JURNAL MATEMATIKA, STATISTIKA & KOMPUTASI E-ISSN: 2614-8811
https://journal.unhas.ac.id/index.php/jmsk/index
Vol. 17, No. 3, 405-417, May, 2021
DOI: 10.20956/j.v17i3.12227

A Two-Dimensional Mathematical Model of Carbon Dioxide (CO_2) Transport in Concrete Carbonation Process

M N Hidayat[1], J Kusuma[2], and N Aris[3]

Abstract

A new two-dimensional mathematical model was developed to describe the transport phenomena of carbon dioxide in concrete structures. By treating transport phenomena as a concrete carbonation process, a two-dimensional linear partial differential equation was derived based on the principle of mass balance and convective-dispersive Equation. It was found the analytical solution by the separation of variables method combined with some substitution approaches. The numerical results from the analytical or exact solution are presented to illustrate the practical application of this model.

Keywords: Concrete carbonation, carbon dioxide, transport phenomena, diffusion equation, and separation of variables method.

1. INTRODUCTION

Carbonation in concrete is very costly and has a significant impact on the economies of industrial nations. A 2002 study by Koch *et al.* (see [2]) reported that the annual direct cost of corrosion on U.S. highway bridges was estimated at $8.3 billion overall, with $4.0 billion the capital cost and maintenance of reinforced concrete highway bridge decks and substructures. Indirect costs due to traffic delays were calculated to be more than ten times the direct costs.

There are numerous studies on concrete carbonation investigations, aiming at developing empirical or semiempirical relations for the prediction of the rate carbonation (see [5]), and the service life of reinforced concrete under chloride environment (see [1]). Using statistical modelling, Silva *et al.* [6] investigated the estimation of the carbonation coefficient, and consequently the carbonation as a function of the variables considered statistically significant in explaining the concrete carbonation phenomenon. Based on physio-chemical mechanisms, Zhang [7] proposed a mathematical model of carbonation process in porous concrete materials. Liang and Lin [3] was developed a one-dimensional mathematical model to describe the transport phenomena of carbon dioxide in concrete structures. This model helps to identify the materials and environmental parameters that affect the rate of carbonation and can be used for parametric studies of their effect on this rate.

In this paper, we developed mathematical modeling of carbon dioxide transport in the concrete carbonation process into a two-dimensional linear partial differential equation. We found the analytical or exact solution by the separation of variables method combined with some

[1,2,3] *Department of Mathematics, Hasanuddin University, Indonesia*
E-mail: *muh.nurhidayat378@gmail.com[1], jeffry.kusuma@gmail.com[2], and newima@gmail.com[3]*

substitution approaches. Later, the numerical results are presented to illustrate the practical application of this model.

2. THEORETICAL MODELING OF CONCRETE CARBONATION

The rate at which carbon dioxide (CO_2) enters into concrete structures can be decided utilizing several transport components. These instruments regularly act at the same time on the concrete structures and may incorporate such forms as convection, diffusion, dispersion, and first-order production or decay. Liang and Lin [3] proposed a one-dimensional mathematical model using these factors. The mathematical model considers the relationships among unsteady state and diffusion, pore-water convective effect and chemical reaction and is shown in Table 1 in Liang and Lin [3].

Similarly, two-dimensional transport phenomena of concrete carbonation can be developed as:

$$R\frac{\partial C(x,y,t)}{\partial t} = D_s\left(\frac{\partial^2 C(x,y,t)}{\partial x^2} + \frac{\partial^2 C(x,y,t)}{\partial y^2}\right) - v\left(\frac{\partial C(x,y,t)}{\partial x} + \frac{\partial C(x,y,t)}{\partial y}\right) - K_T C(x,y,t) - r, \qquad (2.1)$$

where C is the concentration of carbon dioxide, D_s is the diffusion coefficient, R is the retardation factor (dimensionless), v is the pore-water velocity, K_T is the rate constant for first-order decay at a given temperature T, r is the rate constant for zero-order production, x, y is space and t is time.

Initial and boundary conditions are $C(x,y,0) = C_i, C(0,y,t) = C_a, C(m,y,t) = C_b, C(x,0,t) = C_c, C(x,n,t) = C_d$ where $C_i, C_a, C_b, C_c,$ and C_d are the initial concentration of carbon dioxide in concrete, on the surface of the concrete structures, and at the interface between the concrete and steel, respectively. m, n are the concrete cover thickness on the reinforcing steel.

Assuming $R = 1$ (This means that the carbonation phenomenon is only concerned in this study) and $r = 0$ (This means that in the carbonated zone the reduction of concrete absorbed CO_2 has been finished, in other words, the absorbed CO_2 mass per unit volume per unit time equal zero), Equation (2.1) becomes

$$\frac{\partial C(x,y,t)}{\partial t} = D_s\left(\frac{\partial^2 C(x,y,t)}{\partial x^2} + \frac{\partial^2 C(x,y,t)}{\partial y^2}\right) - v\left(\frac{\partial C(x,y,t)}{\partial x} + \frac{\partial C(x,y,t)}{\partial y}\right) - K_T C(x,y,t). \qquad (2.2)$$

3. THE ANALYTICAL SOLUTIONS

In order to solve the concrete carbonation problem modeled by Equation (2.2), first of all, one assumes

$$C(x,y,t) = e^{\alpha x+\beta y+\gamma t}\phi(x,y,t), \qquad (3.1)$$

where α, β and γ are the constant parameters. $\phi(x,y,t)$ is a new function of CO_2 concentration.

