ADVANCING DIFFUSION MODEL FOR DIFFUSION IN A CUBE OF MEDIUM

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ABSTRACT

A solution based on an advancing model for the content of diffusion material in a cube of medium is derived. The cube is assumed to be surrounded by diffusion material, and the diffusion material penetrates through all six surfaces and diffuses toward the center of the cube. The model accounts for the interaction between the diffusions in the three principle coordinates of the Cartesian coordinate system. For the first time, an exact solution of the content of the diffusion material based on the advancing model is derived in a clean form for a three-dimensional case.

Keywords: Advancing model, Diffusion.

1. INTRODUCTION

Fick's law has been used in many cases to interpret diffusion phenomena. The content of diffusion material in a medium is dependent on location, diffusion duration, material properties and environmental conditions.

Conventional solutions for the content of diffusion material do not take diffusion depth into consideration. Carslaw and Jaeger used a technique from Neumann to derive the solution of the content of diffusion material with an advancing boundary in a semi-infinite medium [1] named advancing model. Advancing model is a modification of conventional model. By applying a correction factor to the complementary solution of the conventional model, the solution of content of diffusion material in medium is adjusted to become a continuous function with a positive part and a negative part. The negative part does not make any sense physically. By forcing the negative part to be zero, the solution becomes a combination of a positive function and a zero zone. The boundary of the zero zone turns out to be the diffusion front. The diffusion depth is then defined mathematically. Since the diffusion front is moving continuously toward the depth of the medium, Carslaw and Jaeger named the diffusion front as moving boundary, and that does not appear in the conventional model. Chang, Wang, and Tsai applied the revised model to a case in which diffusion material penetrates symmetrically through both surfaces of a plate medium toward the opposite surface and named the solution based on the algorithm of moving boundary as advancing boundary model [2], advancing model in short. After the diffusion material reaches the center of the plate, the content distribution of the diffusion material can be derived by the TSAI (Two Sides' Anti-symmetric Images) technique [2,3].

Advancing model has never been applied in multi-dimensional cases such as cubic medium. This work applies the advancing model to a case of diffusion involving the three principle directions of the Cartesian coordinate system in diffusion problem for the first time. The solution of the content of the diffusion material in a cube medium is derived.

2. THEORY

When the initial content of the diffusion is zero, the governing equation of Fick's second diffusion law [1] is

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

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where, c is the content of the diffusion material in the medium, t is the diffusion duration, and D is diffusivity which is a positive constant. In the 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 of the Cartesian coordinate system. In an one dimensional case, Eq. (2) becomes

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

The boundary conditions are that the surfaces of the medium contacting the diffusion material saturate instantly and remain so through the whole diffusion process [1].

2.1 Semi-Infinite Medium

In a semi-infinite case, the medium exists only in the area where $x \geq 0$, and the diffusion material travels from $x = 0$ toward the depth of the medium (Fig. 1). The surface of the medium is assumed to become saturated instantly when the diffusion material contacts it. The solution of c is [1]

$$c(t; x) = c_{\infty L}\left[1 - \frac{2}{\sqrt{\pi}}\sum_{m=0}^{\infty}\frac{(-1)^m\left(\dfrac{x}{2\sqrt{Dt}}\right)^{2m+1}}{m!(2m+1)}\right] \tag{4}$$

where, $c_{\infty L}$ is the saturated c corresponding to the environmental conditions of the left hand side space where $x < 0$, and m is the index of the series in Eq. (4). The first part in parentheses on the right hand side of Eq. (4) is a constant which is a particular solution for Eq. (3), while the second part is a complementary solution depending on t and x. Equation (4) satisfies the boundary conditions that $c = c_{\infty L}$ at $x = 0$ once the diffusion starts.

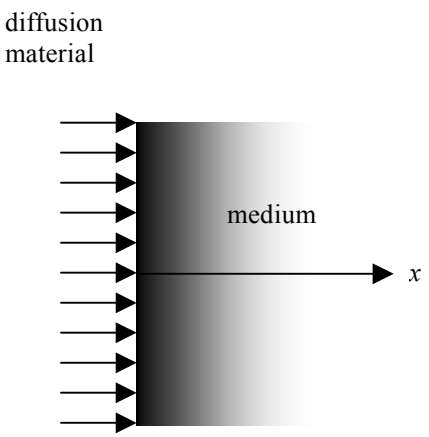


Fig. 1 Diffusion in A Semi-Infinite Medium

Based on the advancing model [1,2], Eq. (4) should be adjusted to

$$c(t; x) = c_{\infty L}\left[1 - \frac{\displaystyle\sum_{m=0}^{\infty}\frac{(-1)^m \xi^{2m+1}\nu^{2m+1}}{m!(2m+1)}}{\displaystyle\sum_{m=0}^{\infty}\frac{(-1)^m \nu^{2m+1}}{m!(2m+1)}}\right] \tag{5}$$

where $\xi = \min\left(\dfrac{x}{2\nu\sqrt{Dt}}, 1\right)$, and ν is a dimensionless constant named Neumann's constant after Franz Neumann [1]. The particular solution for Eq. (5) is the same as that for Eq. (4), and the complementary solution takes the same form as that of Eq. (4) but with a different constant coefficient. ξ is defined delicately to make Eq. (5) a continuous function when $x \leq 2\nu\sqrt{Dt}$ and zero when $x \geq 2\nu\sqrt{Dt}$, meaning that $2\nu\sqrt{Dt}$ is the diffusion depth, indicating the diffusion material has not yet reached a location deeper than $2\nu\sqrt{Dt}$. This result does not exist in Eq. (4) which is a asymptotic solution that approaches zero when x increases, but never becomes zero no mater the depth of x is or the shortness of t. Equation (5) also satisfies the boundary conditions that $c = c_{\infty L}$ at $x = 0$ once the diffusion starts. The complementary solution of Eq. (5) is zero at $x = 0$, which is a very important result and can be used in multi-dimensional cases.

