

**SOLUTIONS OF DIFFUSION EQUATION WITH CONSTANT
DIFFUSION AND SURFACE EMISSION COEFFICIENTS**

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ABSTRACT

Closed-form solutions of the non-steady state diffusion equation with constant transport coefficients are presented. The diffusion coefficient is assumed to be finite, but the surface emission coefficient can be either finite or infinite. Mathematical conditions are established for the transport coefficients to be constant. When these conditions are met, the transport coefficients can then be easily evaluated. Diffusion test data can be compared against these conditions to determine whether or not the transport coefficients are constant. Desorption test data of northern red oak indicate that initial moisture content in wood and equilibrium moisture content in the environment are closely related to the constancy of the transport coefficients.

INTRODUCTION

This paper presents closed-form solutions of the non-steady state diffusion equation with the transport coefficients specified as (1) diffusion coefficient is constant and finite and surface emission coefficient is infinite and (2) both diffusion and surface emission coefficients are constant and finite. The solution of the former is contained in that of the latter. Infinite-series solutions for these cases are quoted by Carslaw and Jaeger [3], Crank [7], and others.

In the mathematical theory of diffusion, the diffusion coefficient can be taken as constant in some cases, such as diffusion in dilute solutions. In other cases, such as diffusion in high polymers the diffusion coefficient depends very markedly on the concentration of diffusing substance [7]. For moisture diffusion in wood, inconsistent observations *or assumptions exist in the literature*. Some authors have reported a strong moisture dependence of the diffusion coefficient (e.g., Høugen et al. [9], Meroney [13], Simpson [18], Skaar [20], Van Arsdell [23]), while others have taken the diffusion coefficient as constant (e.g., Avramidis and Siau [1], Choong and Skaar [5], Droin et al. [8], Mounji et al. [15], Soderstrom and Salin [21]). The surface emission coefficient, defined as a constant of proportionality [7], has been reported to depend on the ambient or environmental conditions either completely (e.g., Avramidis and Siau [1], Wadso [24]) or in combination with material surface conditions (e.g., Choong and Skaar [5], Liu and Simpson [12], Rosen [17], Simpson [18], Simpson and Liu [19]). In addition, some authors have chosen to set the surface emission coefficient equal to infinity in analyzing their test data (e.g., Biggerstaff [2], Choong and Fogg [4], Cornstock [6], McNamara and Hart [14]).

To a great extent, this lack of consistency is due to the limited information that can be derived from the infinite-series solutions. With the closed-form solutions of the diffusion equation established in the present study, we also derived the mathematical conditions under which the diffusion and surface emission coefficients can be taken as constant. By comparing any diffusion test data against those conditions, it can easily be seen whether or not the transport coefficients are constant. Resorption data of northern red oak (*Quercus rubra*) are included to demonstrate the application of the derived equations.

BASIC EQUATIONS AND ANALYSES

In a one-dimensional formulation with the diffusing substance moving in the direction normal to a sheet of medium of thickness $2a$, the diffusion equation can be written as

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial X} \left(D \frac{\partial C}{\partial X} \right) \quad (0 < X < a, t > 0) \quad (1)$$

where C is concentration of the diffusing substance, t is time, D is diffusion coefficient assumed to be constant in this study, and X is space coordinate measured from the center of the sheet.

Let the initial condition be

$$C = C_0 \quad (0 < X < a, t = 0) \quad (2)$$

where C_0 is a constant concentration in the medium, and let the boundary conditions be

$$\frac{\partial C}{\partial X} = 0 \quad (X = 0, t \geq 0) \quad (3)$$

$$D \frac{\partial C}{\partial X} = S(C_e - C) \quad (X = a, t > 0) \quad (4)$$

where S is surface emission coefficient and C_e is equilibrium concentration

corresponding to the vapor pressure in the environment remote from the surface of the sheet. Note that Equation (4) prescribes the boundary condition just within the surface of the sheet [7].

