- Technical Paper -

COMPARISON OF COMPUTATIONAL MODELS FOR CHLORIDE PENETRATION INTO CONCRETE SUBJECTED TO AIRBORNE SALT

Devi NURALINAH[*1], Takumi SHIMOMURA[*2]

ABSTRACT
Time-dependent chloride penetration into concrete subjected to airborne salt was examined by the manufactured wind tunnel. Surface chloride and diffusion coefficient were experimentally derived. Chloride penetration into concrete was recalculated by several computational models. It was clarified that the combination of concentration-dependent diffusion coefficient and natural type of boundary condition can simulate well chloride profiles in both short and long term chloride profiles.
Keywords : airborne salt, surface chloride, diffusion coefficient, chloride ingress, wind tunnel

1. INTRODUCTION

Chloride penetration into concrete is predominant process for service-life of concrete structures since it initiates corrosion of steel reinforcement embedded in concrete. Airborne salt originating from sea water is major sauce of external chlorides for coastal concrete structures. In order to develop a computational model for time-dependent chloride penetration into concrete that can take into account the effect of airborne salt adequately, reliable test data are necessary. Considering this, the authors' research group developed a new laboratory test method using a wind tunnel for chloride penetration into concrete subjected to airborne salt [1].

In the previous paper, surface chloride and diffusion coefficient in concrete derived from wind tunnel test result were presented. Applicability of several mathematical models, which employ constant and time-dependent surface chloride and diffusion coefficient, were examined [2]. It was found that experimentally obtained surface chloride in concrete depends on the intensity of airborne salt to which the concrete is exposed. The combination of time-dependent surface chloride and time-dependent diffusion coefficient can well estimate chloride content in concrete in both short and long term. It was also confirmed that, if the surface chloride and diffusion coefficient are adequately determined, chloride content at the reinforcement position at the specified time can be estimated with satisfactory accuracy even by the combination of constant surface chloride and constant diffusion coefficient.

In this paper, computational models which employ natural type of boundary condition having an analogy with that for heat transfer phenomena and concentration-dependent diffusion coefficient derived by Boltzman-Matano method, are examined.

2. COMPUTATIONAL MODELS

One-dimensional Fick's diffusion equation is used as a typical and general method to estimate chloride penetration into concrete.

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \tag{1}$$

where C = chloride content in unit concrete volume (kg/m^3); t = time (day); x = depth from the exposed surface (mm); D = chloride diffusion coefficient in concrete (m^2/s).

Diffusion coefficient is a material parameter which represents characteristics of concrete in chloride penetration. It has been confirmed by the authors [2] as well as many other researchers that experimentally obtained diffusion coefficient decreases with increasing in time of exposure. This fact implies the possibilities either that concrete pore structure changes during the exposure or that transport process of chloride in concrete cannot be described by ideal diffusion theory. In this study, three types of diffusion coefficient models are examined: constant diffusion coefficient D, time-dependent diffusion coefficient $D(t)$ and concentration-dependent diffusion coefficient $D(C)$. In the previous paper, experimental constant diffusion coefficient D and time-dependent diffusion coefficient $D(t)$ were examined on the basis of the wind tunnel test. In this paper, concentration-dependent diffusion coefficient $D(C)$ is focused.

As boundary conditions for chloride penetration into concrete, chloride content at the surface is usually given according to environmental conditions.

$$C(0,t) = C_0 \tag{2}$$

In the previous paper, constant surface chloride content C_0 and time-dependent surface chloride content $C_0(t)$ were examined on the basis of the wind tunnel test [2].