2.2 Plate Medium

For the case of a plate-shaped medium, the medium material exists in the area $-h_x / 2 \leq x \leq h_x / 2$, and diffusion material travels from $x = -h_x / 2$ toward the center of the medium. The boundary condition for the left surface is the same as that found in the previous case, and c at the right surface remains zero due to the environmental conditions on the right hand side (Fig. 2). Before $2\nu\sqrt{Dt} > h_x$, the solution of c is the same as that for Eq. (5), but with a different location for the x coordinate.

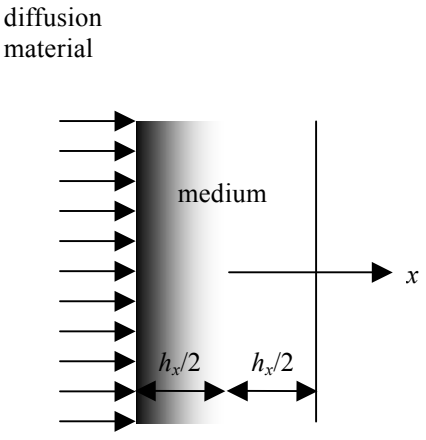


Fig. 2 Diffusion from Left Surface toward The Center of A Plate Shape Medium

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$$c(t;x)=c_{\infty L}\left[1-\frac{\sum_{m=0}^{\infty}\frac{(-1)^m\xi_1^{2m+1}\nu^{2m+1}}{m!(2m+1)}}{\sum_{m=0}^{\infty}\frac{(-1)^m\nu^{2m+1}}{m!(2m+1)}}\right] \tag{6}$$

where

$$\xi_1=\min\left(\frac{h_x/2+x}{2\nu\sqrt{Dt}},1\right) \tag{7a}$$

Equation (6) satisfies the boundary conditions that $c = c_{\infty L}$ at $x = -h_x / 2$, and $c = 0$ at $x = h_x / 2$ due to Eq. (7a).

If the diffusion material travels from $x = h_x / 2$ toward the center of the medium (Fig. 3), c becomes

$$c(t;x)=c_{\infty R}\left[1-\frac{\sum_{m=0}^{\infty}\frac{(-1)^m\xi_2^{2m+1}\nu^{2m+1}}{m!(2m+1)}}{\sum_{m=0}^{\infty}\frac{(-1)^m\nu^{2m+1}}{m!(2m+1)}}\right] \tag{8}$$

where

$$\xi_2=\min\left(\frac{h_x/2-x}{2\nu\sqrt{Dt}},1\right) \tag{7b}$$

and $c_{\infty R}$ is the saturated c corresponding to the environmental condition on the right hand side space where $x > 0$. Equation (8) satisfies the boundary conditions that $c = 0$ at $x = -h_x / 2$, and $c = c_{\infty R}$ at $x = h_x / 2$.

If the diffusion material travels from both surfaces toward the center of the medium (Fig. 4), c should be the combination of Eqs. (6) and (8).

$$\begin{aligned}c(t;x)=&c_{\infty L}\left[1-\frac{\sum_{m=0}^{\infty}\frac{(-1)^m\xi_1^{2m+1}\nu^{2m+1}}{m!(2m+1)}}{\sum_{m=0}^{\infty}\frac{(-1)^m\nu^{2m+1}}{m!(2m+1)}}\right]\\&+c_{\infty R}\left[1-\frac{\sum_{m=0}^{\infty}\frac{(-1)^m\xi_2^{2m+1}\nu^{2m+1}}{m!(2m+1)}}{\sum_{m=0}^{\infty}\frac{(-1)^m\nu^{2m+1}}{m!(2m+1)}}\right]\end{aligned} \tag{9a}$$

Rearrange Eq. (9a) to obtain

$$\frac{c(t;x)}{c_{\infty L}}=1-\frac{\sum_{m=0}^{\infty}\frac{(-1)^m\left(\xi_1^{2m+1}+\frac{c_{\infty R}}{c_{\infty L}}\xi_2^{2m+1}-\frac{c_{\infty R}}{c_{\infty L}}\right)\nu^{2m+1}}{m!(2m+1)}}{\sum_{m=0}^{\infty}\frac{(-1)^m\nu^{2m+1}}{m!(2m+1)}} \tag{9b}$$

Equation (9b) contains two parts, a particular solution, one, and a complementary solution. Equation (9b) satisfies the boundary conditions that $c = c_{\infty L}$ at $x = -h_x / 2$, and $c = c_{\infty R}$ at $x = h_x / 2$. The most important result is that the complementary solution is zero at $x = \pm h_x / 2$.

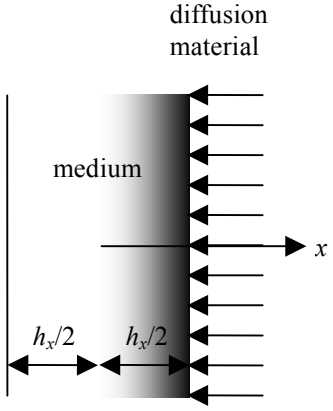


Fig. 3 Diffusion from Right Surface toward The Center of A Plate Shape Medium

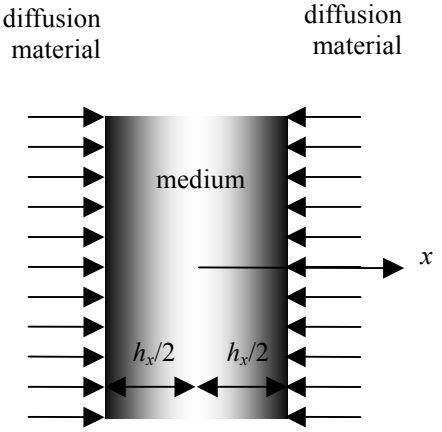


Fig. 4 Diffusion from Both Surfaces toward The Center of A Plate Shape Medium

At the critical moment when the diffusion material reaches the center of the plate