Equations (1) to (4) apply to sorption and desorption. When sorption defines diffusing substance entering the medium and resorption defines diffusing substance leaving the medium [7], these equations are the same in dimensionless formulation. However, when sorption defines diffusing substance entering the medium but resorption defines diffusing substance remaining in the medium (Liu [10], Talbot and Kitchener [22]), these equations are not the same in dimensionless formulation for sorption and resorption.

Sorption

$$\text{Let } c = (C - C_0)/(C_e - C_0), \quad \tau = Dt/a^2, \text{ and } x = X/a.$$

Equations (1) to (4) can be put in dimensionless form in the same order as previously presented

$$\frac{\partial c}{\partial \tau} = \frac{\partial^2 c}{\partial x^2} \quad (0 < x < 1, \tau > 0) \quad (5)$$

$$c = 0 \quad (0 < x < 1, \tau = 0) \quad (6)$$

$$\frac{\partial c}{\partial x} = 0 \quad (x = 0, \tau \geq 0) \quad (7)$$

$$\frac{1}{L} \frac{\partial c}{\partial x} + c = 1 \quad (x = 1 - \epsilon, \tau > 0) \quad (8)$$

Desorption

Let $c = (C - C_e)/(C_0 - C_e)$, $\tau = Dt/a^2$ and $x = X/a$. Equations (1) to (4) can likewise be put in dimensionless form in the same order as previously

presented:

$$\frac{\partial c}{\partial \tau} = \frac{\partial^2 c}{\partial x^2} \quad (0 < x < 1, \tau > 0) \tag{9}$$

$$c = 1 \quad (0 < x < 1, \tau = 0) \tag{10}$$

$$\frac{\partial c}{\partial x} = 0 \quad (x = 0, \tau \geq 0) \tag{11}$$

$$\frac{1}{L} \frac{\partial c}{\partial x} + c = 0 \quad (x = 1 - \epsilon, \tau > 0) \tag{12}$$

MATHEMATICAL DEVELOPMENT

The transport coefficients D and S are both positive and, in the present study, constant. However, the cases where S is either finite or infinite are treated separately in the literature.

Sorption with $S = \infty$

Let

$$M(\tau) = \int_0^{1-\epsilon} c(\tau, x) dx \quad (\epsilon \rightarrow 0) \tag{13}$$

The fraction of total concentration in the medium, E , [7] is

$$E = \frac{M(\tau)}{M(\infty)} = 1 - \frac{8}{\pi^2} \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} \exp \left[- \left(n + \frac{1}{2} \right)^2 \pi^2 \tau \right] \tag{14}$$

which can be expressed in closed form as follows [10]:

$$\tau = \frac{\pi E^2}{4} \quad E \leq 0.52 \tag{15a}$$

and

$$\tau = \frac{4}{\pi^2} \ln \left[\frac{\pi^2 (1-E)}{8} \right] \quad E > 0.52 \quad (15b)$$

The largest deviation of Equations (15) from Equation (14) occurs at $E = 0.52$, where Equation (14) gives $\tau = 0.2131$ and Equation (15a) gives $\tau = 0.2124$, the error being about 0.3%.

Desorption with $S = \infty$

From the dimensionless concentration defined for sorption in Equations (5) to (8) and for desorption in Equations (9) to (12), we obtain

$$E + E' = 1 \quad (16)$$

where E is defined in Equation (14) for sorption and E' is the corresponding quality for desorption. We therefore have

$$E' = \frac{M(\tau)}{M(0)} = \frac{8}{\pi^2} \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} \exp \left[- \left(n + \frac{1}{2} \right)^2 \pi^2 \tau \right] \quad (17)$$

which can be expressed in closed form as follows:

$$\tau = \frac{\pi(1-E')^2}{4} \quad E' \geq 0.48 \quad (18a)$$

$$\tau = -\frac{4}{\pi^2} \ln \left(\frac{\pi^2 E'}{8} \right) \quad E' < 0.48 \quad (18b)$$

Talbot and Kitchener [22] also derived the approximate formula relating E'

to τ

$$\theta = -\ln x + \frac{q}{p} + \frac{rq^2}{2p^3} \quad (19)$$

where $\theta = \pi^2 \tau/4$, $x = \frac{1}{4} \pi^2 E$ and $p = 1 + x^8 + x^{24}$, $q = \frac{1}{9} x^8 + \frac{1}{25} x^{24}$ and $r = 1 - 9x^8 + 25x^{24}$. Equation (19) is correct to four significant figures when $E < \frac{2}{3}$, but is more complicated than Equations (18).

