfr) is assumed to be depending on factor F as

$$Ccfr = F \bullet Cfix \qquad (4)$$

where Cfix is fixed chloride concentration before carbonation. Factor F, requiring quantitative study, is assumed to vary with humidity in concrete pore and concentration of CO2 and Fig.2 shows the assumed function shape. Then free chloride after carbonation (C'fr) becomes

$$C'fr = Cfr + Ccfr \qquad (5)$$

where Cfr is free chloride concentration before the onset of carbonation. Fixed chloride concentration after carbonation (C'fix) is then

$$C'fix = Cfix - Ccfr \qquad (6)$$

and total chloride after carbonation (C') is

$$C' = C'fix + C'fr \qquad (7)$$

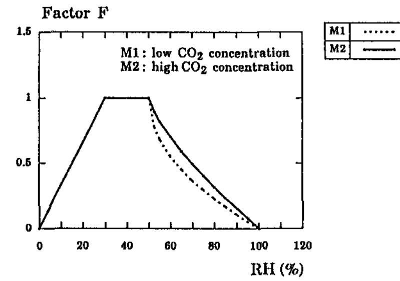

Fig.2 Assumed curve for factor F

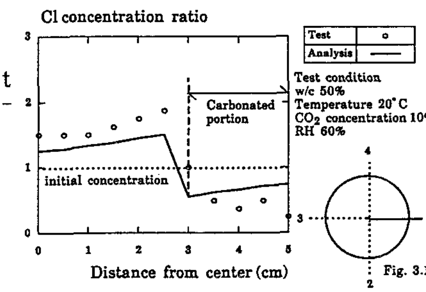

Fig.3 Distribution of Chloride concentration along the radius of mortar specimen

5. COMPARISON BETWEEN ANALYTICAL AND TEST RESULTS

Analytical results were compared with test results from Kobayashi et.al[1]. In their test, mortar specimen (φ5x10 cm.) was cast with sea sand and undergone accelerated carbonation test for 8 weeks before being analyzed for chloride concentration. In Fig.3, test result of distribution of chloride concentration ratio along the radial direction of mortar specimen was the average of 4 radial distributions (1 to 4 in Fig.3.1). Chloride concentration ratio means the ratio of chloride concentration after test to that before test. To obtain analytical result, initial chloride incorporated in the specimen and depth of carbonation were assumed to be 1.0% and 1.0 cm., respectively according to their test (the average chloride concentration after test was 1.0% which can be thought as initial concentration since total chloride in the specimen can be considered unchanged in that test). Chloride condensation in the inner part of concrete was caused by the dissolving of Friedel's salt of the carbonated portion, resulting in higher free chloride concentration in the carbonated portion than in the inner portion. This causes free chloride concentration gradient between the larger concentration in the carbonated portion and the smaller concentration in the inner one. Free chloride then diffuse according to the concentration gradient causing the inner portion to have higher total chloride concentration than the near-surface portion[1]. The occurrence of chloride condensation can be simulated as can be seen from the bold line in Fig.3.

6. CONCLUDING REMARKS

The following conclusions can be made based on the content of this study.

1) The model for simulating chloride movement in hardened concrete taking into account the effect of carbonation was proposed.
2) The idea for computing additional free chloride released by carbonation was introduced.
3) The occurrence of chloride condensation due to carbonation can be simulated by using the introduced idea.
4) Further studies are still needed for quantitative simulation.

REFERENCES

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2) Nagataki, S., Otsuki, N. and Wee, T.H., "Condensation and Binding of Intruded Chloride Ion in Hardened Cement Matrix Materials," Proc. of JSCE, No.414/V-12 (Concrete Eng. and Pavement), Feb. 1989