$$t=t_{cx}=h_x^2/(16\nu^2D) \tag{10a}$$

Equation (9a) becomes

$$\begin{aligned}c(t_{cx};x)=&c_{\infty L}\left[1-\frac{\sum_{m=0}^{\infty}\frac{(-1)^m\xi_{1c}^{2m+1}\nu^{2m+1}}{m!(2m+1)}}{\sum_{m=0}^{\infty}\frac{(-1)^m\nu^{2m+1}}{m!(2m+1)}}\right]\\&+c_{\infty R}\left[1-\frac{\sum_{m=0}^{\infty}\frac{(-1)^m\xi_{2c}^{2m+1}\nu^{2m+1}}{m!(2m+1)}}{\sum_{m=0}^{\infty}\frac{(-1)^m\nu^{2m+1}}{m!(2m+1)}}\right]\end{aligned} \tag{11}$$

where

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$$\xi_{1c} = \min\left(1 + \frac{x}{h_x/2}, 1\right) \tag{12a}$$

$$\xi_{2c} = \min\left(1 - \frac{x}{h_x/2}, 1\right) \tag{12b}$$

when diffusion material reaches the center of the plate, the diffusion material from both surfaces starts to interact, and Eq. (9a) is no longer correct. c must be resolved based on the condition of Eq. (11) after $t \geq t_{cx}$.

By separation variable, let $c(t; x) = T(t)\, X(x)$, where T is a function of t, and X is a function of x. Equation (3) becomes

$$\dot{T}X = DTX'' \quad \text{or} \quad \frac{1}{D}\frac{\dot{T}}{T} = \frac{X''}{X} \tag{13}$$

The left hand side of the second term of Eq. (13) depends on t only, while the right hand side depends on x only. To make them compatible in one equation, let

$$\frac{1}{D}\frac{\dot{T}}{T} = \frac{X''}{X} = -k, \;\; k: \text{constant} \quad \text{or} \quad \begin{cases} \dot{T} + kDT = 0 \\ X'' + kX = 0 \end{cases} \tag{14}$$

For $k = 0$,

$$\begin{cases} T = K_1, \quad K_1: \text{constant} \\ X = K_2 + K_3 x, \quad K_2, K_3: \text{constants} \end{cases} \tag{15}$$

For this particular condition, the solution of c is

$$c(t; x) = K_1 K_2 + K_1 K_3 x = \alpha_0 + \alpha_1 x, \quad \alpha_0, \alpha_1: \text{constants} \tag{16}$$

For $k \neq 0$, let

$$T = K_4\, e^{-kDt}, \quad K_4: \text{constant} \tag{17}$$

$$X = K_5 \cos(\sqrt{k}x) + K_6 \sin(\sqrt{k}x), \quad K_5, K_6: \text{constants} \tag{18}$$

The solutions of c is

$$\begin{aligned} c(t; x) &= K_4 K_5 e^{-kDt} \cos(\sqrt{k}x) + K_4 K_6 e^{-kDt} \sin(\sqrt{k}x) \\ &= \alpha_2\, e^{-kDt} \cos(\sqrt{k}x) + \alpha_3\, e^{-kDt} \sin(\sqrt{k}x), \\ &\quad \alpha_2, \alpha_3: \text{constants} \end{aligned} \tag{19}$$

To ensure that T does not become ∞ as t approaches ∞, k must be positive for the positive D. For the multi-value of k, k_n, $n = 1, 2, 3, \ldots$.

$$c(t; x) = \sum_{n=1}^{\infty}\left[\alpha_{2n}\, e^{-k_n Dt} \cos(\sqrt{k_n}x) + \alpha_{3n}\, e^{-k_n Dt} \sin(\sqrt{k_n}x)\right], \quad k_n, \alpha_{2n}, \alpha_{3n}: \text{constants} \tag{20}$$

The general form of c is the combination of Eqs. (16) and (20).

$$c(t; x) = \alpha_0 + \alpha_1 x + \sum_{n=1}^{\infty}\left[\alpha_{2n}\, e^{-k_n Dt} \cos(\sqrt{k_n}x) + \alpha_{3n}\, e^{-k_n Dt} \sin(\sqrt{k_n}x)\right] \tag{21}$$

At $t = t_{cx}$, Eq. (21) becomes

$$c(t_{cx}; x) = \alpha_0 + \alpha_1 x + \sum_{n=1}^{\infty}\left[\alpha_{2n}\, e^{-k_n Dt_{cx}} \cos(\sqrt{k_n}x) + \alpha_{3n}\, e^{-k_n Dt_{cx}} \sin(\sqrt{k_n}x)\right] \tag{22}$$

Rearrange Eq. (22) to produce

$$c(t_{cx}; x) - \alpha_0 - \alpha_1 x = \sum_{n=1}^{\infty}\left[\alpha_{2n}\, e^{-k_n Dt_{cx}} \cos(\sqrt{k_n}x) + \alpha_{3n}\, e^{-k_n Dt_{cx}} \sin(\sqrt{k_n}x)\right] \tag{23}$$

The TSAI technique [2] is adopted herein. Let

$$\begin{cases} \alpha_0 = \dfrac{c_{\infty R} + c_{\infty L}}{2} \\ \alpha_1 = \dfrac{c_{\infty R} - c_{\infty L}}{h_x} \end{cases} \tag{24}$$

to make $c(t_{cx}; x) - \alpha_0 - \alpha_1 x = 0$ at $x = \pm h_x / 2$. Equation (23) becomes

$$c(t_{cx}; x) - \frac{c_{\infty R} + c_{\infty L}}{2} - \frac{c_{\infty R} - c_{\infty L}}{h_x} x = \sum_{n=1}^{\infty}\left[\alpha_{2n}\, e^{-k_n Dt_{cx}} \cos(\sqrt{k_n}x) + \alpha_{3n}\, e^{-k_n Dt_{cx}} \sin(\sqrt{k_n}x)\right] \tag{25}$$