Sorption with $S \neq \infty$

The solution to Equation (5) under the conditions of Equations (6) to (8) can be found in Crank [7] as

$$E = 1 - 2L^2 \sum_{n=1}^{\infty} \frac{\exp(-\beta_n^2 \tau)}{\beta_n^2 (\beta_n^2 + L^2 + L)} \tag{20}$$

in which β_n are the positive roots of

$$\beta_n \tan \beta_n = L \tag{21}$$

Closed-form solution can be found in Liu [11] as

$$\tau = \frac{\pi E^2}{4} - \frac{1}{L} \ln(1 - E) \quad E \leq 0.52 \tag{22a}$$

and

$$\tau = -\frac{4}{\pi^2} \ln \left[\frac{\pi^2 (1 - E)}{8} \right] - \frac{1}{L} \ln(1 - E) \quad E > 0.52 \tag{22b}$$

Approximation in Equations (22) exist only in the first terms on the right-hand side, which, as mentioned before, are less than 0.3%.

Desorption with $S \neq \infty$

since Equation (16) is valid no matter what constant value S may take, the solution to Equation (9) under the conditions of Equations (10) to (12) is

$$E' = 2L^2 \sum_{n=1}^{\infty} \frac{\exp(-\beta_n^2 \tau)}{\beta_n^2 (\beta_n^2 + L^2 + L)} \quad (23)$$

with in defined the same as in Equation (21).

Closed-form solution can be found in Liu [10] as

$$\tau = \frac{\pi(1-E')^2}{4} - \frac{1}{L} \ln E' \quad E' \geq 0.48 \quad (24a)$$

and

$$\tau = -\frac{4}{\pi^2} \ln \left(\frac{\pi^2 E'}{8} \right) - \frac{1}{L} \ln E' \quad E' < 0.48 \quad (24b)$$

For this case, numerical results of Equations (24) are plotted in Figure 1; these results agree with those from Equation (23) reported by Newman [16].

APPLICATION OF DERIVED EQUATIONS

Since the derived equations apply to the whole range of E or E from 0 to 1, there is no need to use the so-called half-time technique [7] to estimate the constant value of D . Also, since Equations (15) are just a special case of Equations (22), Equations (18) are a special case of Equations (24), and Equations (22) bear close similarity with Equations (24), we can demonstrate the application of these equations by considering Equation (22a) only.

Rewrite Equation (22a) with $\tau = Dt/a^2$ and $L = aS/D$ as

$$\frac{Dt}{a^2} = \frac{\pi E^2}{4} - \frac{D}{aS} \ln(1-E)$$

or

$$\frac{t}{a^2} = \frac{\pi E^2}{4D} - \frac{1}{aS} \ln(1-E) \quad (25)$$

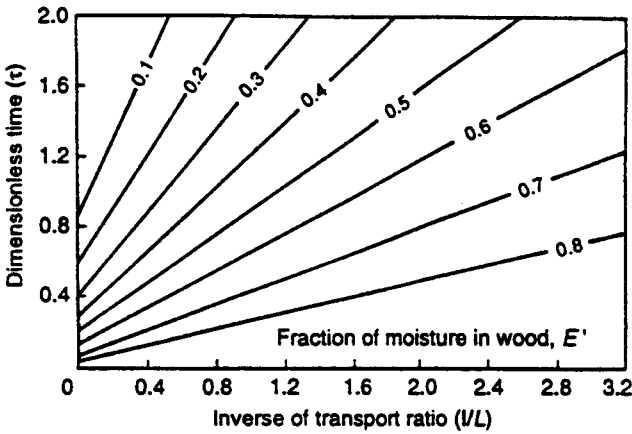


FIGURE 1. Dimensionless time versus inverse of transport ratio for various values of fraction of diffusing substance in medium. (ML 88 5382)