*1 Graduate School of Engineering, Nagaoka University of Technology, JCI Member
*2 Associate Prof., Dept. of Civil and Environmental Eng., Nagaoka University of Technology, Dr. E., JCI Member

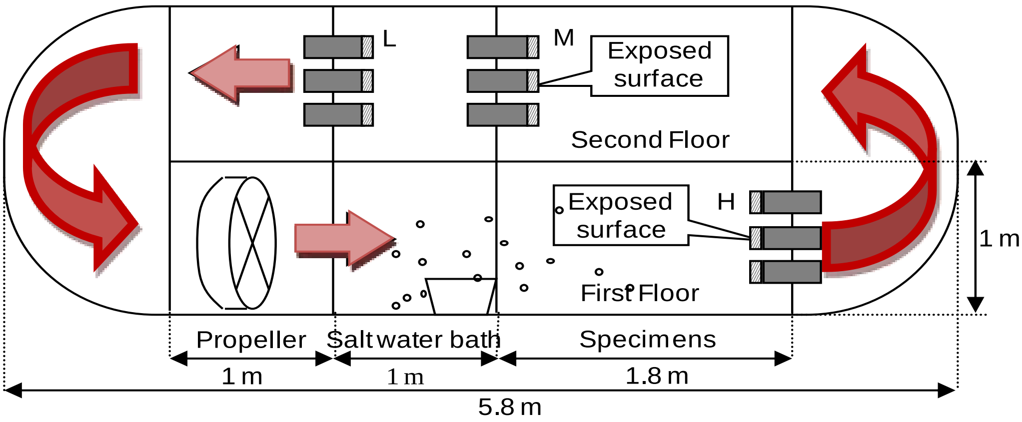

Fig. 1 Outline of the wind tunnel

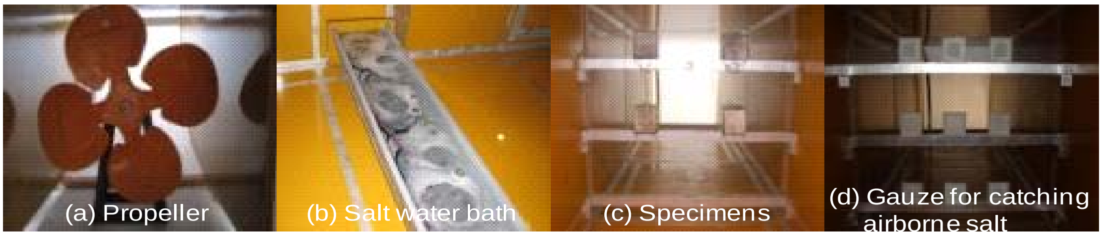

Fig. 2 Inside views of the wind tunnel

In this paper, a natural boundary condition assuming an analogy with heat transfer phenomena is tried [3].

$$J = \alpha (C(0,t) - C_{ext}) \qquad (3)$$

where J = mass flux of chloride through the boundary surface (kg/m^2/s); α = experimental coefficient for surface transfer rate (m/s); C_{ext} = equivalent chloride concentration in concrete under the given environment (kg/m^3). The coefficient α specifies the magnitude of mass flux of chlorides through the surface, which is similar with a heat transfer coefficient. The equivalent chloride concentration in concrete C_{ext} will be dependent of intensity of arriving airborne salt, removal of surface chlorides by rainfall or splash and properties of concrete.

3. EXPERIMENTAL METHOD

The wind tunnel that simulates coastal environment involving airborne salt in the laboratory is shown in Fig.1 and Fig. 2. Size of the cross section inside of the wind tunnel is 1 m x 1 m. The length of wind path is about 12 m in one round. Air flow is generated by a propeller driven by electric motor. Particles of salt water are produced by putting fine air bubbles into the salt water bath. Concrete specimens are set and exposed to airborne salt in both the first and the second floor in the wind tunnel. Wind velocity in the tunnel was 1.5 m/s in average. The measured airborne salt per unit area per unit time was 5 to 68.2 mdd (mg/dm^2/day) depending on the testing position in the wind tunnel. Value of airborne salt is expressed in terms of amount of Natrium Chloride.

Concrete specimen used in the exposure test is shown in Fig. 3. Two types of concrete mix whose water-cement ratio is 40% and 60% were used. Specimens were cured in water for 28 days. After curing, five surfaces of each specimen except one exposed surface were coated with tar epoxy to ensure one-dimensional chloride ingress into concrete from the exposed surface. Six specimens in Table 1 were tested. During the exposure test, specimens were taken out from the wind tunnel periodically and chloride content was measured by sampling concrete powder with drill from the specimens. Value of chloride content in concrete is expressed in terms of amount of chloride ion per unit volume. After measurement of chloride content, specimens were exposed again in the wind tunnel.