Replacing the first term on the left hand side of Eq. (25) with Eq. (11), the left hand side of Eq. (25) becomes

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$$
\begin{cases}
c_{\infty L}\left[1-\dfrac{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\left(1+\dfrac{x}{h_x/2}\right)^{2m+1}\nu^{2m+1}}{m!(2m+1)}}{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\nu^{2m+1}}{m!(2m+1)}}\right]-\dfrac{c_{\infty R}+c_{\infty L}}{2}-\dfrac{c_{\infty R}-c_{\infty L}}{h_x}x, -\dfrac{h_x}{2}\le x\le 0\\
c_{\infty R}\left[1-\dfrac{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\left(1-\dfrac{x}{h_x/2}\right)^{2m+1}\nu^{2m+1}}{m!(2m+1)}}{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\nu^{2m+1}}{m!(2m+1)}}\right]-\dfrac{c_{\infty R}+c_{\infty L}}{2}-\dfrac{c_{\infty R}-c_{\infty L}}{h_x}x, 0\le x\le\dfrac{h_x}{2}
\end{cases}
$$

$$
=\begin{cases}
-\dfrac{c_{\infty R}-c_{\infty L}}{2}\left(1+\dfrac{x}{h_x/2}\right)-c_{\infty L}\dfrac{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\left(1+\dfrac{x}{h_x/2}\right)^{2m+1}\nu^{2m+1}}{m!(2m+1)}}{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\nu^{2m+1}}{m!(2m+1)}}, -\dfrac{h_x}{2}\le x\le 0\\
\dfrac{c_{\infty R}-c_{\infty L}}{2}\left(1-\dfrac{x}{h_x/2}\right)-c_{\infty R}\dfrac{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\left(1-\dfrac{x}{h_x/2}\right)^{2m+1}\nu^{2m+1}}{m!(2m+1)}}{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\nu^{2m+1}}{m!(2m+1)}}, 0\le x\le\dfrac{h_x}{2}
\end{cases}
\tag{26}
$$

Expand Eq. (26) into a stepwise periodic function with a period of $2h_x$.

$$
\begin{cases}
-\left[-\dfrac{c_{\infty R}-c_{\infty L}}{2}\left(1+\dfrac{-h_x-x}{h_x/2}\right)-c_{\infty L}\dfrac{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\left(1+\dfrac{-h_x-x}{h_x/2}\right)^{2m+1}\nu^{2m+1}}{m!(2m+1)}}{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\nu^{2m+1}}{m!(2m+1)}}\right], & -h_x\le x\le-\dfrac{h_x}{2}\\
-\dfrac{c_{\infty R}-c_{\infty L}}{2}\left(1+\dfrac{x}{h_x/2}\right)-c_{\infty L}\dfrac{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\left(1+\dfrac{x}{h_x/2}\right)^{2m+1}\nu^{2m+1}}{m!(2m+1)}}{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\nu^{2m+1}}{m!(2m+1)}}, & -\dfrac{h_x}{2}\le x\le 0\\
\dfrac{c_{\infty R}-c_{\infty L}}{2}\left(1-\dfrac{x}{h_x/2}\right)-c_{\infty R}\dfrac{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\left(1-\dfrac{x}{h_x/2}\right)^{2m+1}\nu^{2m+1}}{m!(2m+1)}}{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\nu^{2m+1}}{m!(2m+1)}}, & 0\le x\le\dfrac{h_x}{2}\\
-\left[\dfrac{c_{\infty R}-c_{\infty L}}{2}\left(1-\dfrac{h_x-x}{h_x/2}\right)-c_{\infty R}\dfrac{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\left(1-\dfrac{h_x-x}{h_x/2}\right)^{2m+1}\nu^{2m+1}}{m!(2m+1)}}{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\nu^{2m+1}}{m!(2m+1)}}\right], & \dfrac{h_x}{2}\le x\le h_x
\end{cases}
\tag{27}
$$

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Equation (27) is anti-symmetric with respect to $x = -h_x / 2$ and $x = h_x / 2$, while in the area of $-h_x / 2 \le x \le h_x / 2$, Eq. (27) is exactly the same as Eq. (26) which is the left hand side of Eq. (25). Express Eq. (27) by Fourier series.

$$a_0 + \sum_{n=1}^{\infty}\left[a_n \cos\left(\frac{2n\pi}{2h_x}x\right) + b_n \sin\left(\frac{2n\pi}{2h_x}x\right)\right] \tag{28}$$

where a_0, a_n and b_n are coefficients of Fourier series, n is the index of the series, and

$$a_0 = 0 \tag{29}$$

$$a_n = (c_{\infty R} + c_{\infty L})\frac{\sum_{m=0}^{\infty}\frac{(-1)^m a_{mn}\nu^{2m+1}}{m!(2m+1)}}{\sum_{m=0}^{\infty}\frac{(-1)^m \nu^{2m+1}}{m!(2m+1)}}, \quad n = 1, 3, 5, \ldots \tag{30}$$

where

$$a_{mn} = (2m+1)!\sum_{r=0}^{m}\left[\frac{(-1)^{r+1}}{(2m-2r)!(n\pi/2)^{2r+2}}\right] \tag{31}$$

where, r is the index of the series, and $a_n = 0$ when $n = 2, 4, 6, \ldots$

$$b_n = (c_{\infty R} - c_{\infty L})\frac{\sum_{m=0}^{\infty}\frac{(-1)^m b_{mn}\nu^{2m+1}}{m!(2m+1)}}{\sum_{m=0}^{\infty}\frac{(-1)^m \nu^{2m+1}}{m!(2m+1)}}, \quad n = 2, 4, 6, \ldots \tag{32}$$