Let $a' = \frac{t}{a^2}$, $b' = \frac{\pi E^2}{4}$, and $c' = \frac{\ln(1-E)}{a}$, in which t and E are test data and a is

half-thickness of the sheet. Equation (25) becomes

$$a'/b' = 1/D - 1/S (c'/b') \tag{26}$$

For D and S to be constant and positive, we must have

$$a'/b' > 1/D \tag{27}$$

since a' and b' are positive and c' is negative. Also, the plot of a'/b' vs. c'/b' must form a straight line so that

with the intercept $a'/b' = 1/D$ at $c'/b' = 0$. When a'/b' is independent of c'/b' , $S =$

∞ .

Or, multiplying through Equation (26) by b'/c' , we obtain

$$a'/c' = 1/D (b'/c') - 1/S \quad (29)$$

The plot of a'/c' versus b'/c' must also form a straight line so that

$$\frac{d(a'/c')}{d(b'/c')} = \frac{1}{D} \quad (30)$$

and $a'/c' = 1/S$ when $b'/c' = 0$. The values of a' , b' , and c' must satisfy the requirements specified by Condition (27) and Equations (28) and (30) for D and S to be constant and positive.

Expressions for a' , b' , and c' for Equations (22b), (24a), and (24b) can likewise be derived and their requirements remain the same.

RESORPTION DATA FOR NORTHERN RED OAK

Resorption test data for northern red oak (*Quercus rubra*) by Simpson [18] can conveniently be used for numerical analysis. Tests were conducted in a chamber attached to a generator unit for temperature and relative humidity (RH) conditioning to set the desired equilibrium moisture content (EMC). The chamber was maintained at 43°C and was equipped with an adjustable blower for air flow. A perforated plate was installed just in front of the specimens to create uniform air flow. Air speed was 5 m/s. Other input data are shown in Table 1.

Figure 2 presents the variation of a'/b' with c'/b' for each data set in Table 1. For each set, the data points can be approximately represented by two straight lines (not plotted), the first line inclining downward and the second line rising upward, from left to right. Clearly, the first line gives a positive value of S and the second line a negative value of S according to Equation (28). Since S is defined

TABLE 1. DESORPTION OF NORTHERN RED OAK

Set	Specimens	Specimen thickness, $2a$ (mm)	Initial moisture content, C_0 (%)	EMC, C_e (%)	RH (%)
1	5	25.0	35.89	5.5	33
2	5	24.2	28.97	8.3	53
3	5	25.4	32.11	11.8	70
4	5	25.0	25.92	15.9	83