By this assumption, we will eliminate each and every one of these objections with a suitable change of variables. The plan is to change variables to reduce the equation (2.2) to the diffusion equation, and then to use the known solution of the diffusion equation to represent the solution, and change variables back. This is a standard technique of solution in partial differential equations, and none of the transformations we are making are strange, unmotivated, or unknown.

Substitution Equation (3.1) into Equation (2.2) gives

$$\frac{\partial \phi}{\partial t} = D_s\left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2}\right) + (2\alpha D_s - v)\frac{\partial \phi}{\partial x} + (2\beta D_s - v)\frac{\partial \phi}{\partial y} + (D_s(\alpha^2 + \beta^2) - v(\alpha + \beta) - K_T - \gamma)\phi. \tag{3.2}$$

To reduce Equation (3.2) as a standard form of the two-dimensional diffusion equation, the coefficients of the second, third, and fourth terms on the right-hand side should be equal to zero, in other words,

$$2\alpha D_s - v = 2\beta D_s - v = D_s(\alpha^2 + \beta^2) - v(\alpha + \beta) - K_T - \gamma = 0.$$

Simplified, one obtains

$$\alpha = \beta = \frac{v}{2D_s}, \gamma = -\left(\frac{v^2}{2D_s} + K_T\right).$$

The solution method of Separation of Variables is described in the following.

3.1. Separation of Variables Method

Now the problem formulated by Equation (3.2) changes into the control equation with initial and boundary conditions.

$$\frac{\partial \phi}{\partial t} = D_s\left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2}\right) \tag{3.3}$$

$$\phi(x, y, 0) = C_i e^{-\alpha x - \beta y} \tag{3.4}$$

$$\phi(0, y, t) = C_a e^{-\beta y - \gamma t} \tag{3.5}$$

$$\phi(m, y, t) = C_b e^{-\alpha m - \beta y - \gamma t} \tag{3.6}$$

$$\phi(x, 0, t) = C_c e^{-\alpha x - \gamma t} \tag{3.7}$$

$$\phi(x, n, t) = C_d e^{-\alpha x - \beta n - \gamma t}. \tag{3.8}$$

For solving the problem of concrete carbonation modeled by Equations (3.3) – (3.8), we must modify the problem in order to introduce homogenous boundary conditions to the problem. We do this by using the physical observance that as $t \to \infty$, the concrete's temperature does not depend on t. Hence,

$$\lim_{t\to\infty} \phi(x, y, t) = \varphi(x, y),$$

where we call $\varphi(x, y)$ in the above Equation the **steady-state temperature.** Therefore, we let

$$\phi(x, y, t) = \Phi(x, y, t) + \varphi(x, y), \tag{3.9}$$

where $\Phi(x, y, t)$ is called the **variable or transient temperature.**
Substitution Equation (3.9) into Equations (3.3) – (3.8) yields

$$\frac{\partial \Phi}{\partial t} = D_s\left(\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2}\right) + D_s\left(\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2}\right) \tag{3.10}$$

$$\phi(x,y,0) = \Phi(x,y,0) + \varphi(x,y) \quad (3.11)$$
$$\phi(0,y,t) = \Phi(0,y,t) + \varphi(0,y) = C_a e^{-\beta y-\gamma t} \quad (3.12)$$
$$\phi(m,y,t) = \Phi(m,y,t) + \varphi(m,y) = C_b e^{-\alpha m-\beta y-\gamma t} \quad (3.13)$$
$$\phi(x,0,t) = \Phi(x,0,t) + \varphi(x,0) = C_c e^{-\alpha x-\gamma t} \quad (3.14)$$
$$\phi(x,n,t) = \Phi(x,n,t) + \varphi(x,n) = C_d e^{-\alpha x-\beta n-\gamma t}. \quad (3.15)$$

One chooses $\varphi(x,y)$ as a solution to the problem. We get two-dimensional Laplace's Equation with nonhomogeneous boundary conditions. Notice that, for concrete carbonation problems, where the diffusion process runs from the outside to the in. The exterior's initial state is always the same so that the function t can be considered constant and is combined to the constant values of C_a, C_b, C_c, and C_d in Equations (3.17) – (3.20)

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} = 0 \quad (3.16)$$
$$\varphi(0,y) = C_a e^{-\beta y-\gamma t} \quad (3.17)$$
$$\varphi(m,y) = C_b e^{-\alpha m-\beta y-\gamma t} \quad (3.18)$$
$$\varphi(x,0) = C_c e^{-\alpha x-\gamma t} \quad (3.19)$$
$$\varphi(x,n) = C_d e^{-\alpha x-\beta n-\gamma t}. \quad (3.20)$$

The solution method of Laplace's Equation of Separation of Variables is described in the following.