where

$$b_{mn} = (2m+1)!\sum_{r=0}^{m}\left[\frac{(-1)^{r+1}}{(2m+1-2r)!(n\pi/2)^{2r+1}}\right] \tag{33}$$

and $b_n = 0$ when $n = 1, 3, 5, \ldots$. Compare the right hand side of Eq. (25) with Eq. (28) to obtain

$$\begin{cases} \sqrt{k_n} = \dfrac{n\pi}{h_x} \quad \text{or} \quad k_n = \left(\dfrac{n\pi}{h_x}\right)^2 \\ \alpha_{2n} = e^{k_n Dt_{cx}} a_n, \quad n = 1, 3, 5, \ldots \\ \alpha_{3n} = e^{k_n Dt_{cx}} b_n, \quad n = 2, 4, 6, \ldots \end{cases} \tag{34}$$

Equation (21) becomes

$$\begin{aligned} c(t;x) = {} & \frac{c_{\infty R} + c_{\infty L}}{2} + \frac{c_{\infty R} - c_{\infty L}}{h_x}x \\ & + (c_{\infty R} + c_{\infty L})\frac{\sum_{n=1,3,5,\ldots}^{\infty}\left[e^{-\left(\frac{n\pi}{h_x}\right)^2 D(t-t_{cx})}\sum_{m=0}^{\infty}\frac{(-1)^m a_{mn}\nu^{2m+1}}{m!(2m+1)}\cos\left(\frac{n\pi}{h_x}x\right)\right]}{\sum_{m=0}^{\infty}\frac{(-1)^m \nu^{2m+1}}{m!(2m+1)}} \\ & + (c_{\infty R} - c_{\infty L})\frac{\sum_{n=2,4,6,\ldots}^{\infty}\left[e^{-\left(\frac{n\pi}{h_x}\right)^2 D(t-t_{cx})}\sum_{m=0}^{\infty}\frac{(-1)^m b_{mn}\nu^{2m+1}}{m!(2m+1)}\sin\left(\frac{n\pi}{h_x}x\right)\right]}{\sum_{m=0}^{\infty}\frac{(-1)^m \nu^{2m+1}}{m!(2m+1)}} \end{aligned} \tag{35}$$

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As a result,

$$c(t;x)=\begin{cases} c_{\infty L}\left[1-\dfrac{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\xi_1^{2m+1}\nu^{2m+1}}{m!(2m+1)}}{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\nu^{2m+1}}{m!(2m+1)}}\right]+c_{\infty R}\left[1-\dfrac{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\xi_2^{2m+1}\nu^{2m+1}}{m!(2m+1)}}{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\nu^{2m+1}}{m!(2m+1)}}\right], & t\le t_{cx} \\ \dfrac{c_{\infty R}+c_{\infty L}}{2}+\dfrac{c_{\infty R}-c_{\infty L}}{h_x}x \\ +(c_{\infty R}+c_{\infty L})\dfrac{\displaystyle\sum_{n=1,3,5,\ldots}^{\infty}\left[e^{-\left(\frac{n\pi}{h_x}\right)^2 D(t-t_{cx})}\sum_{m=0}^{\infty}\dfrac{(-1)^m a_{mn}\nu^{2m+1}}{m!(2m+1)}\cos\left(\dfrac{n\pi}{h_x}x\right)\right]}{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\nu^{2m+1}}{m!(2m+1)}} \\ +(c_{\infty R}-c_{\infty L})\dfrac{\displaystyle\sum_{n=1,3,5,\ldots}^{\infty}\left[e^{-\left(\frac{n\pi}{h_x}\right)^2 D(t-t_{cx})}\sum_{m=0}^{\infty}\dfrac{(-1)^m b_{mn}\nu^{2m+1}}{m!(2m+1)}\sin\left(\dfrac{n\pi}{h_x}x\right)\right]}{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\nu^{2m+1}}{m!(2m+1)}}, & t\ge t_{cx} \end{cases} \tag{36}$$

In the special case, where the boundary conditions are $c_{\infty L}=c_{\infty R}=c_\infty$, Eq. (36) becomes

$$c(t;x)=\begin{cases} c_\infty\left[1-\dfrac{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\xi_1^{2m+1}\nu^{2m+1}}{m!(2m+1)}}{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\nu^{2m+1}}{m!(2m+1)}}\right]+c_\infty\left[1-\dfrac{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\xi_2^{2m+1}\nu^{2m+1}}{m!(2m+1)}}{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\nu^{2m+1}}{m!(2m+1)}}\right], & t\le t_{cx} \\ c_\infty\left\{1+2\dfrac{\displaystyle\sum_{n=1,3,5,\ldots}^{\infty}\left[e^{-\left(\frac{n\pi}{h_x}\right)^2 D(t-t_{cx})}\sum_{m=0}^{\infty}\dfrac{(-1)^m a_{mn}\nu^{2m+1}}{m!(2m+1)}\cos\left(\dfrac{n\pi}{h_x}x\right)\right]}{\displaystyle\sum_{m=0}^{\infty}\dfrac{(-1)^m\nu^{2m+1}}{m!(2m+1)}}\right\}, & t\ge t_{cx} \end{cases} \tag{37a}$$

Rearrange Eq. (37a) to obtain

$$\frac{c(t;x)}{c_\infty}=1-\frac{\displaystyle\sum_{m=0}^{\infty}\frac{(-1)^m\Phi_{mx}\nu^{2m+1}}{m!(2m+1)}}{\displaystyle\sum_{m=0}^{\infty}\frac{(-1)^m\nu^{2m+1}}{m!(2m+1)}} \tag{37b}$$

where

$$\Phi_{mx}=\begin{cases}\xi_1^{2m+1}+\xi_2^{2m+1}-1, & t\le t_{cx}\\ (-2)\displaystyle\sum_{n=1,3,5,\ldots}^{\infty}a_{mn}\,e^{-\left(\frac{n\pi}{h_x}\right)^2 D(t-t_{cx})}\cos\left(\dfrac{n\pi}{h_x}x\right), & t\ge t_{cx}\end{cases} \tag{38a}$$

