



DIFFUSION IN A SOLID CYLINDER PART I: ADVANCING MODEL

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Recommended Citation

Tsai, Cho-Liang and Lin, Ching-Chang (2015) "DIFFUSION IN A SOLID CYLINDER PART I: ADVANCING MODEL," *Journal of Marine Science and Technology*. Vol. 23: Iss. 2, Article 1.

DOI: 10.6119/JMST-014-0117-1

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Acknowledgements

The authors would like to thank the National Science Council of the Republic of China, Taiwan for financially supporting this research under Contract No. (NSC97-2221-E-224-054).

DIFFUSION IN A SOLID CYLINDER PART I: ADVANCING MODEL

Cho-Liang Tsai¹ and Ching-Chang Lin²

Key words: advancing model, diffusion.

ABSTRACT

An advanced diffusion model is used to calculate the concentration of a substance diffused in a solid cylindrical medium. The mathematical process in this study adopts Neumann's algorithm for applying the advancing model to revise the solution derived by Carslaw and Jaeger. The modified solution clearly indicates a diffusion front which does not exist in the original model. Calculating the diffusion depth becomes possible and is novel for a solid cylindrical medium. The major contribution of this study is the application of the advancing model to solve the diffusion problem of a cylindrical medium in cylindrical coordinate system.

I. INTRODUCTION

Fick's diffusion law is widely used for studying diffusion mechanisms. The concentration of a diffusing substance in a medium depends on the location in the medium, the diffusion duration, the geometry of the medium, the environmental conditions and the material properties of both the diffusing substance and medium.

Carslaw and Jaeger (1959) applied Laplace transform to solve the temperature of a semi-infinite space in a case that the heat is conducted from the surface of the space toward its depth. By assuming the solution to be a uni-formed function, Carslaw and Jaeger formulated the solution as an asymptotic function. When the solution was applied to the diffusion problem of the same medium, which has the same governing equation as that of heat conduction problem, the solution indicated that the concentration in the medium infinitely approached zero as the diffusing substance moved along its path inward but can never be zero regardless of the duration (Crank, 1975). The solution reveals no diffusion front, and

the diffusion depth is impossible to be calculated. However, transporting molecules of a diffusing substance in a medium takes time. The molecules of a diffusing substance do not appear deep inside the medium immediately after the diffusion begins. The Crank's solution is inapplicable for diffusion in semi-infinite space in practice even if it is mathematically correct.

Carslaw and Jaeger (1959) presented Neumann's solution for heat conduction of a semi-infinite space with a moving boundary. When the famous Neumann's solution was applied to the diffusion in the case of a semi-infinite medium with a moving boundary, the model was called the advancing model (Crank, 1975; Chang et al., 2008; Wang, 2010; Lin et al., 2012). The solution of this model is a bi-formed and continuous but not a smooth function. The solution is in a series form in the contaminated zone which is close to the surface, while it is zero in the uncontaminated zone which is deeper than the contaminated zone. The bi-formed solution clearly indicates a diffusion front and enables calculation of the diffusion depth.

Carslaw and Jaeger (1959) also presented the solution of the temperature for heat conduction in a solid cylindrical medium in terms of the Bessel function without the advancing model. For the past half century, the high complexity of the cylindrical coordinate system has prevented researchers from deriving the solution of the temperature for heat conduction or the solution of the concentration of the diffusing substance for diffusion by using the advancing model.

This study successfully applied the Neumann's algorithm to the cylindrical coordinate system by focusing on the local diffusion around the surface of a cylindrical medium and correlating the modification factors of the advancing model for both Cartesian and cylindrical coordinate systems. Similar to the solution with the advancing model, presented by Crank for the diffusion in a semi-infinite medium, the solution clearly shows the diffusion front. The result can be used to characterize the diffusion parameters of a cylindrical specimen medium, which is very common for concrete specimens.

II. THEORY

The governing equation of Fick's second diffusion law (Crank, 1975) is

Paper submitted 01/28/13; revised 01/07/14; accepted 01/17/14. Author for correspondence: Ching-Chang Lin (e-mail: cclin@fcu.edu.tw).

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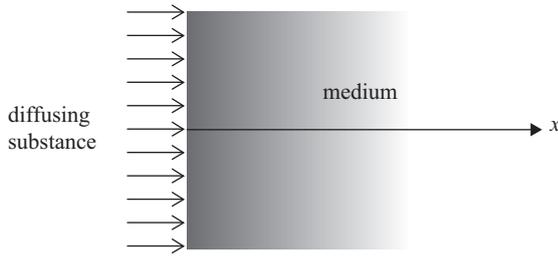


Fig. 1. Diffusion in a semi-infinite medium.

$$\frac{\partial c}{\partial t} = D\nabla^2 c \tag{1}$$

where c is the concentration of the diffusing substance in a medium defined as the mass of a diffusing substance in unit volume of medium, t is the diffusion duration, and D is the diffusivity, which is a positive constant. In a three-dimensional Cartesian coordinate system, Eq. (1) becomes

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2}\right) \tag{2}$$

where x , y and z are the three coordinates.