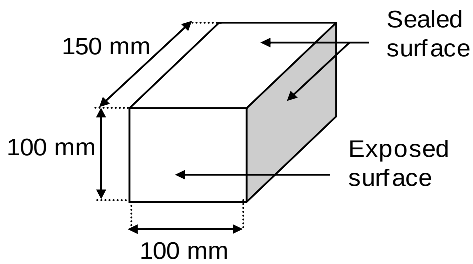

Fig. 3 Concrete specimen

Table 1 Test condition of specimens

Specimen	W/C (%)	Airborne salt (mdd)	Installation position
H-40	40	60.6	First floor
M-40	40	14.7	Second floor
L-40	40	4.9	Second floor
H-60	60	68.2	First floor
M-60	60	15.2	Second floor
L-60	60	5	Second floor

4. EXPERIMENTAL SURFACE CHLORIDES

Fig. 4 shows experimental time-dependent profiles of chloride contents in the specimen obtained by the wind tunnel test during 240 days of exposure. Though six specimens were tested, the result of specimen H-40 is demonstrated here as an example. Based on these results, surface chloride content is determined by following procedure.

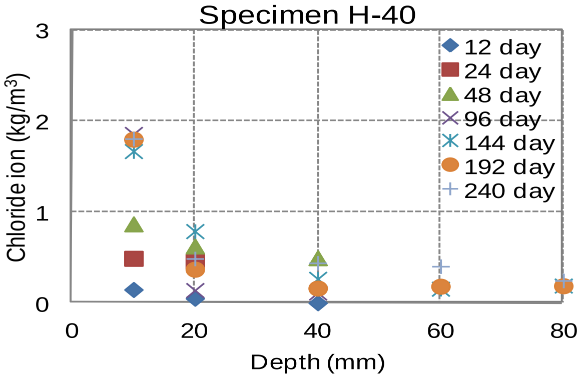

Fig. 4 Experimental time-dependent profiles of chloride contents in specimen H-40

The surface chloride content at time t_j is estimated by extrapolating the experimental inner chloride profile by Lagrange polynomial as shown in Fig. 5. The obtained surface chloride content $C_0(t_j)$ as a function of the sampling time of each specimen is plotted in Fig. 6. It is regarded in Fig. 6 that surface chloride increases with increasing of exposure time and approaches to a certain value in all cases. Regression curves of time-dependent surface chloride content $C_0(t)$ are drawn using Eq. (4).

$$C_0(t) = C_{ext}(1 - e^{-bt}) \tag{4}$$

where C_{ext} and b are parameters for time-dependent surface chloride content determined by least square method. C_{ext} represents an extrapolated surface chloride after a long exposing time. Therefore, C_{ext} is also adopted as an equivalent chloride concentration in concrete under the given environment in natural boundary condition model.

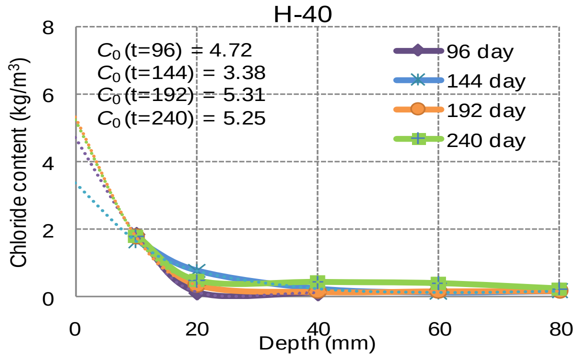

Fig. 5 Extrapolated surface chloride content from inner chloride content in specimen H-40

Mean surface chloride is calculated by averaging $C_0(t)$ with respect to time during the exposure by Eq. (5).

$$C_0 = \frac{1}{T}\int_0^T C_0(t)\,dt \tag{5}$$

where T is length of time of exposure (day) .

The experimentally obtained time-dependent and mean surface chloride content of all specimens are shown in Table 1.