Equations (37b) and.(38a) indicate that c changes its form at the critical moment t_{cx}. When $t\le t_{cx}$, two terms in Eq. (37a) stand for two groups of diffusion material moving from both surfaces toward the center of the plate. In each term, there is a constant and a function depending on t and x. At the critical moment t_{cx}, the diffusion material of the two groups reaches the center of the plate and starts to interact. Equation (37b) shows that the solution of c includes two parts: A constant particular solution, one, and a complementary solution. Equation (37b) satisfies the boundary conditions that $c=c_\infty$ at $x=\pm h_x/2$, where the complementary solution of Eq. (37b) is zero.

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2.3 Cubic Medium

In a three-dimensional case, the governing equation should be Eq. (2), and c depends not only on t and x, but also on y and z. Let $c = c(t; x, y, z)$. For a cube of medium, the medium material exists in the area $-h_x / 2 \le x \le h_x / 2$, $-h_y / 2 \le y \le h_y / 2$, and $-h_z / 2 \le z \le h_z / 2$ (Fig. 5). The specimen is surrounded by diffusion material which penetrates the six surfaces and travels toward the center. Once the boundaries contact diffusion material around the specimen, they are assumed to become saturated instantly and remain so through the whole diffusion process. The saturated c is c_∞, which depends on the environmental condition around the specimen. Based on separation variable technique, let

$$\frac{c(t; x, y, z)}{c_\infty} = 1 + F(t; x)F(t; y)F(t; z) \tag{39}$$

where 1 is the particular solution, as shown in Eq. (37b). $F(t; x)$ is a function depending on t and x, $F(t; y)$ is a function depending on t and y, $F(t; z)$ is a function depending on t and z, and because all the conditions in x, y and z directions are the same, these three terms should be in the same form. The combination, $F(t; x)\,F(t; y)\,F(t; z)$, is the complementary solution. Both the particular solution and complementary solution satisfy Eq. (2).

$$\begin{aligned}&\frac{\partial F(t; x)}{\partial t}F(t; y)F(t; z) + F(t; x)\frac{\partial F(t; y)}{\partial t}F(t; z)\\&+F(t; x)F(t; y)\frac{\partial F(t; z)}{\partial t}\\&= D\left[\frac{\partial^2 F(t; x)}{\partial x^2}F(t; y)F(t; z)\right.\\&\left.+F(t; x)\frac{\partial^2 F(t; y)}{\partial y^2}F(t; z) + F(t; x)F(t; y)\frac{\partial^2 F(t; z)}{\partial z^2}\right]\end{aligned} \tag{40}$$

Rearrange Eq. (40) to obtain

$$\begin{aligned}&\frac{\dfrac{\partial F(t; x)}{\partial t} - D\dfrac{\partial^2 F(t; x)}{\partial x^2}}{F(t; x)} + \frac{\dfrac{\partial F(t; y)}{\partial t} - D\dfrac{\partial^2 F(t; y)}{\partial y^2}}{F(t; y)}\\&+\frac{\dfrac{\partial F(t; z)}{\partial t} - D\dfrac{\partial^2 F(t; z)}{\partial z^2}}{F(t; z)} = 0\end{aligned} \tag{41}$$

To make the three terms on the left hand side of Eq. (41) compatible in one equation, they must all be zero.

$$\frac{\partial F(t; x)}{\partial t} - D\frac{\partial^2 F(t; x)}{\partial x^2} = 0 \tag{42a}$$

$$\frac{\partial F(t; y)}{\partial t} - D\frac{\partial^2 F(t; y)}{\partial y^2} = 0 \tag{42b}$$

$$\frac{\partial F(t; z)}{\partial t} - D\frac{\partial^2 F(t; z)}{\partial z^2} = 0 \tag{42c}$$

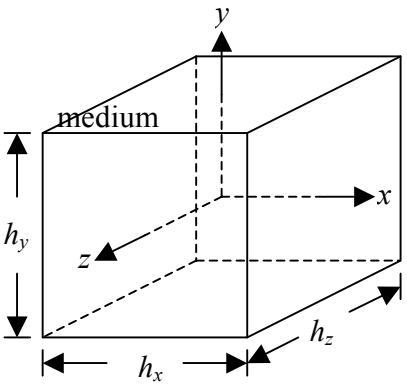


Fig. 5 A Cube of Medium

The particular solution is accounted for in Eq. (39). Since Eqs. (42a), (42b) and (42c) are exactly the same as Eq. (3), and the boundary conditions for all the six surfaces are the same as those for a plate specimen with symmetric diffusion, the solution for $F(t; x)$, $F(t; y)$ and $F(t; z)$ should take the form of the complementary solutions of Eq. (37b). As a result, Eq. (39) becomes

$$\begin{aligned}&\frac{c(t; x, y, z)}{c_\infty}\\&= 1 - \frac{\displaystyle\sum_{m=0}^{\infty}\frac{(-1)^m \Phi_{mx}\nu^{2m+1}}{m!(2m+1)}\sum_{m=0}^{\infty}\frac{(-1)^m \Phi_{my}\nu^{2m+1}}{m!(2m+1)}\sum_{m=0}^{\infty}\frac{(-1)^m \Phi_{mz}\nu^{2m+1}}{m!(2m+1)}}{\left[\displaystyle\sum_{m=0}^{\infty}(-1)^m\frac{\nu^{2m+1}}{m!(2m+1)}\right]^3}\end{aligned} \tag{43}$$

