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**Autor:** Liang, Ming-Te / Hong, Chao-liang / Liang, Chih-Hsin  
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## Mathematical Modeling and Prediction Method of Concrete Carbonation

Ming-Te LIANG  
Associate Professor  
Taiwan Ocean University  
Keelung, Taiwan

Ming-te Liang, born 1948.  
received his Ph.D. from  
Aberdeen University in 1986.

Chao-liang HONG  
Hong Post Graduate  
Taiwan Ocean University  
Keelung, Taiwan

Chao-liang Hong  
received his Master degree from  
Taiwan Ocean University in 1998.

Chih-Hsin LIANG  
Structural Engineer,  
Sinotech Engineering Consultants Ltd  
Taipei, Taiwan

Chih-hsin Liang, born in 1963.  
received his Master degree from  
Center University in 1991.

### Summary

This carbonation process of concrete is principally a diffusion phenomenon. The penetration rate of carbon dioxide depends mainly on the concrete quality and the exposure condition. Based on both the Fick first and second laws of linear diffusion equations, the three-dimensional equation of conservation of mass is derived. This equation can be reduced to two- and one-dimensional equations of conservation of mass for which provide to predict the carbonation depth beneath the corner and the general surface of concrete structures. The result of present study indicates that the maximum carbonation depth of concrete at corner is large than  $\sqrt{2}$  times that of general surface under the conditions of homogeneous, isotropic and noncrack concrete. The carbonation depth predicted by the statistical method have to use large data and should be multiplied the modified coefficient for obtaining the approximate result.

### 1. Introduction

The reinforcing steel bars embedded in concrete are protected from corrosion by a thin oxide film that forms on their surface due to the highly alkaline, with pH values above 12.5, environment of the surrounding concrete. This alkalinity is due to calcium hydroxide ( $Ca(OH)_2$ ) produced during the reaction between water and the constituents of cement which occurs the hardening and development of strength of cement and concrete. Carbon dioxide ( $CO_2$ ) in the air penetrates concrete and reduces the pH value to less than 11, rendering it conducive to the corrosion of embedded reinforcing steel bars which cause concrete to spall or split. This process is called carbonation and is principally a diffusion phenomenon and the rate of penetration of  $CO_2$  depends mainly on the concrete quality and the exposure condition.

The objectives of this paper are to determine the carbonation depth at the surface and the corner of a concrete member and to predict the carbonation depth by using a statistical method. In order to investigate the concrete carbonation problem, the three-dimensional equation of carbonation of mass based on the Fick second law can be reduced to a one-dimensional diffusion equation of which the solution is simplified as an empirical formula. This empirical formula associated with the statistical method can predict the carbonation depth of the concrete.

## 2. Mathematical modeling of concrete carbonation

Assume that concrete is a kind of homogeneous and isotropic material and is free of crack. According to Fick's first law and applying the concept of mass conservation, the mass flux per unit volume (Fig. 1) is written in the three-dimensional equation of conservation of mass as

$$\frac{\partial C}{\partial t} + \frac{\partial \eta_{CO_2,x}}{\partial x} + \frac{\partial \eta_{CO_2,y}}{\partial y} + \frac{\partial \eta_{CO_2,z}}{\partial z} = \gamma_{CO_2} \quad (1)$$

where  $C$  is the  $CO_2$  mass of unit volume concrete, i. e.,  $CO_2$  concentration,  $\eta_{CO_2,x}$ ,  $\eta_{CO_2,y}$ ,  $\eta_{CO_2,z}$  the mass flux of  $CO_2$  in the x-, y-, z-direction, respectively,  $t$  time and  $\gamma_{CO_2}$  the absorbed  $CO_2$  mass per unit volume per unit time or the absorbed  $CO_2$  velocity per unit volume. Eq. (1) can be expressed in terms of vector form

$$\frac{\partial C}{\partial t} + \nabla \cdot \eta_{CO_2} = \gamma_{CO_2} \quad (2)$$

Where  $\nabla$  the Laplacian operator.