3.1.1. The Solution of Laplace's Equation

Let us notice that while the partial differential equation is both linear and homogenous, the boundary conditions are only linear and are not homogenous. This boundary creates a problem because the separation of variables requires homogenous boundary conditions. To completely solve Laplace's Equation, we are going to have to solve it four times. Each time we solve it, only one of the four boundary conditions can be nonhomogeneous, while the remaining three will be homogeneous. The following equations show the four problems.

$$\frac{\partial^2 \varphi_1}{\partial x^2} + \frac{\partial^2 \varphi_1}{\partial y^2} = 0, \varphi_1(x,0) = f_1, \varphi_1(0,y) = \varphi_1(m,y) = \varphi_1(x,n) = 0 \quad (3.21)$$
$$\frac{\partial^2 \varphi_2}{\partial x^2} + \frac{\partial^2 \varphi_2}{\partial y^2} = 0, \varphi_2(0,y) = f_2, \varphi_2(x,0) = \varphi_2(m,y) = \varphi_2(x,n) = 0 \quad (3.22)$$
$$\frac{\partial^2 \varphi_3}{\partial x^2} + \frac{\partial^2 \varphi_3}{\partial y^2} = 0, \varphi_3(x,n) = g_1, \varphi_3(0,y) = \varphi_3(m,y) = \varphi_3(x,0) = 0 \quad (3.23)$$
$$\frac{\partial^2 \varphi_4}{\partial x^2} + \frac{\partial^2 \varphi_4}{\partial y^2} = 0, \varphi_4(m,y) = g_2, \varphi_4(0,y) = \varphi_4(x,0) = \varphi_4(x,n) = 0, \quad (3.24)$$

where
$f_1(x) = C_c e^{-\alpha x-\gamma t}, f_2(y) = C_a e^{-\beta y-\gamma t}, g_1(x) = C_d e^{-\alpha x-\beta n-\gamma t}, g_2(y) = C_b e^{-\alpha m-\beta y-\gamma t}$.
Now, once we solve all four of these problems the solution to our original system, will be

$$\varphi(x,y) = \varphi_1(x,y) + \varphi_2(x,y) + \varphi_3(x,y) + \varphi_4(x,y).$$

First, we are going to solve Equation (3.21)
Start by assuming that our solution will be in the form,

$$\varphi_1 = X(x)Y(y), \tag{3.25}$$

where $X(x)$ and $Y(y)$ are the functions of the independent variables of x and y, respectively. Substituted Equation (3.25) into Equation (3.21), one obtains

$$\frac{X''(x)}{X(x)} = -\frac{Y''(y)}{Y(y)} = K, \tag{3.26}$$

where K is an unknown constant.
Equation (3.26) and the boundary conditions from Equation (3.21) can be rewritten as two ordinary differential equations that we will need to solve.

$$X'' - KX = 0, X(0) = 0, X(m) = 0 \tag{3.27}$$
$$Y'' + KY = 0, Y(n) = 0. \tag{3.28}$$

We have three cases to deal with, and only $K < 0$ came up with the nontrivial solution.
Now, one assumes $K = -\lambda^2$.
From Equation (3.27), we have

$$\lambda = \frac{p\pi}{m}, K = -(\lambda)^2 = -\left(\frac{p\pi}{m}\right)^2, p = 0,1,2,3, \dots$$

and

$$X(x) = A\sin\left(\frac{p\pi x}{m}\right). \tag{3.29}$$

Substituting $K = -\left(\frac{p\pi}{m}\right)^2$ into Equation (3.28). The general solution for Equation (3.28) is

$$Y(y) = B\sinh\frac{p\pi}{m}(y-n). \tag{3.30}$$

Substituting Equations (3.29) and (3.30) into Equation (3.25), one obtains

$$\varphi_1(x,y) = E\sin\left(\frac{p\pi x}{m}\right)\sinh\left(\frac{p\pi}{m}(y-n)\right),$$

where $E = AB$ is constant.
Using The principle of Superposition, we get

$$\varphi_1(x,y) = \sum_{p=0}^{\infty} E_p \sin\left(\frac{p\pi x}{m}\right)\sinh\left(\frac{p\pi}{m}(y-n)\right). \tag{3.31}$$

Substituting the initial condition in Equation (3.21) into Equation (3.31), one has

$$f_1(x) = \sum_{p=0}^{\infty} F_p \sin\left(\frac{p\pi x}{m}\right), \tag{3.32}$$

where $F_p = -E_p \sinh\left(\frac{p\pi n}{m}\right)$.
Equation (3.32) is the Fourier sine series. Thus, one chooses

$$F_p = \frac{2}{m}\int_0^m \sin\left(\frac{p\pi x}{m}\right) f_1(x)dx. \tag{3.33}$$