where

$$\Phi_{my} = \begin{cases}\xi_3^{2m+1} + \xi_4^{2m+1} - 1, & t \le t_{cy}\\ (-2)\displaystyle\sum_{n=1,3,5,\ldots}^{\infty} a_{mn}\, e^{-\left(\frac{n\pi}{h_y}\right)^2 D(t-t_{cy})}\cos\left(\frac{n\pi}{h_y}y\right), & t \ge t_{cy}\end{cases} \tag{38b}$$

$$\Phi_{mz} = \begin{cases}\xi_5^{2m+1} + \xi_6^{2m+1} - 1, & t \le t_{cz}\\ (-2)\displaystyle\sum_{n=1,3,5,\ldots}^{\infty} a_{mn}\, e^{-\left(\frac{n\pi}{h_z}\right)^2 D(t-t_{cz})}\cos\left(\frac{n\pi}{h_z}z\right), & t \ge t_{cz}\end{cases} \tag{38c}$$

$$\xi_3 = \min\left(\frac{h_y/2 + y}{2\nu\sqrt{Dt}}, 1\right) \tag{7c}$$

$$\xi_4 = \min\left(\frac{h_y/2 - y}{2\nu\sqrt{Dt}}, 1\right) \tag{7d}$$

$$\xi_5 = \min\left(\frac{h_z/2 + z}{2\nu\sqrt{Dt}}, 1\right) \tag{7e}$$

$$\xi_6 = \min\left(\frac{h_z/2 - z}{2\nu\sqrt{Dt}}, 1\right) \tag{7f}$$

$$t_{cy} = h_y^2/(16\nu^2 D) \tag{10b}$$

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$$t_{cz} = h_z^2 /(16\nu^2 D) \tag{10c}$$

Equation (39) is based on the fact that all the complementary solutions are zero at all the boundaries so that Eq. (43) satisfies the boundary conditions that $c = c_\infty$ at all the boundaries.

If the initial c in the medium is not zero but c_i [1,4], Eq. (43) becomes

$$\frac{c(t; x, y, z) - c_i}{c_\infty - c_i} = 1 - \frac{\sum_{m=0}^{\infty} \frac{(-1)^m \Phi_{mx} \nu^{2m+1}}{m!(2m+1)} \sum_{m=0}^{\infty} \frac{(-1)^m \Phi_{my} \nu^{2m+1}}{m!(2m+1)} \sum_{m=0}^{\infty} \frac{(-1)^m \Phi_{mz} \nu^{2m+1}}{m!(2m+1)}}{\left[\sum_{m=0}^{\infty} (-1)^m \frac{\nu^{2m+1}}{m!(2m+1)}\right]^3} \tag{44}$$

3. DISCUSSION

Equation (44) is a very clean function carrying a particular solution, one, and a complementary solution. The complementary solution includes three parts of the same form standing for the effects from diffusion in the x, y and z directions. The numerator and denominator of each part are almost identical, except that the numerator has an extra term which changes its form at the critical diffusion duration.

For the case that $h_x = h_y = h_z$, $t_{cx} = t_{cy} = t_{cz}$. At the center of a equal-sided cube where $x = y = z = 0$, $\xi_1 = \xi_2 = \xi_3 = \xi_4 = \xi_5 = \xi_6 = 1$, Equation (44) becomes zero when $t \le t_{cx}$, and

$$\frac{c(t; 0, 0, 0) - c_i}{c_\infty - c_i} = 1 - \left[\frac{\sum_{m=0}^{\infty} \frac{(-1)^m \Phi_{mx} \nu^{2m+1}}{m!(2m+1)}}{\sum_{m=0}^{\infty} (-1)^m \frac{\nu^{2m+1}}{m!(2m+1)}}\right]^3, \quad t \ge t_{cx} \tag{45}$$

where

$$\Phi_{mx} = \Phi_{my} = \Phi_{mz} = (-2) \sum_{n=1,3,5,\ldots}^{\infty} a_{mn} e^{-\left(\frac{n\pi}{h_x}\right)^2 D(t - t_{cx})} \tag{46}$$

The conventional solution for the same case [1,3] is

$$\frac{c(t; 0, 0, 0) - c_i}{c_\infty - c_i} = 1 - \frac{64}{\pi^3} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \sum_{r=0}^{\infty} \frac{(-1)^{m+n+r} e^{-\frac{\pi^2 D\left[(2m+1)^2 + (2n+1)^2 + (2r+1)^2\right] t}{h_x^2}}}{(2m+1)(2n+1)(2r+1)} \tag{47}$$

Equation (45) has two material properties, ν and D, while there is only one property in Eq. (47), D. Figure 6 plots $[c(t; 0, 0, 0) - c_i]/(c_\infty - c_i)$ versus Dt / h_x^2 calculated from Eqs. (45) and (47). When $Dt / h_x^2 = 0.16$,

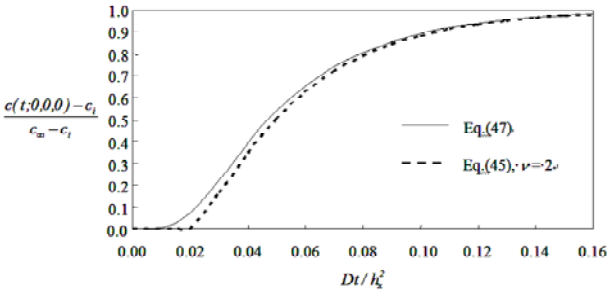


Fig. 6 Change Ratio of Content of Diffusion Material versus Dt/h_x^2 at The Center of A Cube of Medium

$c(t; 0, 0, 0)$ is very close to that of saturated status, and $[c(t; 0, 0, 0) - c_i]/(c_\infty - c_i)$ is just 2% less than 1. Define ν to be 2 to make Dt_{cx} / h_x^2 roughly equal 10% of 0.16.