Table 1 Mean and time-dependent surface chloride

Series	C_{air} (mdd)	W/C	Mean C_0 (kg/m^3)	$C_0(t)$ (kg/m^3)
H-40	60.6	40	3.90	$6.66(1-e^{-0.007t})$
M-40	14.7	40	3.57	$4.45(1-e^{-0.015t})$
L-40	4.9	40	3.09	$4.43(1-e^{-0.01t})$
H-60	68.2	60	4.34	$7.10(1-e^{-0.008t})$
M-60	15.2	60	3.94	$6.76(1-e^{-0.007t})$
L-60	5.0	60	2.73	$4.53(1-e^{-0.007t})$

mdd = mg/dm^2/day

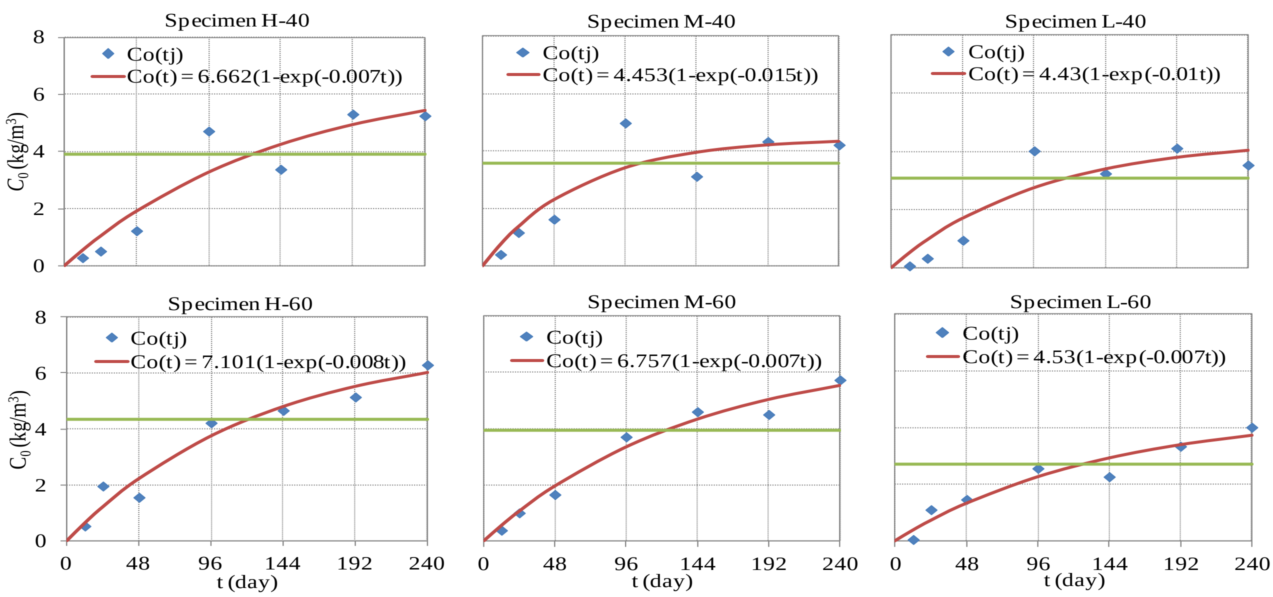

Fig. 6 Time-dependent and mean surface chloride contents

5. CONCENTRATION-DEPENDENT DIFFUSION COEFFICIENT

It is well-known that experimentally obtained apparent diffusion coefficient for chlorides in concrete decreases with increasing in exposure time. One of the practical ways to express this tendency in computational model is that diffusion coefficient is regarded as a function of time, as taken in many previous studies. If the reason of decreasing diffusion coefficient is change of pore structure of concrete, time-dependent diffusion coefficient is reasonable. However, if the reason is attributable to difference of transport mechanism from pure diffusion, another way of mathematical expression is worth being tried. Hence, concentration-dependent diffusion coefficient is examined in this study. Diffusion coefficient is regarded as a function of chloride concentration in concrete, such as nonlinear diffusion model for moisture transport in concrete [4].