In a one-dimensional case, Eq. (2) becomes

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} \tag{3}$$

For the semi-infinite case, the medium exists only in the region where $x \geq 0$ and is initially free of the diffusing substance. The diffusing substance exists in the region where $x < 0$ and is transported inward from the surface of the medium at $x = 0$ according to Fick's diffusion law (Fig. 1). In this typical one-dimensional diffusion case, c is a function of t and x , represented as $c(t, x)$. The assumed boundary condition is that, when the diffusing substance comes into contact with the medium at the boundary, the boundary is instantly saturated and remains so throughout the process of diffusion (Crank, 1975).

$$c(t; 0) = c_\infty \tag{4}$$

where c_∞ is the saturated c . The initial condition is

$$c(0; x) = 0 \tag{5}$$

Accordingly, $c(t, x)$ was solved as

$$\frac{c(t, x)}{c_\infty} = 1 - \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} (-1)^n \frac{\left(\frac{x}{2\sqrt{Dt}}\right)^{2n+1}}{n!(2n+1)} \tag{6}$$

The right side of Eq. (6) has two parts, a unit constant, which is a particular solution, and a complementary function of the solution. Both parts satisfy the governing equation, Eq. (3).

Next modify Eq. (6) by dividing the complementary function by a modification factor C . Eq. (6) then becomes

$$\frac{c(t, x)}{c_\infty} = 1 - \frac{\frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} (-1)^n \frac{\left(\frac{x}{2\sqrt{Dt}}\right)^{2n+1}}{n!(2n+1)}}{C} \tag{7}$$

where C is a constant such that the governing equation and boundary condition are satisfied. If $C = 1$, Eq. (7) is identical to Eq. (6). Since C and c_∞ are constants, Eq. (7) satisfies both Eq. (3) and the boundary condition represented by Eq. (4). Neumann defined C for Eq. (7) as

$$C = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} (-1)^n \frac{\nu^{2n+1}}{n!(2n+1)} \tag{8}$$

where ν is Neumann's constant named after Neumann, F. (Carslaw and Jager, 1959; Crank, 1975; Wang et al., 2011).

Therefore, Eq. (7) becomes

$$\begin{aligned} \frac{c(t, x)}{c_\infty} &= 1 - \frac{\frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} (-1)^n \frac{\left(\frac{x}{2\sqrt{Dt}}\right)^{2n+1}}{n!(2n+1)}}{\frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} (-1)^n \frac{\nu^{2n+1}}{n!(2n+1)}} \\ &= 1 - \frac{\sum_{n=0}^{\infty} (-1)^n \frac{\left(\frac{x}{2\sqrt{Dt}}\right)^{2n+1}}{n!(2n+1)}}{\sum_{n=0}^{\infty} (-1)^n \frac{\nu^{2n+1}}{n!(2n+1)}} \end{aligned} \tag{9}$$

Eq. (9) implies a very interesting result in that it vanishes at

$$\frac{x}{2\sqrt{Dt}} = \nu \quad \text{or} \quad x = 2\nu\sqrt{Dt} \tag{10}$$

and becomes negative at any location deeper than $2\nu\sqrt{Dt}$. A negative concentration is illogical. Redefine Eq. (10) as a bi-formed equation (Crank, 1975; Tsai et al., 2014).

$$\frac{c(t, x)}{c_\infty} = \begin{cases} 1 - \frac{\sum_{n=0}^{\infty} (-1)^n \frac{\left(\frac{x}{2\sqrt{Dt}}\right)^{2n+1}}{n!(2n+1)}}{\sum_{n=0}^{\infty} (-1)^n \frac{\nu^{2n+1}}{n!(2n+1)}}, & 0 \leq x \leq 2\nu\sqrt{Dt} \\ 0, & 2\nu\sqrt{Dt} \leq x \end{cases} \tag{11}$$

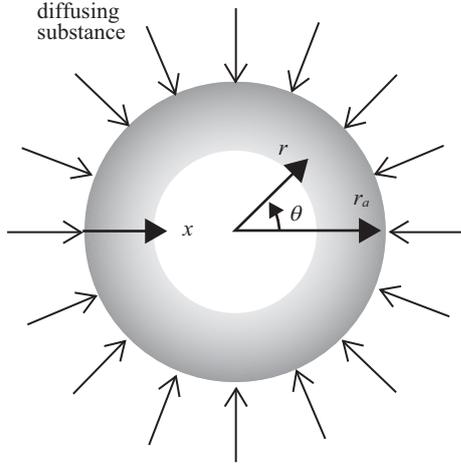


Fig. 2. Diffusion in a cylindrical medium.

Since transport of the diffusing substance starts from $x = 0$, $2\sqrt{Dt}$ stands for the diffusion depth.

For a cylindrical coordinate system, Eq. (1) becomes

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r} + \frac{1}{r^2} \frac{\partial^2 c}{\partial \theta^2} + \frac{\partial^2 c}{\partial z^2}\right) \quad (12)$$

where r and θ are the polar coordinates and z is the axial coordinate. In the case of axially symmetrical diffusion in an infinitely long solid cylinder with radius r_a , c is dependent only on t and r , $c(t,r)$, and Eq. (12) becomes

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r}\right) \quad (13)$$

Again, assume that the concentration of the diffusing substance in the cylinder is initially zero.

$$c(0;r) = 0 \quad (14)$$

The diffusing substance exists in the surrounding environment, penetrates the surface when the diffusion process starts and diffuses toward the center of the cylinder (Fig. 2). As in the previous case, the assumed boundary condition is that, when the diffusing substance contacts the medium at the boundary, the boundary is instantly saturated and then remains so throughout the diffusion process.

$$c(t;r_a) = c_\infty \quad (15)$$

By separation variable, let $c(t,r) = R(r)T(t)$ where $R(r)$ is a function of r and where $T(t)$ is a function of t . Eq. (13) becomes

$$R \frac{dT}{Dt} = T\left(\frac{d^2 R}{dr^2} + \frac{1}{r} \frac{dR}{dr}\right) \quad (16)$$

or

$$\frac{\frac{dT}{Dt}}{DT} = \frac{\frac{d^2 R}{dr^2} + \frac{1}{r} \frac{dR}{dr}}{R} \quad (17)$$