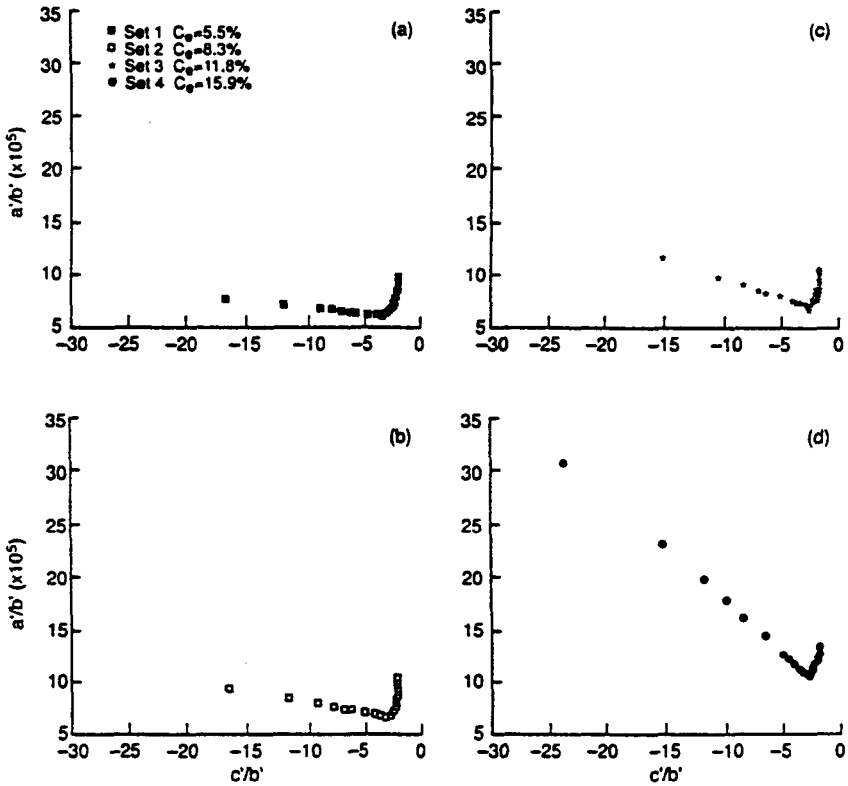


FIGURE 2. Variation of a'/b' with c'/b' .

as positive, at most we can use the diffusion equation with constant transport coefficients for the range covered by only the first line of each data set.

To obtain the value of D , we plot the variation of a'/c' with b'/c' for each data set. These are shown in Figure 3. Here again we see that the data points for each set can be represented by two straight lines (not plotted) corresponding to the two lines in Figure 2. We should use the line corresponding to the first line in Figure 2 to obtain the value of D using Equation (3), since D and S are coupled both mathematically and physically; i.e., either two of them are acceptable or none of them is acceptable. The line corresponding to the first line in Figure 2 is the one inclining downward from right to left in the upper part of Figure 3,

The values of D and S for the four sets of data are presented in Table 2.

From the data in Tables 1 and 2, we find a strong dependence of S on C_e as demonstrated in Figure 4. Since C_e is a constant in each test, such a dependence is theoretically acceptable. It has been suggested that S may also be dependent on C_0 . According to the present observation, if such a dependence does exist, it must be very weak. The results in Figure 4 are in qualitative agreement with those reported by Avramidis and Siau [1]. The diffusion coefficient D appears to be dependent on C_0 as shown in Figure 5, which is not unexpected in an isothermal desorption environment. As C_0 approaches the fiber saturation point, D tends to level off toward a constant value.

The drying curves in Figure 6 show the variation of fraction of total moisture content in wood with time. The calculated results were based on the D and S values in Table 2. Close agreement between test data and calculated results exists in all cases when the moisture fraction reaches about 50%. Beyond that, the deviation increases with decreasing EMC or increasing S . For a relatively large EMC value as in set 3 or 4, the close agreement could extend well below a