The reduction of Eq. (2) into two-dimensional case (see Fig. 2) is

$$\frac{\partial C}{\partial t} = D \nabla^2 C + \gamma_{CO_2} \quad (3)$$

where  $\eta_{CO_2,x} = -D \frac{\partial C}{\partial x}$ ,  $\eta_{CO_2,y} = -D \frac{\partial C}{\partial y}$  and  $D$  is the diffusion coefficient of  $CO_2$  in the concrete. Fig. 3 show that the cross-sectional area of concrete located in the air can be divided into carbonated, carbonation reaction and uncarbonated zones. In the carbonated zone, the reduction of concrete absorbed  $CO_2$  has been finished, i. e.,  $\gamma_{CO_2} = 0$  in Eq. (3). Thus, Eq. (3) changes to

$$\frac{\partial C}{\partial t} = D \nabla^2 C \quad (4)$$

Eq. (4) is called the Fick second law of linear diffusion equation.

Assume that the ability of concrete absorbed  $CO_2$  in unit volume is  $m_0$  ( $kg/m^3$ ). Using the



Fick first law, the carbonation front in reaction zone at any time  $t$  is

$$m_0 dx_0 dy_0 = -D \left[ dy_0 \frac{\partial C}{\partial x} \Big|_{(x_0, y_0)} + dx_0 \frac{\partial C}{\partial y} \Big|_{(x_0, y_0)} \right] dt \quad (5)$$

Consider the carbonation front  $x_{j0}$  at  $x_0 = y_0$  at any time  $t$ . We know

$$\frac{\partial C}{\partial x} \Big|_{(x_0=y_0)} = \frac{\partial C}{\partial y} \Big|_{(x_0=y_0)} = -\frac{C_0}{x_0} = -\frac{C_0}{y_0} \quad (6)$$

where  $C_0$  is  $CO_2$  concentration at the outer edge of cross section of concrete structures.

The substitution of Eq. (6) into Eq. (5) yields

$$m_0 dx_0 = 2D \frac{C_0}{x_0} dt \text{ or } m_0 dy_0 = 2D \frac{C_0}{y_0} dt \quad (7)$$

with initial condition  $x_0 = 0$  and  $y_0 = 0$  when  $t = 0$  (Chiu, 1995). We obtain the solution of Eq. (7)

$$x_{j0} = 2 \sqrt{\frac{DC_0}{m_0} t} = B\sqrt{t} \quad (8)$$

where  $B = 2 \sqrt{\frac{DC_0}{m_0}}$  is the coefficient of carbonation rate at the corner of the concrete structure.

Eq. (5) can be reduced into a one-dimensional problem as shown in Fig. 4 and can be written as

$$m_0 dx_0 = -D \frac{\partial C}{\partial x_0} \Big|_{x_0} dt \quad (9)$$

Consider the depth of carbonation front at time  $t$ . We know

$$\frac{\partial C}{\partial x_0} \Big|_{x_0} = -\frac{C_0}{x_0} \quad (10)$$

Substituting Eq. (10) into Eq. (9) and considering the initial condition (Tsaour, 1989), we have

$$\frac{dx_0}{dt} = \frac{DC_0}{m_0} \frac{1}{x_0}, \quad x_0 = 0 \text{ when } t = 0 \quad (11)$$

We obtain the solution of Eq. (11)

$$x_0 = \sqrt{\frac{2DC_0}{m_0} t} = A\sqrt{t} \quad (12)$$

where  $A = \sqrt{\frac{2DC_0}{m_0}}$  is the coefficient of carbonation rate under the general surface of concrete structures.

Comparing Eq. (8) with Eq. (12), we get

$$B = \sqrt{2}A \quad (13)$$

Eq. (13) denotes that the maximum carbonation depth of concrete structures at corner is large than  $\sqrt{2}$  times that of the general surface of concrete structures.