Because $F_p = -E_p \sinh\left(\frac{p\pi n}{m}\right)$, we get

$$E_p = \frac{-2}{m\sinh\left(\frac{p\pi n}{m}\right)} \int_0^m \sin\left(\frac{p\pi x}{m}\right) f_1(x)dx. \tag{3.34}$$

Substituting Equation (3.34) into (3.31), yields

$$\varphi_1(x,y) = \sum_{p=0}^{\infty}\left(\left[\frac{-2}{m\sinh\left(\frac{p\pi n}{m}\right)}\int_0^m \sin\left(\frac{p\pi\xi}{m}\right) f_1(\xi)d\xi\right]\sin\left(\frac{p\pi x}{m}\right)\sinh\left(\frac{p\pi}{m}(y-n)\right)\right). \tag{3.35}$$

The next three problems are similar to the first problem, one obtains

$$\varphi_2(x,y) = \sum_{p=0}^{\infty}\left\{\frac{-2}{n\sinh\left(\frac{p\pi m}{n}\right)}\int_0^n \sin\left(\frac{p\pi\zeta}{n}\right) f_2(\zeta)d\zeta\right\}\sin\left(\frac{p\pi y}{n}\right)\sinh\left(\frac{p\pi}{n}(x-m)\right) \tag{3.36}$$

$$\varphi_3(x,y) = \sum_{p=0}^{\infty}\left\{\frac{2}{m\sinh\left(\frac{p\pi n}{m}\right)}\int_0^m \sin\left(\frac{p\pi\xi}{m}\right) g_1(\xi)d\xi\right\}\sin\left(\frac{p\pi x}{m}\right)\sinh\left(\frac{p\pi y}{m}\right) \tag{3.37}$$

$$\varphi_4(x,y) = \sum_{p=0}^{\infty}\left\{\frac{2}{n\sinh\left(\frac{p\pi m}{n}\right)}\int_0^n \sin\left(\frac{p\pi\zeta}{n}\right) g_2(\zeta)d\zeta\right\}\sin\left(\frac{p\pi y}{n}\right)\sinh\left(\frac{p\pi x}{n}\right). \tag{3.38}$$

After solving the integral, adding Equations (3.35) – (3.38), and change back the value of the boundary conditions, we get the general solution of the Laplace's Equation.

$$\begin{aligned}\varphi(x,y) = \sum_{p=0}^{\infty} \sin\left(\frac{p\pi x}{m}\right)\Bigg\{&\left\{\frac{-2C_c p\pi e^{-\gamma t}(1-e^{-\alpha m}\cos(p\pi))}{\sinh\left(\frac{p\pi n}{m}\right)((\alpha m)^2+(p\pi)^2)}\right\}\sinh\left(\frac{p\pi}{m}(y-n)\right) \\ &+\left\{\frac{-2C_d p\pi e^{-\beta n-\gamma t}(1-e^{-\alpha m}\cos(p\pi))}{\sinh\left(\frac{p\pi n}{m}\right)((\alpha m)^2+(p\pi)^2)}\right\}\sinh\left(\frac{p\pi y}{m}\right)\Bigg\} \\ &+\sin\left(\frac{p\pi y}{n}\right)\Bigg\{\left\{\frac{-2C_b p\pi e^{-\alpha m-\gamma t}(1-e^{-\beta n}\cos(p\pi))}{\sinh\left(\frac{p\pi m}{n}\right)((\beta n)^2+(p\pi)^2)}\right\}\sinh\left(\frac{p\pi}{n}(x-m)\right) \\ &+\left\{\frac{-2C_a p\pi e^{-\gamma t}(1-e^{-\beta n}\cos(p\pi))}{\sinh\left(\frac{p\pi m}{n}\right)((\beta n)^2+(p\pi)^2)}\right\}\sinh\left(\frac{p\pi x}{n}\right)\Bigg\}.\end{aligned} \quad (3.39)$$

3.2. Solution of Diffusion Equation with Homogenous Boundary Conditions
From Equations (3.10) – (3.15), one has

$$\frac{\partial \Phi}{\partial t} = D_s\left(\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2}\right) \quad (3.40)$$

$$\Phi(x,y,0) = \phi(x,y,0) - \varphi(x,y) = C_i e^{-\alpha x - \beta y} - \varphi(x,y) = f(x,y) \quad (3.41)$$

$$\Phi(0,y,t) = 0 \quad (3.42)$$

$$\Phi(m,y,t) = 0 \quad (3.43)$$

$$\Phi(x,0,t) = 0 \quad (3.44)$$

$$\Phi(x,n,t) = 0. \quad (3.45)$$

In order to solve the concrete carbonation problem modeled by Equations (3.40) – (3.45), the separation of variables method is used, in other words,

$$\Phi(x,y,t) = X(x)Y(y)T(t), \quad (3.46)$$

where $X(x), Y(y)$ and $T(t)$ are the functions of the independent variables of x, y and t, respectively. Substituted Equation (3.27) into Equation (3.21), one obtains

$$XYT' = D_s(X''YT + XY''T). \quad (3.28)$$

Equation (3.28) can be written as

$$\frac{T'}{D_s T} = \frac{X''}{X} + \frac{Y''}{Y} = -k^2, \quad (3.29)$$

where $k > 0$ is an unknown constant to be determined.
Equation (3.30) can be rewritten as three ordinary differential equations.