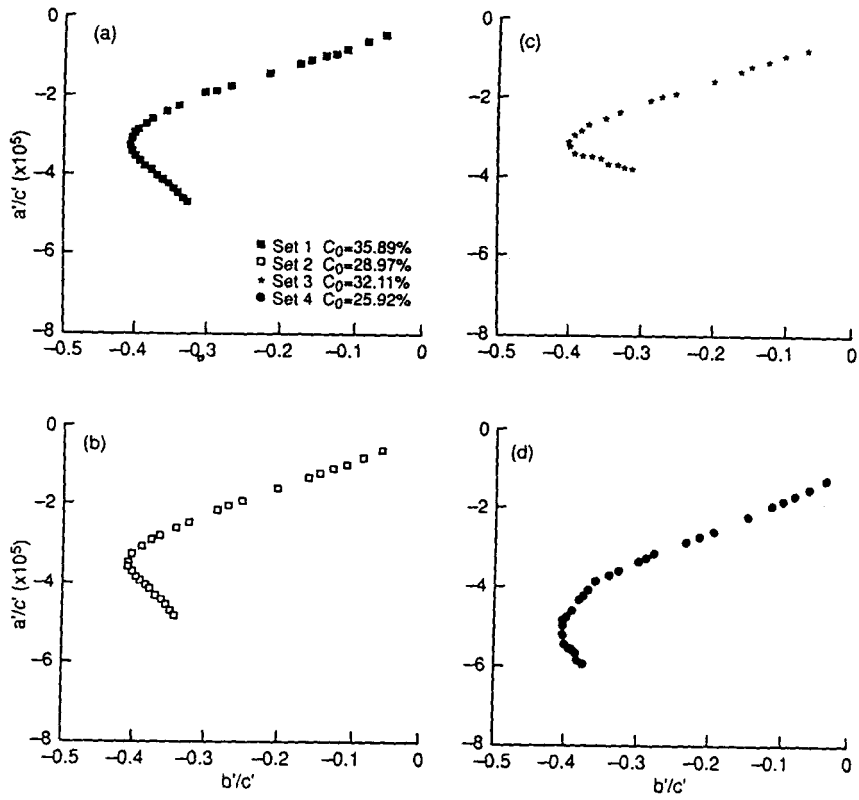


FIGURE 3. Variation of a'/c' with b'/c' .

TABLE 2. DIFFUSION AND SURFACE EMISSION COEFFICIENTS

Set	Surface emission coefficient S (cm/s)	Diffusion coefficient D (cm ² /s)
1	8.7358×10^{-5}	1.7044×10^{-6}
2	5.6892×10^{-5}	1.4661×10^{-6}
3	3.0689×10^{-5}	1.5573×10^{-6}
4	1.0492×10^{-5}	1.1626×10^{-6}

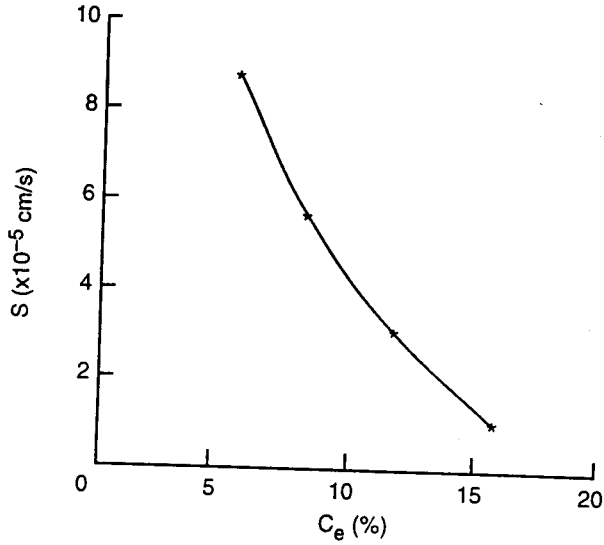


FIGURE 4. Dependence of surface emission coefficient S on equilibrium moisture content (EMC).

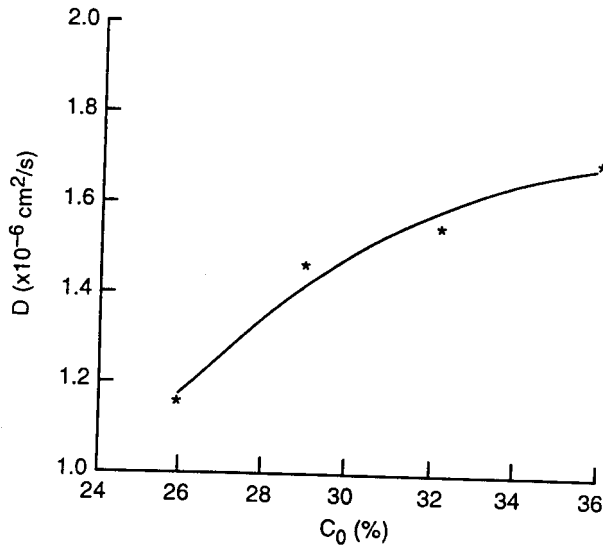


FIGURE 5. Dependence of diffusion coefficient D on initial moisture content.