The left side of Eq. (17) is a function of t only, and the right side is a function of r only. Both sides must be constant to be compatible in one equation. Let

$$\frac{\frac{dT}{Dt}}{DT} = -k = \frac{\frac{d^2 R}{dr^2} + \frac{1}{r} \frac{dR}{dr}}{R}, \quad k : \text{constant} \quad (18)$$

when $k = 0$,

$$\frac{dT}{dt} = 0 \quad (19)$$

$$\frac{d^2 R}{dr^2} + \frac{1}{r} \frac{dR}{dr} = 0 \quad \text{or} \quad \frac{1}{r} \frac{d\left(r \frac{\partial R}{\partial r}\right)}{dr} = 0 \quad (20)$$

Eq. (19) implies that T is a constant, and Eq. (20) implies that R is a constant or $\ln(r)$. Since $\ln(r)$ becomes undefined when $r = 0$, $\ln(r)$ is an unacceptable solution for R . In this particular condition, the solution of $c(t;r)$ is a constant.

$$c(t;r) = \beta_0, \quad \beta_0 : \text{constant} \quad (21)$$

when $k \neq 0$,

$$\frac{dT}{dt} + DkT = 0 \quad (22)$$

$$\frac{d^2 R}{dr^2} + \frac{1}{r} \frac{dR}{dr} + kR = 0 \quad \text{or} \quad \frac{1}{r} \frac{d\left(r \frac{dR}{dr}\right)}{dr} + kR = 0 \quad (23)$$

Eq. (23) is a Bessel's differential equation of zero order, and its solution is

$$R(r) = J_0(\sqrt{k_m} r) \quad (24)$$

where m is a multi-value index, k_m is the multi-value k , and J_0 is Bessel function of the first kind of order zero. For Eq. (22), the solution corresponding to the m -th term of $R(r)$ is

$$T(t) = e^{-k_m Dt} \quad (25)$$

The general solution for $c(t;r)$ is the combination of Eq. (21), Eq. (24) and Eq. (25).

$$c(t; r) = \beta_0 + \sum_{m=1}^{\infty} [\beta_m J_0(\sqrt{k_m} r) e^{-k_m D t}], \beta_m : \text{constants} \quad (26)$$

To satisfy the boundary condition, Eq. (15), let

$$\beta_0 = c_{\infty}, \quad k_m = \left(\frac{\alpha_m}{r_a}\right)^2 \quad (27)$$

where α_m is the m -th zero of J_0 , listed in APPENDIX I, which is very close to $(m-1/4)\pi$ when $m > 20$ (Abramowitz and Stegun, 1972). Eq. (26) becomes

$$c(t; r) = c_{\infty} + \sum_{m=1}^{\infty} \left[\beta_m J_0\left(\alpha_m \frac{r}{r_a}\right) e^{-\left(\alpha_m \frac{\sqrt{Dt}}{r_a}\right)^2} \right], \quad \beta_m : \text{constants} \quad (28)$$

The initial condition, Eq. (14), yields

$$c_{\infty} = -\sum_{m=1}^{\infty} \left[\beta_m J_0\left(\alpha_m \frac{r}{r_a}\right) \right] \quad (29)$$

Multiply both sides of Eq. (29) by $r J_0(\alpha_n r/r_a)$, where n is an integer index, and then integrate both sides with respect to r from 0 to r_a (APPENDIX II) to obtain

$$\beta_m = -c_{\infty} \frac{2}{\alpha_m J_1(\alpha_m)} \quad (30)$$

Eq. (26) becomes

$$\frac{c(t; r)}{c_{\infty}} = 1 - \sum_{m=1}^{\infty} \left[\frac{2}{\alpha_m J_1(\alpha_m)} J_0\left(\alpha_m \frac{r}{r_a}\right) e^{-\left(\alpha_m \frac{\sqrt{Dt}}{r_a}\right)^2} \right] \quad (31)$$

Eq. (31) is the normalized $c(t; r)$, an uni-formed solution. The right side of Eq. (31) is separated into two parts, one part being a particular solution which is an unit constant and the other part being a complementary function. Both parts satisfy the governing equation, Eq. (13). For the case of chloride diffusion in a water-logged cylindrical concrete specimen (Wang et al., 2011), assume $c_{\infty} = 0.025 \text{ g/cm}^3$, $D = 0.00758 \text{ cm}^2/\text{day}$, $r_a = 7.5 \text{ cm}$ and the ends of the specimen are painted to block the chloride diffusion through the ends, Fig. 3(a) shows the $c(t; x)/c_{\infty}$ versus r/r_a for different \sqrt{Dt}/r_a .