$$T' + D_s k^2 T = 0 \quad (3.30)$$

$$X'' + p^2 X = 0 \quad (3.31)$$

$$Y'' + q^2 Y = 0, \tag{3.32}$$

where $q^2 = k^2 - p^2$, $p > 0$, and $q > 0$ are others constant.
The general solution of the Equations (3.30) - (3.32) is

$$T(t) = A_1 e^{(-D_s k^2 t)} \tag{3.33}$$
$$X(x) = A_2 \cos(px) + B_2 \sin(px) \tag{3.34}$$
$$Y(y) = A_3 \cos(qy) + B_3 \sin(qy). \tag{3.35}$$

Substituting Equations (3.33) - (3.35) into (3.27), one discovers

$$X(0) = 0, \quad Y(0) = 0, \quad X(m) = 0, \quad Y(n) = 0.$$

Substituting these results into Equations (3.34) and (3.35), we have

$$p = \frac{r\pi}{m}, q = \frac{s\pi}{n}, r = 0,1,2,..,s, = 0,1,2, ...$$

and

$$X(x) = B_2 \sin\left(\frac{r\pi x}{m}\right) \tag{3.36}$$
$$Y(y) = B_3 \sin\left(\frac{s\pi y}{n}\right). \tag{3.37}$$

Because $q^2 = k^2 - p^2$ then Equation (3.33) will be

$$T(t) = A_1 e^{\left(-D_s\left(\left(\frac{r}{m}\right)^2 + \left(\frac{s}{n}\right)^2\right)\pi^2 t\right)}. \tag{3.38}$$

Substituting Equations (3.36), (3.37), and (3.38) into Equation (3.27), one obtains

$$\Phi(x, y, t) = E \sin\left(\frac{r\pi x}{m}\right) \sin\left(\frac{s\pi y}{n}\right) e^{\left(-D_s\left(\left(\frac{r}{m}\right)^2 + \left(\frac{s}{n}\right)^2\right)\pi^2 t\right)},$$

where $E = A_1 B_2 B_3$ is constant.
The principle of Superposition then tells us that a solution to the partial differential equation is,

$$\Phi(x, y, t) = \sum_{s=0}^{\infty} \sum_{r=0}^{\infty} E_{rs} \sin\left(\frac{r\pi x}{m}\right) \sin\left(\frac{s\pi y}{n}\right) e^{\left(-D_s\left(\left(\frac{r}{m}\right)^2 + \left(\frac{s}{n}\right)^2\right)\pi^2 t\right)}. \tag{3.39}$$

Substituting the initial condition in Equation (3.22) into Equation (3.39), one has

$$f(x, y) = \sum_{s=0}^{\infty} \sum_{r=0}^{\infty} E_{rs} \sin\left(\frac{r\pi x}{m}\right) \sin\left(\frac{s\pi y}{n}\right). \tag{3.40}$$

Using the Fourier series, we get the value of the coefficient E_{rs}

$$E_{rs} = \frac{4}{mn} \int_0^n \int_0^m f(x, y) \sin\left(\frac{r\pi x}{m}\right) \sin\left(\frac{s\pi y}{n}\right) dxdy. \tag{3.41}$$

Substituting Equation (3.41) into Equation (3.39)

$$\Phi(x,y,t)=\sum_{s=0}^{\infty}\sum_{r=0}^{\infty}\left(\left[\frac{4}{mn}\int_0^n\int_0^m f(x,y)\sin\left(\frac{r\pi x}{m}\right)\sin\left(\frac{s\pi y}{n}\right)dxdy\right]\sin\left(\frac{r\pi x}{m}\right)\sin\left(\frac{s\pi y}{n}\right)e^{\left(-D_s\left(\left(\frac{r}{m}\right)^2+\left(\frac{s}{n}\right)^2\right)\pi^2 t\right)}\right). \quad (3.42)$$

The substitution of Equations (3.42) and (3.39) into Equation (3.9), yields

$$\phi(x,y,t)=\sum_{s=0}^{\infty}\sum_{r=0}^{\infty}\left(\left[\frac{4}{mn}\int_0^n\int_0^m f(\xi,\zeta)\sin\left(\frac{r\pi\xi}{m}\right)\sin\left(\frac{s\pi\zeta}{n}\right)d\xi d\zeta\right]\sin\left(\frac{r\pi x}{m}\right)\sin\left(\frac{s\pi y}{n}\right)e^{\left(-D_s\left(\left(\frac{r}{m}\right)^2+\left(\frac{s}{n}\right)^2\right)\pi^2 t\right)}\right) + \varphi(x,y). \quad (3.43)$$