### 3. The prediction of concrete carbonation by using statistical method

Under the condition control, we take  $n$  number of  $A_i$  samples and draw the frequency distribution diagram. Based on the frequency distribution diagram, the model of statistical analysis is provided and is verified by the chi-square test or the Kolmogorov-Smirnov test (Ang and Tang, 1975). The value of  $A_i$  is determined by the carbonation depth  $x_i$  of the  $i$ th measurement point, i.e.,  $A_i = x_i / \sqrt{t}$ . Chiu (1995) studied the distribution of coefficient of carbonation rate carbonation coefficient  $A$  and pointed out that  $A$  obeyed the normal distribution  $N(\mu, \sigma)$ , where  $\mu$  is mean value and  $\sigma$  is standard deviation. Thus, the one-dimensional carbonation depth of concrete structure is  $x_0(t)$ ,  $t \in [0, T_s]$ , where  $T_s$  is a determined time. The normal probability density function at any time  $t$  is

$$f(x_0, t) = \frac{1}{\sqrt{2\pi}\sigma_A} \exp\left[-\frac{(x_0 - \mu_A\sqrt{t})^2}{2t\sigma_A^2}\right] \quad (14)$$

where  $\mu_A\sqrt{t}$  is mean value and  $\sqrt{t}\sigma_A$  is standard deviation.  $f(x_0, t)$  determines the possible result of  $x_0$  at any time  $t$ . According to a certain insurance rate  $P$ , the constant of  $\beta$  corresponding to  $P$  is determined from the table of standard normal probability. The depth of concrete carbonation beneath the general surface after service life  $t$  years is

$$x_{p|t} = (\mu_A + \beta\sigma_A)\sqrt{t} \quad (15)$$

Similarly, we can derive the depth of concrete carbonation at the corner after service life  $t$  years is

$$x_{p|t} = (\mu_A + \beta\sigma_A)\sqrt{2t} \quad (16)$$

### 4. Application

The coefficient of carbonation rate  $A$  of a bridge in Taipei city with water-cement 0.45 and concrete compressive strength  $f'_c = 45 \text{ MPa}$  obeyed the normal distribution  $N(\mu_A, \sigma_A) = N(17.32, 5.1)$  ( Fig. 5 ) and the concrete carbonation depth is of insurance rate 95%



(i. e.,  $p = 0.95$ ,  $\beta = 1.645$  obtained from the table of standard normal probability) after using 50 years in service. Then, we obtain from Eq. (15)

$$x_{0.95|50} = (17.32 + 1.645 \times 5.1)\sqrt{50} = 181.79(\text{mm})$$

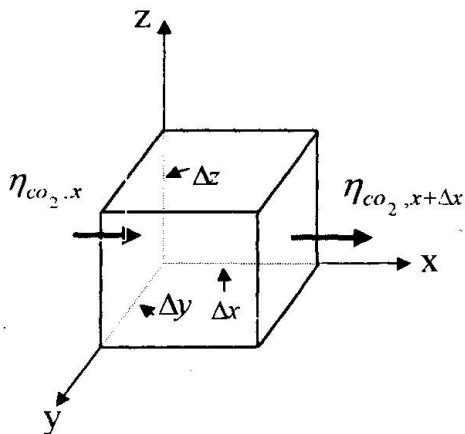
This means that the carbonation depth under general concrete surface is 181.79 mm after service life 50 years. Similarly, the carbonation depth at the concrete corner after using 50 years can be estimated from Eq. (16) as

$$x_{0.95|50} = (17.32 + 1.645 \times 5.1)\sqrt{2 \times 50} = 257.09(\text{mm})$$

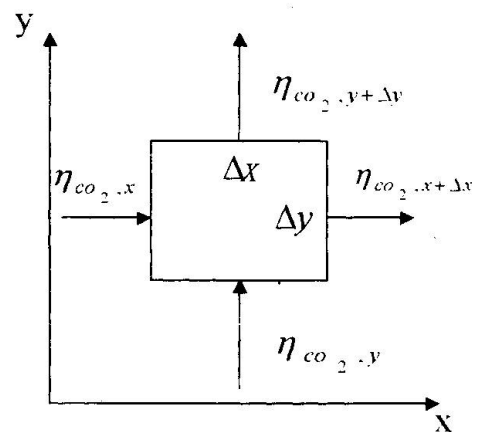
Both carbonation depths mentioned above are obvious too large. This may be due to that only the 12 test samples bored from bridge are used for statistical prediction.