After applying the Neumann's technique to divide the complementary function by a modification factor C , Eq. (31) becomes

$$\frac{c(t; r)}{c_{\infty}} = 1 - \frac{\sum_{m=1}^{\infty} \left[\frac{2}{\alpha_m J_1(\alpha_m)} J_0\left(\alpha_m \frac{r}{r_a}\right) e^{-\left(\alpha_m \frac{\sqrt{Dt}}{r_a}\right)^2} \right]}{C} \quad (32)$$

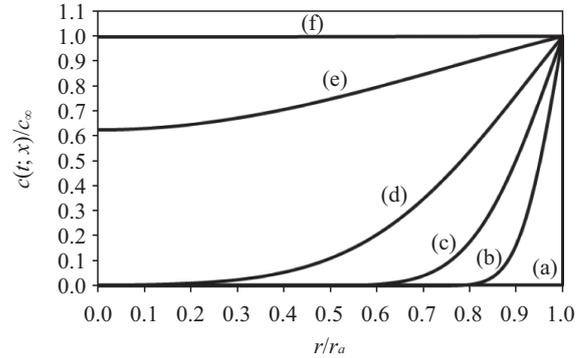


Fig. 3a. $c(t; x)/c_{\infty}$ versus r/r_a in a cylindrical medium for $C = 1$, (a) $\sqrt{Dt}/r_a = 0$, (b) $\sqrt{Dt}/r_a = 0.05$, (c) $\sqrt{Dt}/r_a = 0.1$, (d) $\sqrt{Dt}/r_a = 0.2$, (e) $\sqrt{Dt}/r_a = 0.5$, (f) $\sqrt{Dt}/r_a = 1$.

Since C and c_{∞} are constants, Eq. (32) satisfies Eq. (13) and the boundary condition, Eq. (15).

When r is sufficiently small but t is not sufficiently large, the numerator of the second term on the right side of Eq. (32) could be bigger than its denominator, meaning that Eq. (32) might be negative. A negative concentration value is irrational. Eq. (32) must be set to zero under this condition. As a result, the cross section of the cylinder is separated into two zones, a contaminated zone that is closer to the surface and an uncontaminated core. However, when t is sufficiently large, the cylinder is contaminated thoroughly and there is no uncontaminated core.

Before the medium is thoroughly contaminated, $c(t; x)$ gradually decreases as it approaches the center, becomes zero at a critical location, and is set to zero for the rest area where it is numerically negative. The critical location where $r = r_f$ stands for the diffusion front. The zone where $r \leq r_f$ is the uncontaminated core. The distance between the surface and diffusion front is the diffusion depth, which is not considered in Eq. (31). The location of the diffusion front r_f depends on t and can be calculated numerically by setting Eq. (32) to zero. Define the critical t when the diffusing substance reaches the center, $r_f = 0$, as t_c . When $t \leq t_c$, redefine Eq. (32) as

$$\frac{c(t; r)}{c_{\infty}} = \begin{cases} 1 - \frac{\sum_{m=1}^{\infty} \left[\frac{2}{\alpha_m J_1(\alpha_m)} J_0\left(\alpha_m \frac{r}{r_a}\right) e^{-\left(\alpha_m \frac{\sqrt{Dt}}{r_a}\right)^2} \right]}{C}, & r \geq r_f \\ 0, & r \leq r_f \end{cases} \quad (33)$$

Neumann defined C for Eq. (7) as Eq. (8), and resulted in the diffusion depth as $2\sqrt{Dt}$. Here, the important task is defining C for this cylindrical coordinate system. Before solving C , however, the local diffusion near the surface should be discussed. Eq. (31) is the solution for the normalized

concentration of the cylindrical medium obtained without the advancing model. Let the original point of a unidirectional Cartesian coordinate system be placed on the left edge of the cylinder, with the x -coordinate oriented toward the center of the cylinder (Fig. 2). Clearly, $x = r_a - r$ or $r = r_a - x$. Eq. (31) becomes

$$\frac{c(t; x)}{c_\infty} = 1 - \sum_{m=1}^{\infty} \left[\frac{2}{\alpha_m J_1(\alpha_m)} J_0\left(\alpha_m \left(1 - \frac{x}{r_a}\right)\right) e^{-\left(\alpha_m \frac{\sqrt{Dt}}{r_a}\right)^2} \right] \quad (34)$$

When x is very small, the local geometry around the surface should be very close to a semi-infinite domain, meaning that Eq. (34) should be the same as Eq. (6).

Similarly, the complementary functions on the right side of both Eqs. (34) and (6) should be the same.

$$\begin{aligned} \sum_{m=1}^{\infty} \left[\frac{2}{\alpha_m J_1(\alpha_m)} J_0\left(\alpha_m \left(1 - \frac{x}{r_a}\right)\right) e^{-\left(\alpha_m \frac{\sqrt{Dt}}{r_a}\right)^2} \right] \\ = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} (-1)^n \frac{\left(\frac{x}{2\sqrt{Dt}}\right)^{2n+1}}{n!(2n+1)} \end{aligned} \quad (35)$$

When the advancing model is considered, Eq. (31) becomes Eq. (32). For the diffusion near the area close to the surface of cylinder, Eq. (32) should be very close to Eq. (9). With the aid of Eq. (35), the C in Eq. (32) is proven to be the same as that in Eq. (7) for a Cartesian coordinate system as shown in Eq. (8). Therefore, Eq. (32) becomes

$$\frac{c(t; r)}{c_\infty} = 1 - \frac{\sum_{m=1}^{\infty} \left[\frac{2}{\alpha_m J_1(\alpha_m)} J_0\left(\alpha_m \frac{r}{r_a}\right) e^{-\left(\alpha_m \frac{\sqrt{Dt}}{r_a}\right)^2} \right]}{\frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} (-1)^n \frac{v^{2n+1}}{n!(2n+1)}} \quad (36)$$

and Eq. (33) becomes

$$\frac{c(t; r)}{c_\infty} = \begin{cases} 1 - \frac{\sum_{m=1}^{\infty} \left[\frac{2}{\alpha_m J_1(\alpha_m)} J_0\left(\alpha_m \frac{r}{r_a}\right) e^{-\left(\alpha_m \frac{\sqrt{Dt}}{r_a}\right)^2} \right]}{\frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} (-1)^n \frac{v^{2n+1}}{n!(2n+1)}}, & r \geq r_f \\ 0, & r \leq r_f \end{cases} \quad (37)$$

For the case of a water-logged cylindrical concrete specimen with $r_a = 7.5$ cm, where the two ends are painted, $c_\infty = 0.025$ g/cm³ and $D = 0.00758$ cm²/day, Figs. 3(b)-(d) show the results for $c(t; x)/c_\infty$ versus r/r_a for varying \sqrt{Dt}/r_a , v and C , respectively.