Concentration-dependent diffusion coefficient is experimentally derived by Boltzman-Matano method [5]. Fick's second law is transformed into ordinary homogeneous differential equation. Concentration-dependent diffusion coefficient can be expressed as:

$$D(C') = -\frac{1}{2}\left(\frac{d\lambda}{dC}\right)\Bigg|_{C=C'} \int_0^{C'} \lambda \, dC \qquad (6)$$

where $\lambda = x/\sqrt{t}$ (m/s$^{1/2}$). $D(C')$ is calculated according to following procedure.

Experimental λ and C are plotted in a diagram and regression curve for $\lambda(C)$ is drawn using Eq. (7).

$$\lambda(C) = \frac{v}{C + w} \qquad (7)$$

where v and w are parameters for $\lambda(C)$, which are determined by least square method. $D(C')$ is calculated by substituting Eq. (7) into Eq. (6).

$$D(C') = \frac{0.5v^2}{(C'+w)^2} \ln\left\{\frac{C'+w}{w}\right\} \qquad (8)$$

This calculation is schematically shown in Fig. 7.

Relationship between λ and chloride content C based on the wind tunnel test results and its regression curves are shown in Fig. 8.

Derived concentration-dependent diffusion coefficients $D(C)$ are shown in Fig. 9. There is a tendency in Fig. 9 that diffusion coefficients for the series of 40% of W/C are smaller than 60% of W/C. The curve of $D(C)$ starts from the origin, shows a peak at around C is 0.1 kg/m^3 and thereafter gradually decreases. The configuration of the curve of $D(C)$ is attributable to the type of the function of regression curve for $\lambda(C)$, for which Eq.(7) is used in this study. The influence of pre-peak part of the curve of $D(C)$ on the calculated results of long term chloride transport in concrete will be investigated in Chapter 7.

Diffusion coefficient decreases with increasing of chloride concentration. The reason for this is not clarified at this moment. One of the possible reasons is that resistivity for chloride transport of pore structure increases due to increasing of chemically bound chlorides.

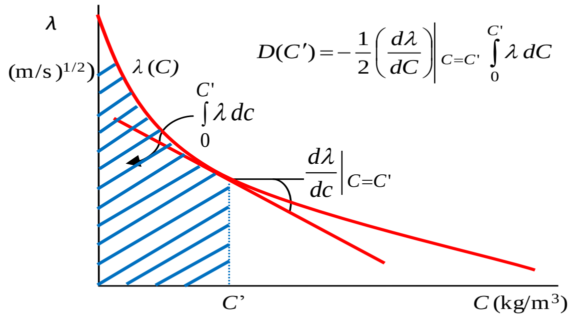

Fig. 7 Determination of $D(C)$ by Boltzman-Matano method

6. NUMERICAL SIMULATION OF CHLORIDE INGRESS INTO CONCRETE

Time-dependent chloride profiles in the concrete specimens in the wind tunnel test were numerically simulated by means of concentrate-dependent diffusion coefficient in Fig. 9 coupled with three types of boundary condition model in Table 3.

Implicit FDM (Finite Difference Method) is employed in numerical analysis. Computational time interval is set as 6 days and size of control volume is set as 5 mm. In natural boudary condition, experimental coefficient for surface transfer rate α in Eq.(3) is set as 10^{-9} m/s. This value is determined by trial and error so that calculated time-dependent chloride profile based on this value is adequate in any cases.

Table 3 Boundary condition models

Method	Boundary Condition
1	$C(0, t) = C_0$
2	$C(0, t) = C_0(t)$
3	$J = \alpha(C(0,t)-C_{ext})$

In fact, chloride profiles in all specimens were calculated. There was, however, no significant difference in qualitative tendencies among calculation results of six specimens. Therefore, only result of specimen H-40 is presented in Fig. 10.

There was no remarkable difference among the calculation results by method 1, 2 and 3 in Fig. 10. All methods can more or less simulate experimental chloride profiles in both short and long time. In detail, the method 2 can estimate chloride content near the surface better than method 1 because of time-dependent surface chloride. Calculated chloride profiles by method 2 and 3 are similar with each other.