## 5. Conclusion

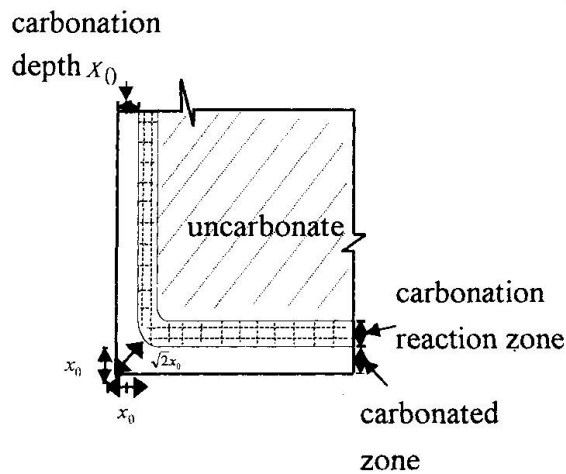
The carbonation depth is an important index for estimating both the damage and durability of concrete structures. This paper has presented the mathematical modeling and prediction methods of the carbonation depth for the concrete structures without any crack. It should be noted that the present study provides the maximum carbonation depth of concrete structures at corner is large than  $\sqrt{2}$  times that of the general surface of concrete structures. In addition, the carbonation depth predicted by the statistical method must use large data and may be multiplied the modified coefficient for obtaining the approximate result.



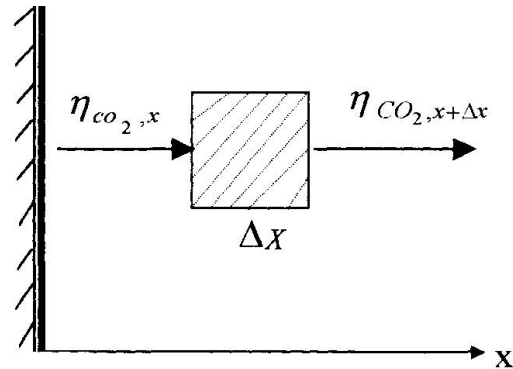
**Fig. 1 Mass flux of x direction in a three-dimensional control element**



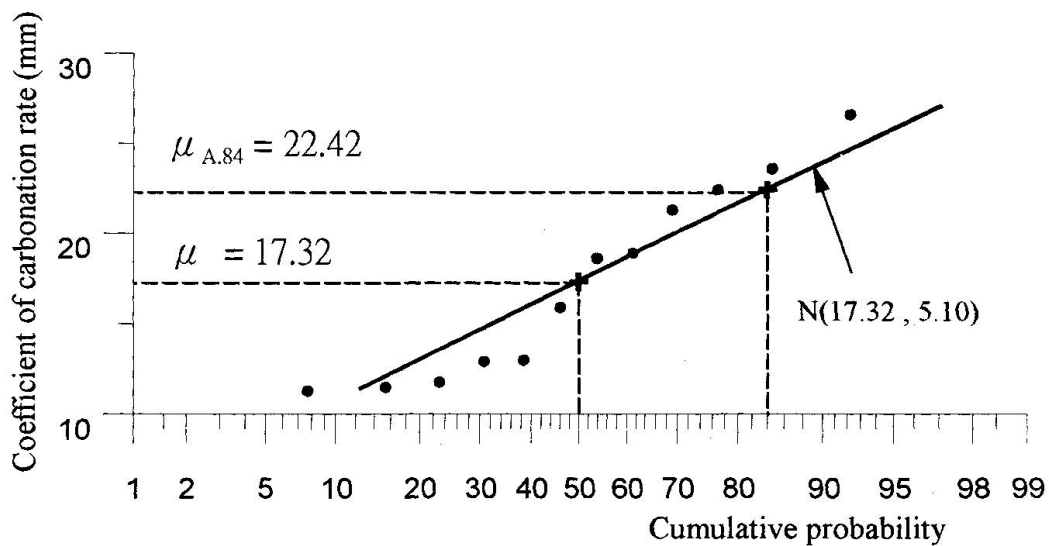
**Fig. 2 CO<sub>2</sub> mass flux in the x- and y-direction**



**Fig. 3 Carbonation distinguish of concrete**



**Fig. 4 CO<sub>2</sub> mass flux in the x-direction**



**Fig 5 Coefficient of carbonation rate plotted on normal probability paper**

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