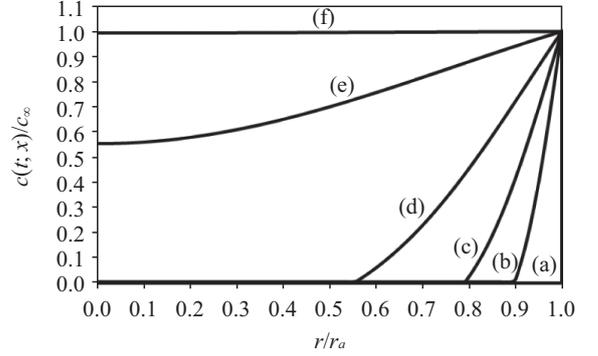


Fig. 3b. $c(t; x)/c_\infty$ versus r/r_a in a cylindrical medium for $\nu = 1$, $C = 0.84$, (a) $\sqrt{Dt}/r_a = 0$, (b) $\sqrt{Dt}/r_a = 0.05$, (c) $\sqrt{Dt}/r_a = 0.1$, (d) $\sqrt{Dt}/r_a = 0.2$, (e) $\sqrt{Dt}/r_a = 0.5$, (f) $\sqrt{Dt}/r_a = 1$.

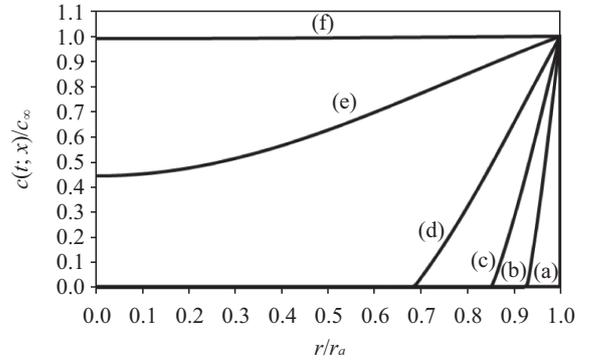


Fig. 3c. $c(t; x)/c_\infty$ versus r/r_a in a cylindrical medium for $\nu = 0.7$, $C = 0.68$, (a) $\sqrt{Dt}/r_a = 0$, (b) $\sqrt{Dt}/r_a = 0.05$, (c) $\sqrt{Dt}/r_a = 0.1$, (d) $\sqrt{Dt}/r_a = 0.2$, (e) $\sqrt{Dt}/r_a = 0.5$, (f) $\sqrt{Dt}/r_a = 1$.

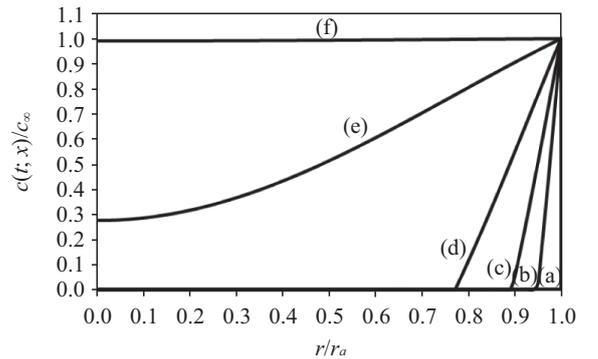


Fig. 3d. $c(t; x)/c_\infty$ versus r/r_a in a cylindrical medium for $\nu = 0.5$, $C = 0.52$, (a) $\sqrt{Dt}/r_a = 0$, (b) $\sqrt{Dt}/r_a = 0.05$, (c) $\sqrt{Dt}/r_a = 0.1$, (d) $\sqrt{Dt}/r_a = 0.2$, (e) $\sqrt{Dt}/r_a = 0.5$, (f) $\sqrt{Dt}/r_a = 1$.

III. DISCUSSION

Along the radius coordinate toward the center of the cylindrical medium, $r = r_f$ is the location where $c(t; r)$ starts to be 0, which is the location of the boundary between the

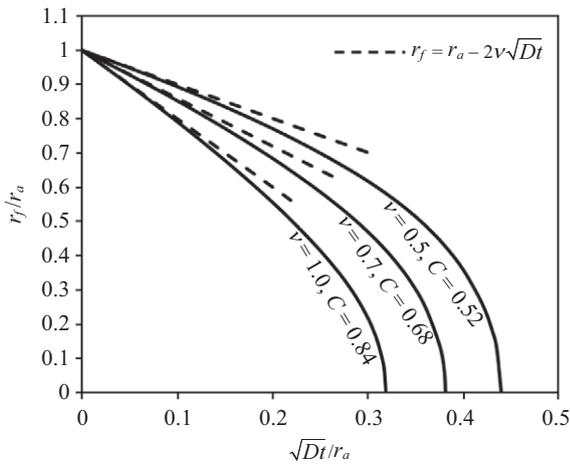


Fig. 4. r_f/r_a versus \sqrt{Dt}/r_a in a cylindrical medium.