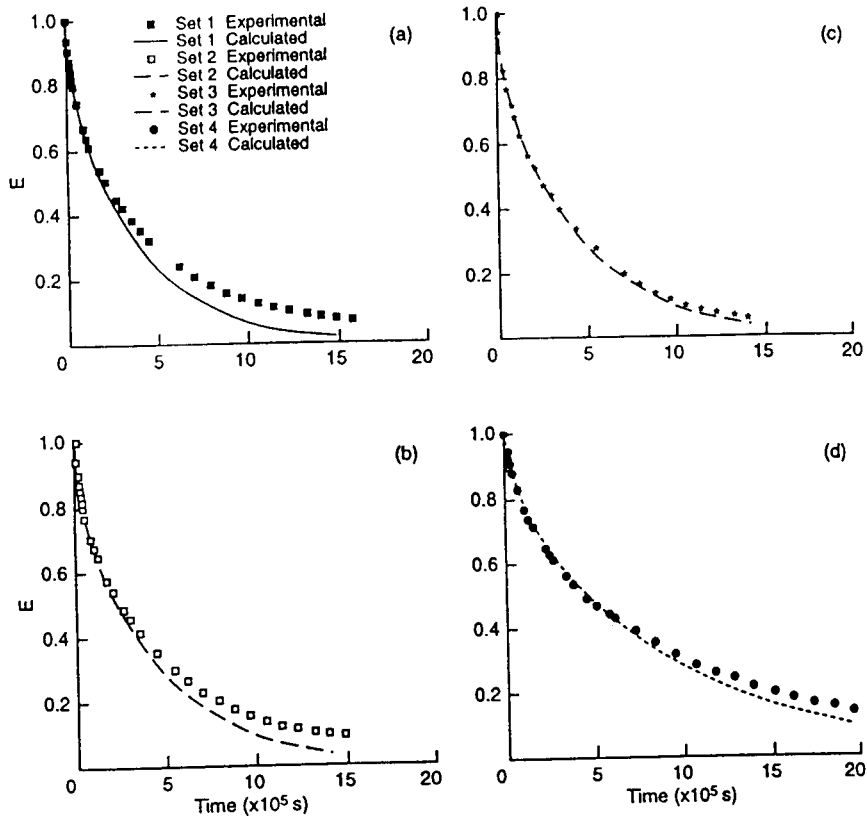


FIGURE 6. Variation of moisture fraction E with time.

moisture fraction of 50%. This suggests that the applicability of the diffusion equation with constant transport coefficients, D and S , depends very much on the magnitude of EMC and, to a somewhat lesser degree, on the initial moisture content, as can be seen from Figures 4 and 5. Under the test conditions considered, the common range of applicability defined by the fraction of total moisture content in wood is about 50% and above.

CONCLUSIONS

The closed-form solutions of the diffusion equation with constant transport coefficients were used to derive the conditions under which the transport coefficients can be taken as constant. Any diffusion test data can be compared against these conditions to determine whether or not the transport coefficients are constant. The resorption data of northern red oak in the present study also reveal another situation—i. e., when the moisture fraction in wood is above a certain value, the transport coefficients can be taken as constant; below this value, they cannot. Where they can be taken as constant, the diffusion coefficient is found to be dependent on the initial moisture content in wood and the surface emission coefficient on the equilibrium moisture content in the environment.

The closed-form solutions of the diffusion equation and the conditions derived therefrom for constant transport coefficients are valid for the whole range of diffusion, which renders unnecessary the half-time technique applied in the literature for several decades.

NOMENCLATURE

- a Half of medium thickness
- a', b', c' Parameters
- C Concentration of diffusing substance
- C_e Equilibrium concentration of diffusing substance
- C_0 Initial concentration of diffusing substance
- c Dimensionless concentration of diffusing substance
- D Diffusion coefficient

E	Fraction of total concentration in medium in sorption
E'	Fraction of total concentration in medium in resorption
L	Transport ratio
M	Total concentration in medium
S	Surface emission coefficient
t	Time
X	Space coordinate
x	Dimensionless space coordinate
ϵ	Positive constant close to zero
τ	Dimensionless time

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