It should be noted that surface chloride and diffusion coefficient adopted here had been derived from the same laboratory test data used in the verification. It is necessary to verify the method using data by actual structure under real environment in further study.

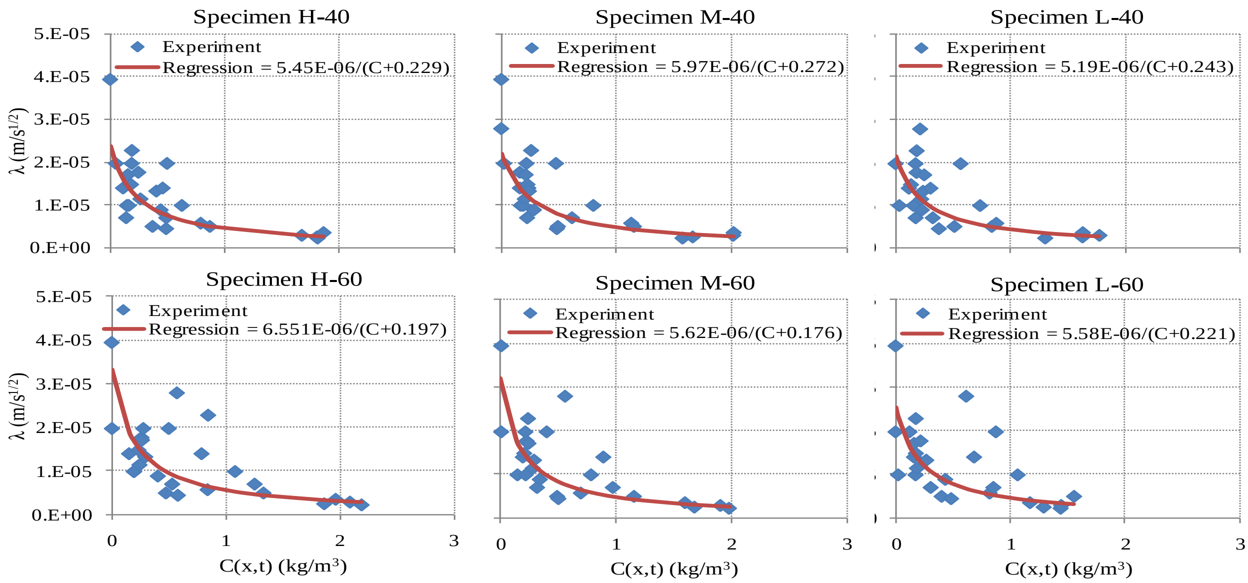

Fig. 8 Experimental $\lambda(C)$ and its regression curve

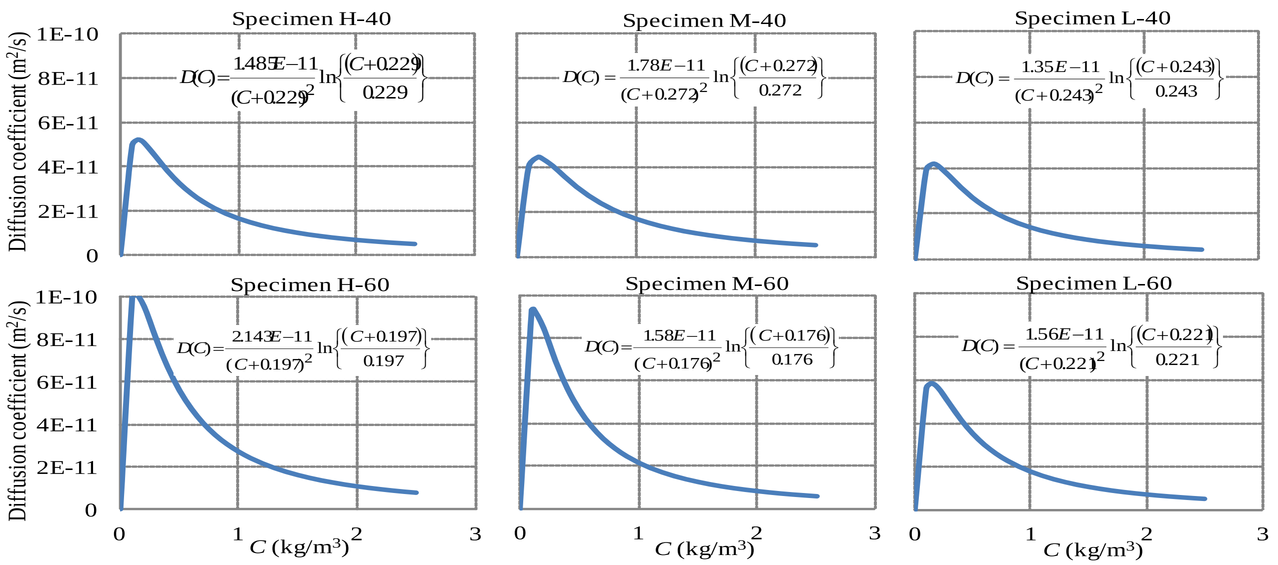

Fig. 9 Concentration-dependent diffusion coefficient *D(C)* by Boltzman-Matano method

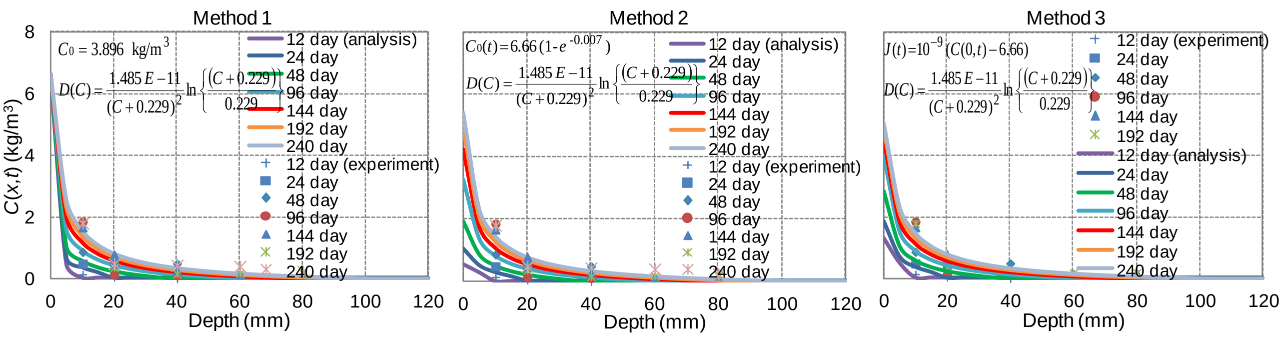

Fig. 10 Calculated time-dependent chloride profiles in specimen H-40

7. SENSITIVITY ANALYSIS ON CURVE OF DIFFUSION COEFFICIENT

The configuration of curve of concentration-dependent diffusion coefficient $D(C)$ is dependent of the configuration of $\lambda(C)$, for which Eq.(7) was adopted. The obtained curve of $D(C)$ has a peak around C = 0.1 kg/m^3. However, the physical meaning of this peak is not clear. In order to investigate the influence of pre-peak part of the curve on calculated results, comparative calculation is conducted. Three types of $D(C)$ curve in Fig. 11, which are original curve, flat and curve and exponential curve, were examined.

Concentration-dependent diffusion coefficient named as flat and curve is composed of two parts expressed by Eq. (9) and (10).