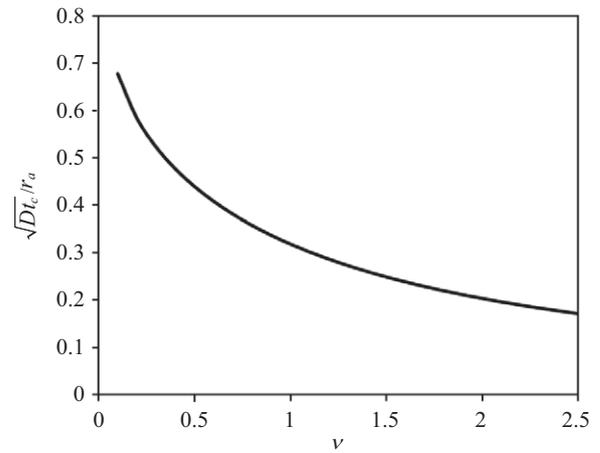


Fig. 5. $\sqrt{Dt_c}/r_a$ versus ν in a cylindrical medium.

contaminated zone and the uncontaminated core. Setting the first term of the right side of Eq. (37) to zero obtains

$$\frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} (-1)^n \frac{\nu^{2n+1}}{n!(2n+1)} = \sum_{m=1}^{\infty} \left[\frac{2}{\alpha_m J_1(\alpha_m)} J_0\left(\alpha_m \frac{r_f}{r_a}\right) e^{-\left(\alpha_m \frac{\sqrt{Dt}}{r_a}\right)^2} \right] \quad (38)$$

The relationship between r_f/r_a and \sqrt{Dt}/r_a can be calculated numerically via Eq. (38) for different ν (Fig. 4).

Clearly, $r_f \approx r_a - 2\nu\sqrt{Dt}$ around the surface of the cylindrical medium where $2\nu\sqrt{Dt}$ is the diffusion depth for a semi-infinite medium. In the cylindrical medium, the speed of the diffusion front increases as it approaches the center. This phenomenon does not occur in a semi-infinite medium. When the diffusing substance approaches the center of the medium, it is thickened because of the smaller space. Fick's first law is that the diffusion rate of a diffusing substance, along a diffusion path, is proportional to the derivative of the concentration of the diffusing substance. When the substance thickens along its path inward toward the center, the derivative of the concentration increases, and the diffusion rate accelerates. Such an inward flow accelerated by the thickening diffusing substance which is named thickening-substance-accelerated-inward flow, TSAI flow in short, will be critical for further studies of reverse osmosis efficiency.

The area deeper than r_f is the uncontaminated zone, where $c(t;r)$ is zero. When $r_f = 0$, the t is defined as the critical duration t_c when the diffusion reaches the center of the medium and Eq. (38) becomes

$$\frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} (-1)^n \frac{\nu^{2n+1}}{n!(2n+1)} = \sum_{m=1}^{\infty} \left[\frac{2}{\alpha_m J_1(\alpha_m)} e^{-\left(\alpha_m \frac{\sqrt{Dt_c}}{r_a}\right)^2} \right] \quad (39)$$

The relationship between $\sqrt{Dt_c}/r_a$ and ν can be calculated numerically via Eq. (39) (Fig. 5). When $t \leq t_c$, Eq. (37) is applied to get the concentration of the diffusing substance. When $t \geq t_c$, Eq. (36) is applied because there is no uncontaminated core. Future studies can extend Eqs. (36) and (37) to a cylindrical specimen with finite length, which is very common for concrete specimens.

Values of r_f and t_c depend on t , ν , D and r_a and must be calculated numerically from Eqs. (38) and (39). The process is tedious and needs further study for simplification, which will be included in the future work.

Cylindrical specimens are commonly used in compression test to determine the strength of concrete. If the specimen is placed in an environment full of chloride or other diffusing substance before the compression test, the concentration of chloride in the specimen can be measured by using the broken specimen after the compression test. Strength and chloride concentration can be obtained from the same specimen. By fitting the result of this work to the data of chloride concentration in the cylindrical concrete specimens, the parameters of chloride diffusion in the concrete will be obtained as well as its strength. In addition, the results can also be used to study the influence of chloride concentration on the concrete strength, and this should be another interesting work for the future.

IV. APPENDIX

1. Appendix I: Zeros of J_0

m	α_m	m	α_m
1	2.4048255604	51	159.4366111649
2	5.5200781056	52	162.5781886695
3	8.6537279135	53	165.7197667486
4	11.7915344396	54	168.8613453698
5	14.9309177091	55	172.0029245037
6	18.0710639685	56	175.1445041225

m	α_m	m	α_m
7	21.2116366305	57	178.2860842007
8	24.3524715314	58	181.4276647143
9	27.4934791327	59	184.5692456412
10	30.6346064690	60	187.7108269607
11	33.7758202142	61	190.8524086532
12	36.9170983543	62	193.9939907007
13	40.0584257652	63	197.1355730863
14	43.1997917138	64	200.2771557939
15	46.3411883723	65	203.4187388088
16	49.4826098980	66	206.5603221168
17	52.6240518417	67	209.7019057049
18	55.7655107556	68	212.8434895606
19	58.9069839267	69	215.9850736721
20	62.0484691908	70	219.1266580286
21	65.1899648008	71	222.2682426197
22	68.3314693305	72	225.4098274355
23	71.4729816042	73	228.5514124667
24	74.6145006443	74	231.6929977046
25	74.6145006443	75	234.8345831410
26	80.8975558717	76	237.9761687679
27	84.0390907775	77	241.1177545779
28	87.1806298442	78	244.2593405639
29	90.3221726378	79	247.4009267193
30	93.4637187825	80	250.5425130376
31	96.6052679516	81	253.6840995128
32	99.7468198593	82	256.8256861392
33	102.8883742548	83	259.9672729112
34	106.0299309171	84	263.1088598237
35	109.1714896504	85	266.2504468717
36	112.3130502811	86	269.3920340504
37	115.4546126543	87	272.5336213553
38	118.5961766315	88	275.6752087821
39	121.7377420886	89	278.8167963268
40	124.8793089138	90	281.9583839852
41	128.0208770066	91	285.0999717538
42	131.1624462758	92	288.2415596288
43	134.3040166389	93	291.3831476069
44	137.4455880209	94	294.5247356847
45	140.5871603535	95	297.6663238591
46	143.7287335743	96	300.8079121270
47	146.8703076264	97	303.9495004856
48	150.0118824576	98	307.0910889321
49	153.1534580198	99	310.2326774638
50	156.2950342691	100	313.3742660781