No mater how close the data from the two equations end up being, they are quite different from each other at the beginning. Equation (45) shows an initial zero zone at the beginning, but Eq. (47) does not. This result of Eq. (45) makes perfect sense, because it takes time for the molecules of the diffusion material to travel from the surfaces to the center of the cube. It is impossible for any molecule to suddenly appear at the center of the cube as soon as the diffusion process starts. Equation (47) is positive as long as $t > 0$, meaning that some diffusion material suddenly appears at the center of the cube at the start of the diffusion process. The change of content could be small, but is definitely not zero. This result does not make any physical sense.

4. CONCLUSIONS

The algorithm of advancing model for studying diffusion in semi-infinite medium has been presented by Carslaw and Jaeger in 1959, but has never been applied to multi-dimensional cases after that. In reality, specimens used in experiment can never be semi-infinite. Normally, they are cubic, cylinder, plate or rod specimens with finite dimensions. Cubic specimens are popular ones, because preparing them is easy and diffusion process through all six surfaces of a cube is fast.

One of the studies for characterizing the diffusivity of mortar against natural diffusion of chloride needs 5cm × 5cm × 5cm cubic specimens to yield useful data in reasonable time. Analyzing data of content of diffusion material in cubic specimens needs an analytic solution. The multi-dimensional solution presented herein takes into consideration the advancing boundary condition and is novel.

Because the governing equation is exactly the same as that for heat conduction [5], this result can be applied to heating conduction problems for a cubic specimen in an environment with elevated temperatures.

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NOMENCLATURES

a_0, a_n, b_n: Constants of Fourier series

a_{mn} : $a_{mn} = \sum_{r=0}^{m}\left[\frac{(-1)^{r+1}(2m+1)!}{(2m-2r)!}\frac{1}{(n\pi/2)^{2r+2}}\right]$

b_{mn} : $b_{mn} = \sum_{r=0}^{m}\left[\frac{(-1)^{r+1}(2m+1)!}{(2m+1-2r)!}\frac{1}{(n\pi/2)^{2r+1}}\right]$

c : Content of diffusion material in medium
c_i : Initial c
c_∞ : Saturated c
$c_{\infty L}$: c_∞ corresponding to the environmental condition on the left hand side of a plate shape medium
$c_{\infty R}$: c_∞ corresponding to the environmental condition on the right hand side of a plate shape medium
D : Diffusivity
F : A function of t and x (or y, or z)
h_x : Thickness of a plate shape medium or a cubic medium
h_y : Width of a cubic medium
h_z : High of a cubic medium
$K_{1,2,3,4,5,6}$: Constants
k : Constant
k_n : Constants
m, n, r : Indices of series function
T : A function of t
t : Diffusion duration
t_{cx} : $t_{cx} = h_x^2/(16\nu^2 D)$
t_{cy} : $t_{cy} = h_y^2/(16\nu^2 D)$
t_{cz} : $t_{cz} = h_z^2/(16\nu^2 D)$
X : A function of x
x, y, z : Coordinates of Cartesian coordinate system
$\alpha_{0,1,2,3,2n,3n}$: Constants

Φ_{mx} :

$$\Phi_{mx} = \begin{cases} \xi_1^{2m+1} + \xi_2^{2m+1} - 1, & t \le t_{cx} \\ (-2)\sum_{n=1,3,5,\ldots}^{\infty} a_{mn}\, e^{-\left(\frac{n\pi}{h_x}\right)^2 D(t-t_{cx})} \cos\left(\frac{n\pi}{h_x}x\right), & t \ge t_{cx} \end{cases}$$

Φ_{my} :

$$\Phi_{my} = \begin{cases} \xi_3^{2m+1} + \xi_4^{2m+1} - 1, & t \le t_{cy} \\ (-2)\sum_{n=1,3,5,\ldots}^{\infty} a_{mn}\, e^{-\left(\frac{n\pi}{h_y}\right)^2 D(t-t_{cy})} \cos\left(\frac{n\pi}{h_y}y\right), & t \ge t_{cy} \end{cases}$$

Φ_{mz} :

$$\Phi_{mz} = \begin{cases} \xi_5^{2m+1} + \xi_6^{2m+1} - 1, & t \le t_{cz} \\ (-2)\sum_{n=1,3,5,\ldots}^{\infty} a_{mn}\, e^{-\left(\frac{n\pi}{h_z}\right)^2 D(t-t_{cz})} \cos\left(\frac{n\pi}{h_z}z\right), & t \ge t_{cz} \end{cases}$$

ξ : $\xi = \min\left(\frac{x}{2\nu\sqrt{Dt}}, 1\right)$

ξ_1 : $\xi_1 = \min\left(\frac{h_x/2 + x}{2\nu\sqrt{Dt}}, 1\right)$

ξ_{1c} : $\xi_{1c} = \min\left(1 + \frac{x}{h_x/2}, 1\right)$

ξ_2 : $\xi_2 = \min\left(\frac{h_x/2 - x}{2\nu\sqrt{Dt}}, 1\right)$

ξ_{2c} : $\xi_{2c} = \min\left(1 - \frac{x}{h_x/2}, 1\right)$

ξ_3 : $\xi_3 = \min\left(\frac{h_y/2 + y}{2\nu\sqrt{Dt}}, 1\right)$

ξ_4 : $\xi_4 = \min\left(\frac{h_y/2 - y}{2\nu\sqrt{Dt}}, 1\right)$

ξ_5 : $\xi_5 = \min\left(\frac{h_z/2 + z}{2\nu\sqrt{Dt}}, 1\right)$

ξ_6 : $\xi_6 = \min\left(\frac{h_z/2 - z}{2\nu\sqrt{Dt}}, 1\right)$

ν : Neumann's constant

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