Finally, putting Equation (3.43) into Equation (3.1), one obtains the analytical solution for the original problem

$$C(x,y,t)=e^{\alpha x+\beta y+\gamma t}\left(\sum_{s=0}^{\infty}\sum_{r=0}^{\infty}\left(\left[\frac{4}{mn}\int_0^n\int_0^m f(\xi,\zeta)\sin\left(\frac{r\pi\xi}{m}\right)\sin\left(\frac{s\pi\zeta}{n}\right)d\xi d\zeta\right]\sin\left(\frac{r\pi x}{m}\right)\sin\left(\frac{s\pi y}{n}\right)e^{\left(-D_s\left(\left(\frac{r}{m}\right)^2+\left(\frac{s}{n}\right)^2\right)\pi^2 t\right)}\right) + \varphi(x,y)\right), \quad (3.44)$$

where $f(\xi,\zeta)=C_i e^{-\alpha\xi-\beta\zeta}-\varphi(\xi,\zeta)$, and

$$\begin{aligned}\varphi(x,y)=\sum_{p=0}^{\infty}\sin\left(\frac{p\pi x}{m}\right)&\left\{\left\{\frac{-2C_c p\pi e^{-\gamma t}(1-e^{-\alpha m}\cos(p\pi))}{\sinh\left(\frac{p\pi n}{m}\right)((\alpha m)^2+(p\pi)^2)}\right\}\sinh\left(\frac{p\pi}{m}(y-n)\right)\right.\\ &\left.+\left\{\frac{-2C_d p\pi e^{-\beta n-\gamma t}(1-e^{-\alpha m}\cos(p\pi))}{\sinh\left(\frac{p\pi n}{m}\right)((\alpha m)^2+(p\pi)^2)}\right\}\sinh\left(\frac{p\pi y}{m}\right)\right\}\\ &+\sin\left(\frac{p\pi y}{n}\right)\left\{\left\{\frac{-2C_b p\pi e^{-\alpha m-\gamma t}(1-e^{-\beta n}\cos(p\pi))}{\sinh\left(\frac{p\pi m}{n}\right)((\beta n)^2+(p\pi)^2)}\right\}\sinh\left(\frac{p\pi}{n}(x-m)\right)\right.\\ &\left.+\left\{\frac{-2C_a p\pi e^{-\gamma t}(1-e^{-\beta n}\cos(p\pi))}{\sinh\left(\frac{p\pi m}{n}\right)((\beta n)^2+(p\pi)^2)}\right\}\sinh\left(\frac{p\pi x}{n}\right)\right\}.\end{aligned}$$

4. NUMERICAL SIMULATION

The computer package MATLAB [10] was used to show the closed-form solution of Equation (3.44). We divide the simulation into three different parts depending on the depth level of the concrete, namely the depth of 0-0.5 meters, the depth of 0-1 meters, and the depth of 0-1.5 meters. It aims to show the concentration distribution for several values of parameters such as diffusion coefficient and carbonation depth. Notice that, the parameter value used in this study is adapted from the parameter value which is taken from Liang and Lin [3].

Simulation I

In this first simulation from a simple domain that is a square domain with domain areas $0 \le x \le 0.5$ and $0 \le y \le 0.5$, with

$C_i = 0.0\ gm^{-3}, C_a = 0.1\ gm^{-3}, C_b = 0.2\ gm^{-3}, C_c = 0.3\ gm^{-3}, C_d = 0.4\ gm^{-3}, v = 10^{-12}\ m/s$, and $K_T = 10^{-10}\ s^{-1}$. The concentration of CO_2 distribution at $D_s = 10^{-12} m^2 s^{-1}$ and $D_s = 10^{-13} m^2 s^{-1}$ are displayed in figure 1, and figure 2. From figure 1, one knows the carbonation depth $x = y = 0.0263158\ m$ after $t = 14$ days with $C(x, y, t) = 0.1957325\ gm^{-3}$ and $D_s = 10^{-12} m^2 s^{-1}$. For $D_s = 10^{-13} m^2 s^{-1}$, and $C(x, y, t) = 0.2908709\ gm^{-3}$, one needs $t = 24$ days at $x = 0.0263158\ m, y = 0.0526316\ m$ from figure 2.

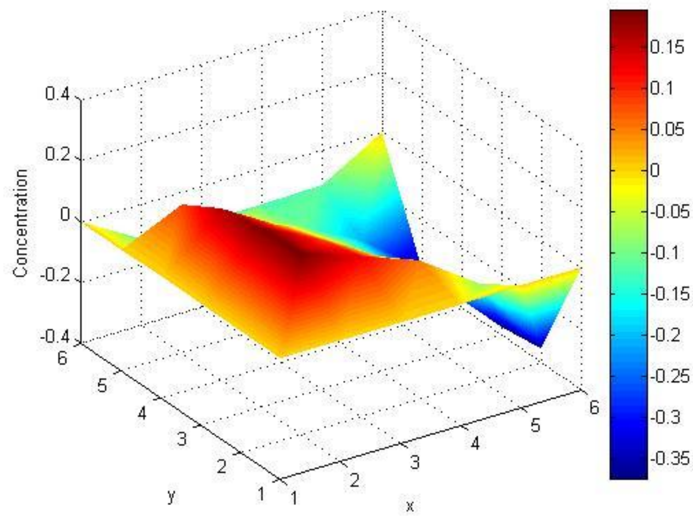

Figure 1. Concentration distribution at $D_s = 10^{-12} m^2 s^{-1}$.