2. Appendix II: Verification of Eq. (30)

Multiply both sides of Eq. (29) by $rJ_0(\alpha_n r/r_a)$, where n is an integer index, and integrate both sides with respect to r from 0 to r_a . The left side becomes

$$\begin{aligned} & \int_0^{r_a} c_\infty r J_0(\alpha_n \frac{r}{r_a}) dr \\ &= c_\infty \int_0^{r_a} r [1 - \frac{(\frac{\alpha_n}{r_a})^2 r^2}{2^2(1!)^2} + \frac{(\frac{\alpha_n}{r_a})^4 r^4}{2^4(2!)^2} - \frac{(\frac{\alpha_n}{r_a})^6 r^6}{2^6(3!)^2} + \dots] dr \\ &= c_\infty [\frac{1}{2} r_a^2 - \frac{(\frac{\alpha_n}{r_a})^2 r_a^4}{2^2 4(1!)^2} + \frac{(\frac{\alpha_n}{r_a})^4 r_a^6}{2^4 6(2!)^2} - \frac{(\frac{\alpha_n}{r_a})^6 r_a^8}{2^6 8(3!)^2} + \dots] \\ &= c_\infty [\frac{\alpha_n}{2} - \frac{\alpha_n^3}{2^2 4(1!)^2} + \frac{\alpha_n^5}{2^4 6(2!)^2} - \frac{\alpha_n^7}{2^6 8(3!)^2} + \dots] \frac{r_a^2}{\alpha_n} \\ &= c_\infty J_1(\alpha_n) \frac{r_a^2}{\alpha_n} \end{aligned} \tag{A1}$$

The right side becomes

$$-\sum_{m=1}^{\infty} [\beta_m \int_0^{r_a} J_0(\alpha_m \frac{r}{r_a}) r J_0(\alpha_n \frac{r}{r_a}) dr] \tag{A2}$$

Since $J_0(\alpha_n r/r_a)$ is one of the solutions of Eq. (23),

$$\frac{1}{r} \frac{d(r \frac{dJ_0(\alpha_n \frac{r}{r_a})}{dr})}{dr} + (\frac{\alpha_n}{r_a})^2 J_0(\alpha_n \frac{r}{r_a}) = 0 \tag{A3}$$

or

$$J_0(\alpha_n \frac{r}{r_a}) = -(\frac{r_a}{\alpha_n})^2 \frac{1}{r} \frac{d[r \frac{dJ_0(\alpha_n \frac{r}{r_a})}{dr}]}{dr} \tag{A4}$$

$\int_0^{r_a} J_0(\alpha_m \frac{r}{r_a}) r J_0(\alpha_n \frac{r}{r_a}) dr$ in Eq. (A2) becomes

$$\begin{aligned} & \int_0^{r_a} J_0(\alpha_m \frac{r}{r_a}) r J_0(\alpha_n \frac{r}{r_a}) dr \\ &= -\int_0^{r_a} J_0(\alpha_m \frac{r}{r_a}) r (\frac{r_a}{\alpha_n})^2 \frac{1}{r} \frac{d[r \frac{dJ_0(\alpha_n \frac{r}{r_a})}{dr}]}{dr} dr \\ &= -(\frac{r_a}{\alpha_n})^2 \int_0^{r_a} J_0(\alpha_m \frac{r}{r_a}) d[r \frac{dJ_0(\alpha_n \frac{r}{r_a})}{dr}] \end{aligned}$$

$$\begin{aligned}
 &= -\left(\frac{r_a}{\alpha_n}\right)^2 \left[J_0\left(\alpha_m \frac{r}{r_a}\right) r \frac{dJ_0\left(\alpha_n \frac{r}{r_a}\right)}{dr} \Big|_0^{r_a} \right. \\
 &\quad \left. - \int_0^{r_a} r \frac{dJ_0\left(\alpha_n \frac{r}{r_a}\right)}{dr} dJ_0\left(\alpha_m \frac{r}{r_a}\right) \right] \\
 &= \left(\frac{r_a}{\alpha_n}\right)^2 \int_0^{r_a} r \frac{dJ_0\left(\alpha_n \frac{r}{r_a}\right)}{dr} \frac{dJ_0\left(\alpha_m \frac{r}{r_a}\right)}{dr} dr \tag{A5}
 \end{aligned}$$

By the same process,

$$\begin{aligned}
 &\int_0^{r_a} J_0\left(\alpha_n \frac{r}{r_a}\right) r J_0\left(\alpha_m \frac{r}{r_a}\right) dr \\
 &= \left(\frac{r_a}{\alpha_m}\right)^2 \int_0^{r_a} r \frac{dJ_0\left(\alpha_m \frac{r}{r_a}\right)}{dr} \frac{dJ_0\left(\alpha_n \frac{r}{r_a}\right)}{dr} dr \tag{A6}
 \end{aligned}$$