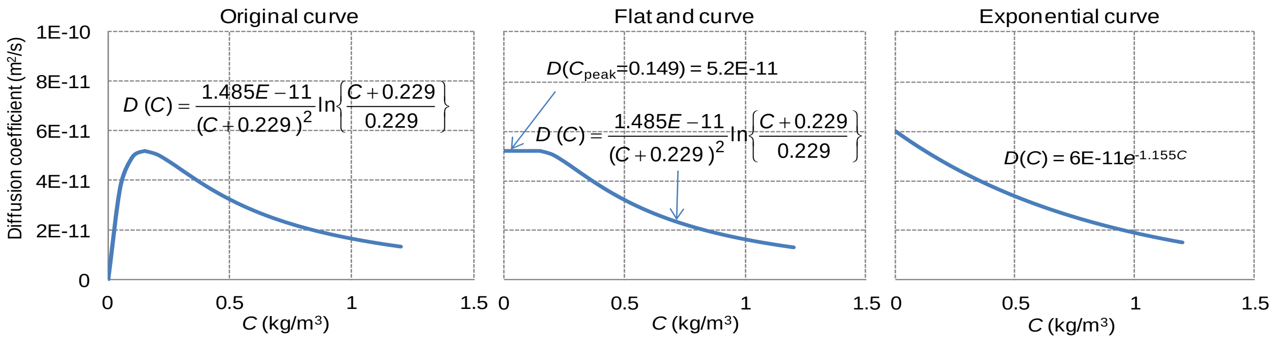

Fig. 11 Three types of $D(C)$ examined

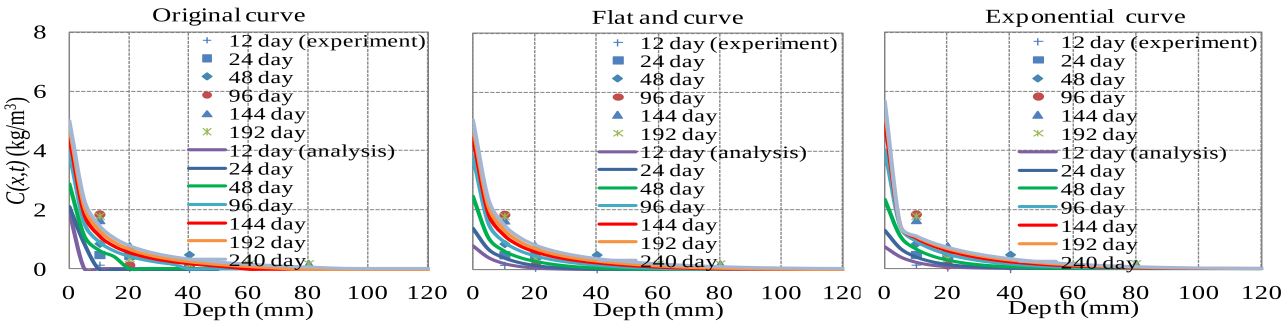

Fig. 12 Chloride profiles in specimen H-40 calculated by three types of $D(C)$

for $0 \le C \le C_{peak}$

$$D(C) = D(C_{peak}) = \frac{v^2}{4w^2e^1} \tag{9}$$

for $C \ge C_{peak}$

$$D(C) = \frac{0.5v^2}{(C+w)^2}\ln\left\{\frac{C+w}{w}\right\} \tag{10}$$

Exponential curve is an approximation of post-peak part of the original $D(C)$ curve.

Calculated time-dependent chloride profiles in specimen H-40 by three types of $D(C)$ are shown in Fig. 12. The results by three methods are similar with one another. Therefore, the pre-peak part of $D(C)$ curve doesn't much affect the chloride profile. The pre-peak part of $D(C)$ is only attributable to the mathematical expression of $\lambda(C)$ by Eq.(7) with less physical importance. Consequently, the important characteristic of $D(C)$ is its post-peak part.

8. CONCLUSIONS

(1) Diffusion coefficient as a function of chloride content in concrete was derived from the exposure test results by the wind tunnel.

(2) Chloride penetration analysis based on concentration-dependent diffusion coefficient with constant surface chloride as boundary condition can estimate chloride profiles in concrete adequately.

(3) Chloride penetration analysis based on concentration-dependent diffusion coefficient with time-dependent surface chloride as boundary condition can estimate chloride profiles better than constant surface chloride particularly at early stage.

(4) The calculated chloride profiles based on concentration-dependent diffusion coefficient with natural type of boundary condition were similar with that based on time-dependent surface chloride as boundary condition.

ACKNOWLEDGEMENTS

The authors wish to express their gratitude to Mr. Kamiura, Mr. Aoki and Mr. Fukuchi, former graduate students of Nagaoka University of Technology, for their contribution in both experimental and analytical work.

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