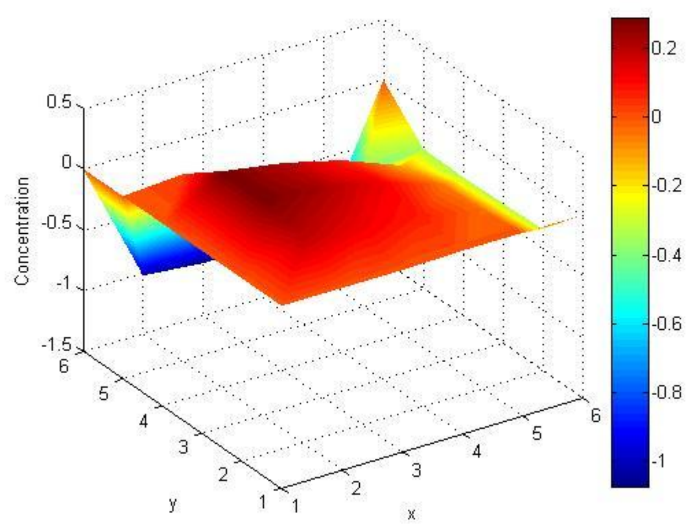

Figure 2. Concentration distribution at $D_s = 10^{-13} m^2 s^{-1}$.

Simulation II

The second simulation, we consider a simple unit square domain $0 \leq x \leq 1$ and $0 \leq y \leq 1$, with $C_i = 0.0\ gm^{-3}, C_a = 0.1\ gm^{-3}, C_b = 0.2\ gm^{-3}, C_c = 0.3\ gm^{-3}, C_d = 0.4\ gm^{-3}, v = 10^{-12}\ m/s$, and $K_T = 10^{-10}\ s^{-1}$. The concentration of CO_2 distribution at $D_s = 10^{-12} m^2 s^{-1}$ and $D_s = 10^{-13} m^2 s^{-1}$ are displayed in figure 3, and figure 4. If one knows $D_s = 10^{-12} m^2 s^{-1}$ and $C(x, y, t) = 0.1986104\ gm^{-3}$, one obtains $x = 0.0526316\ m, y = 0.1052632\ m$ after $t = 127$ days from figure 3. For $D_s = 10^{-13} m^2 s^{-1}$, and $C(x, y, t) = 1.0324499\ gm^{-3}$, one needs $t = 160$ days at $x = y = 0.1578947\ m$ from figure 4.

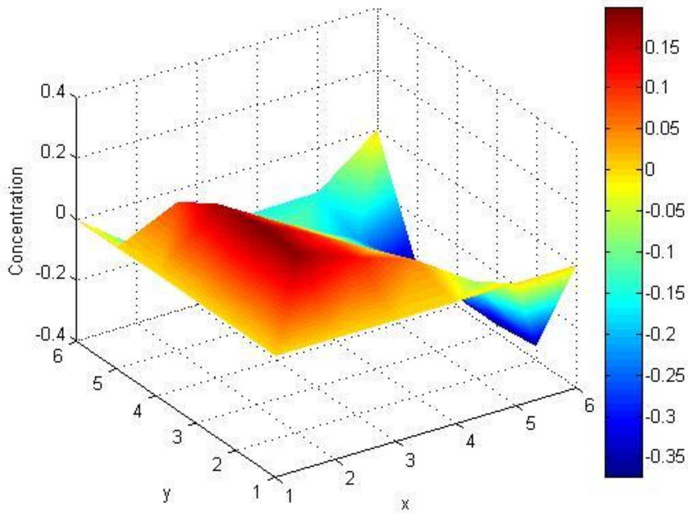

Figure 3. Concentration distribution at $D_s = 10^{-12} m^2 s^{-1}$.