However,

$$\int_0^{r_a} J_0\left(\alpha_m \frac{r}{r_a}\right) r J_0\left(\alpha_n \frac{r}{r_a}\right) dr = \int_0^{r_a} J_0\left(\alpha_n \frac{r}{r_a}\right) r J_0\left(\alpha_m \frac{r}{r_a}\right) dr \tag{A7}$$

Eq. (A5) and Eq. (A6) are the same. Subtract Eq. (A5) by Eq. (A6) to obtain

$$0 = \left(\frac{1}{\alpha_n^2} - \frac{1}{\alpha_m^2}\right) r_a^2 \int_0^{r_a} r \frac{dJ_0\left(\alpha_m \frac{r}{r_a}\right)}{dr} \frac{dJ_0\left(\alpha_n \frac{r}{r_a}\right)}{dr} dr \tag{A8}$$

On the right side of Eq. (A8), either $m = n$ will make the first term zero, or the integration should be zero. Eq. (A8) verifies the orthogonality of Bessel function, meaning that the integration in Eq. (A2) must vanish when $m \neq n$. Eq. (A2) becomes

$$-\beta_n \int_0^{r_a} r J_0^2\left(\alpha_n \frac{r}{r_a}\right) dr \tag{A9}$$

Multiply both sides of Eq. (A4) by $2r \frac{dJ_0(\alpha_n r / r_a)}{dr}$. The left side becomes

$$2r \frac{dJ_0\left(\alpha_n \frac{r}{r_a}\right)}{dr} J_0\left(\alpha_n \frac{r}{r_a}\right) = r \frac{dJ_0^2\left(\alpha_n \frac{r}{r_a}\right)}{dr} \tag{A10}$$

The right side becomes

$$\begin{aligned}
 &-\left(\frac{r_a}{\alpha_n}\right)^2 \frac{1}{r} 2 \left[r \frac{dJ_0\left(\alpha_n \frac{r}{r_a}\right)}{dr} \right] \frac{dJ_0\left(\alpha_n \frac{r}{r_a}\right)}{dr} \\
 &= -\left(\frac{r_a}{\alpha_n}\right)^2 \frac{1}{r} \frac{d\left[r \frac{dJ_0\left(\alpha_n \frac{r}{r_a}\right)}{dr} \right]^2}{dr} \tag{A11}
 \end{aligned}$$

Combine Eq. (A10) and Eq. (A11) to obtain

$$r \frac{dJ_0^2\left(\alpha_n \frac{r}{r_a}\right)}{dr} = -\left(\frac{r_a}{\alpha_n}\right)^2 \frac{1}{r} \frac{d\left[r \frac{dJ_0\left(\alpha_n \frac{r}{r_a}\right)}{dr} \right]^2}{dr} \tag{A12}$$

$$-\left(\frac{r_a}{\alpha_n}\right)^2 \frac{d\left[r \frac{dJ_0\left(\alpha_n \frac{r}{r_a}\right)}{dr} \right]^2}{dr} = r^2 \frac{dJ_0^2\left(\alpha_n \frac{r}{r_a}\right)}{dr} \tag{A13}$$

Integrate both sides of Eq. (A13) with respect to r from 0 to r_a .

$$\begin{aligned}
 &-\left(\frac{r_a}{\alpha_n}\right)^2 \left[r \frac{dJ_0\left(\alpha_n \frac{r}{r_a}\right)}{dr} \right]^2 \Big|_0^{r_a} = \int_0^{r_a} r^2 dJ_0^2\left(\alpha_n \frac{r}{r_a}\right) \\
 &= r^2 J_0^2\left(\alpha_n \frac{r}{r_a}\right) \Big|_0^{r_a} - \int_0^{r_a} J_0^2\left(\alpha_n \frac{r}{r_a}\right) 2r dr = 0 - 2 \int_0^{r_a} r J_0^2\left(\alpha_n \frac{r}{r_a}\right) dr \tag{A14}
 \end{aligned}$$

Eq. (A9) and Eq. (A2) become

$$\begin{aligned}
 &-\beta_n \int_0^{r_a} r J_0^2\left(\alpha_n \frac{r}{r_a}\right) dr = -\beta_n \frac{1}{2} \left(\frac{r_a}{\alpha_n}\right)^2 \left[r \frac{dJ_0\left(\alpha_n \frac{r}{r_a}\right)}{dr} \right]^2 \Big|_0^{r_a} \\
 &= -\beta_n \frac{1}{2} \left(\frac{r_a}{\alpha_n}\right)^2 \left[-r J_1\left(\alpha_n \frac{r}{r_a}\right) \frac{\alpha_n}{r_a} \right]^2 \Big|_0^{r_a} = -\beta_n \frac{1}{2} r_a^2 J_1^2(\alpha_n) \tag{A15}
 \end{aligned}$$

Combine Eq. (A1) and Eq. (A15) to obtain

$$\beta_n = -c_\infty \frac{2}{\alpha_n J_1(\alpha_n)} \tag{A16}$$

or

$$\beta_m = -c_\infty \frac{2}{\alpha_m J_1(\alpha_m)} \quad (\text{A17})$$

ACKNOWLEDGMENTS

The authors would like to thank the National Science Council of the Republic of China, Taiwan for financially supporting this research under Contract No. (NSC97-2221-E-224-054).

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