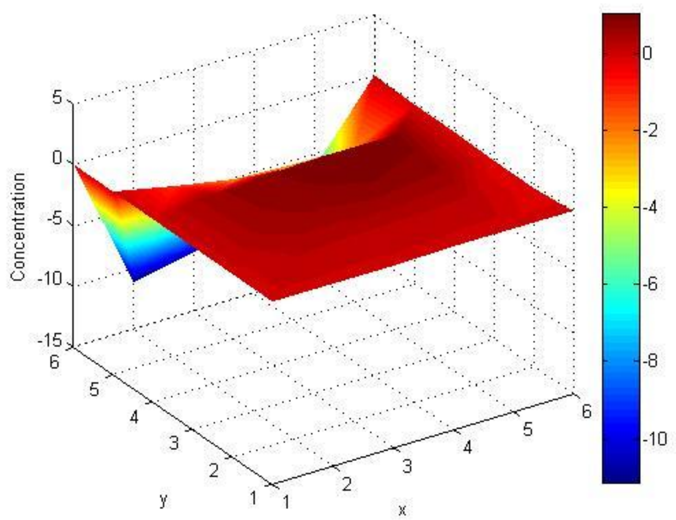

Figure 4. Concentration distribution at $D_s = 10^{-13} m^2 s^{-1}$.

Simulation III

The last simulation, we consider a simple unit square domain $0 \leq x \leq 1.5$ and $0 \leq y \leq 1.5$, with $C_i = 0.0\ gm^{-3}, C_a = 0.1\ gm^{-3}, C_b = 0.2\ gm^{-3}, C_c = 0.3\ gm^{-3}, C_d = 0.4\ gm^{-3}, v = 10^{-12}\ m/s$, and $K_T = 10^{-10}\ s^{-1}$. The concentration of CO_2 distribution at $D_s = 10^{-12} m^2 s^{-1}$ and $D_s = 10^{-13} m^2 s^{-1}$ are displayed in figure 5, and figure 6. From figure 5, one knows the carbonation depth $x = 0.0789474\, m, y = 0.1578947\, m$ after $t = 121$ days with $C(x, y, t) = 0.2060931\, gm^{-3}$ and $D_s = 10^{-12} m^2 s^{-1}$. For $D_s = 10^{-13} m^2 s^{-1}$, and $C(x, y, t) = 5.3363605\, gm^{-3}$, one needs $t = 64$ days at $x = 0.3157895\, m, y = 0.3947368\, m$ from figure 6.

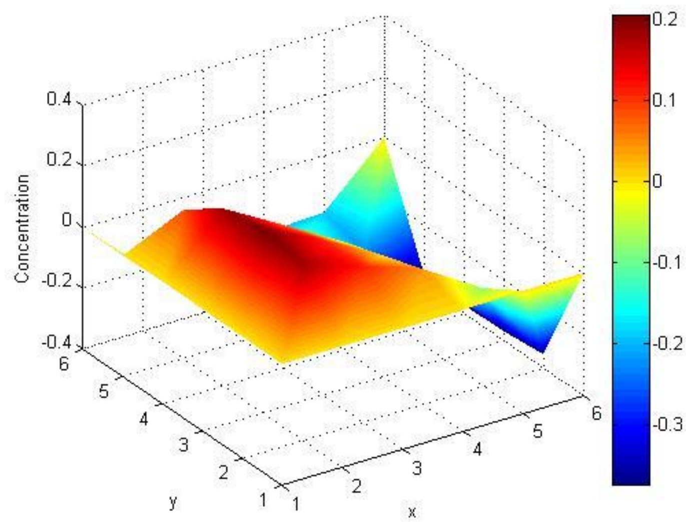

Figure 5. Concentration distribution at $D_s = 10^{-12} m^2 s^{-1}$.

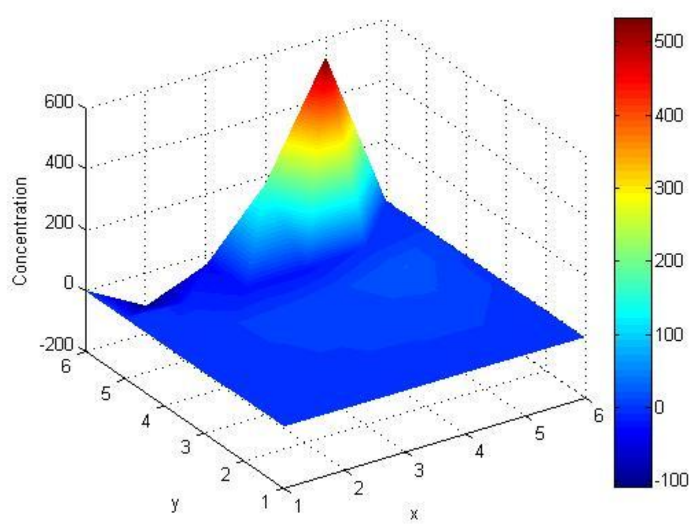

Figure 6. Concentration distribution at $D_s = 10^{-13} m^2 s^{-1}$.

CONCLUSION

We have developed the new two-dimensional mathematical model to describe the transport phenomena of carbon dioxide in concrete structures. The analytical solution for the two-dimensional linear partial differential equation obtained using the separation of variables method combined with some substitution approaches. The numerical results are presented in figures 1,2,3,4,5 and 6 to illustrate the concentration distribution for several values of parameters such as diffusion coefficient and carbonation depth. Based on this research, we can use to analyze the dynamic behavior over a long period of time from a more complex mathematical model of concrete carbonation process.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interest

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