

Engineering Materials MECH 390

Tutorial 3

Chapter 5 Diffusion in Solids

What is it?

Diffusion

Diffusion - Mass transport by atomic motion

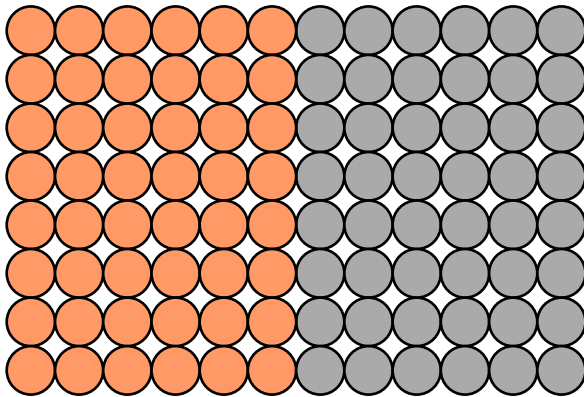
Mechanisms

- Gases & Liquids – random (Brownian) motion
- Solids – vacancy diffusion or interstitial diffusion

Diffusion

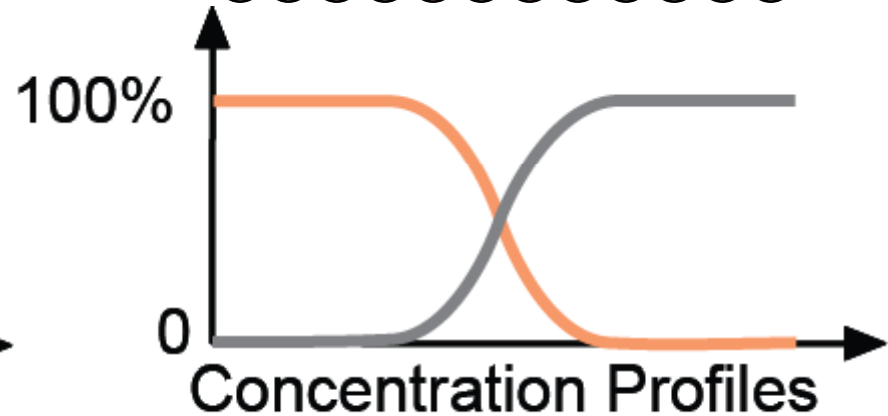
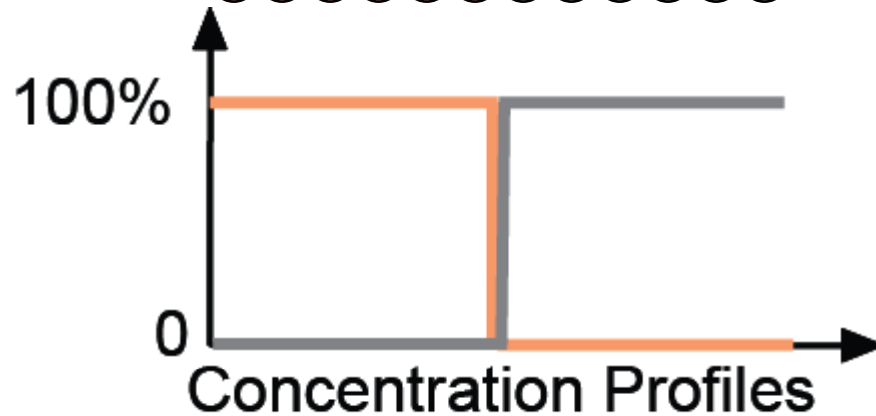
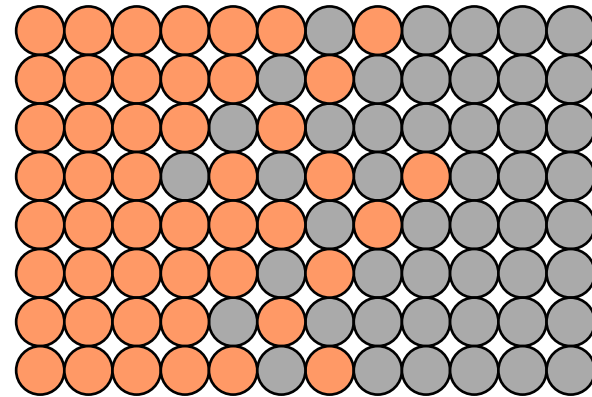
- **Interdiffusion:** In an alloy, atoms tend to migrate from regions of high conc. to regions of low conc.

Initially



Adapted from
Figs. 5.1 and
5.2, Callister
7e.

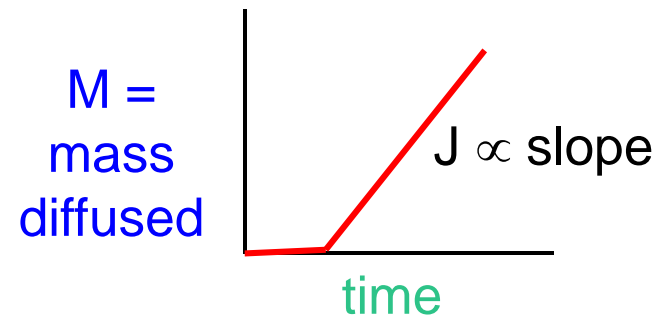
After some time



Diffusion

$$J \equiv \text{Flux} \equiv \frac{\text{moles (or mass) diffusing}}{(\text{surface area})(\text{time})} = \frac{\text{mol}}{\text{cm}^2 \cdot \text{s}} \text{ or } \frac{\text{kg}}{\text{m}^2 \cdot \text{s}} \text{ or } \frac{\text{atoms}}{\text{m}^2 \cdot \text{s}}$$

$$J = \frac{M}{At} = \frac{l}{A} \frac{dM}{dt}$$

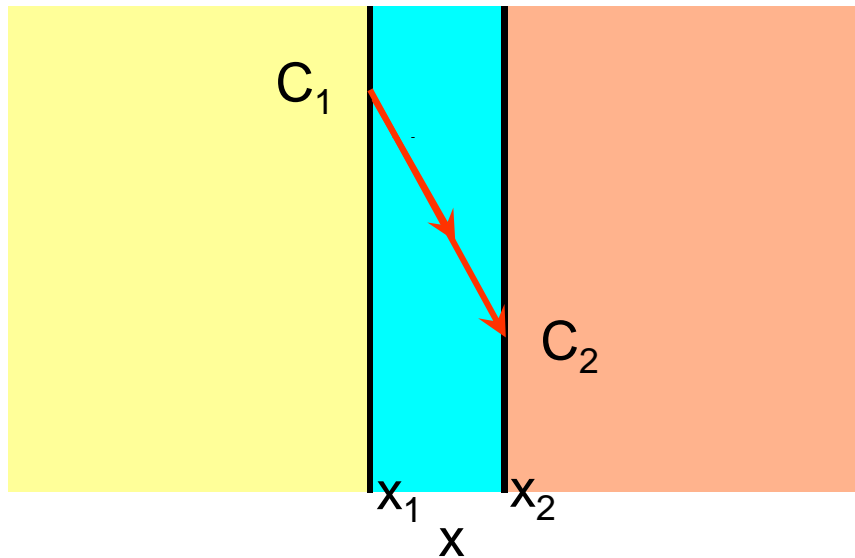


Steady-State Diffusion

Rate of diffusion independent of time

Flux proportional to concentration gradient =

$$\frac{dC}{dx}$$



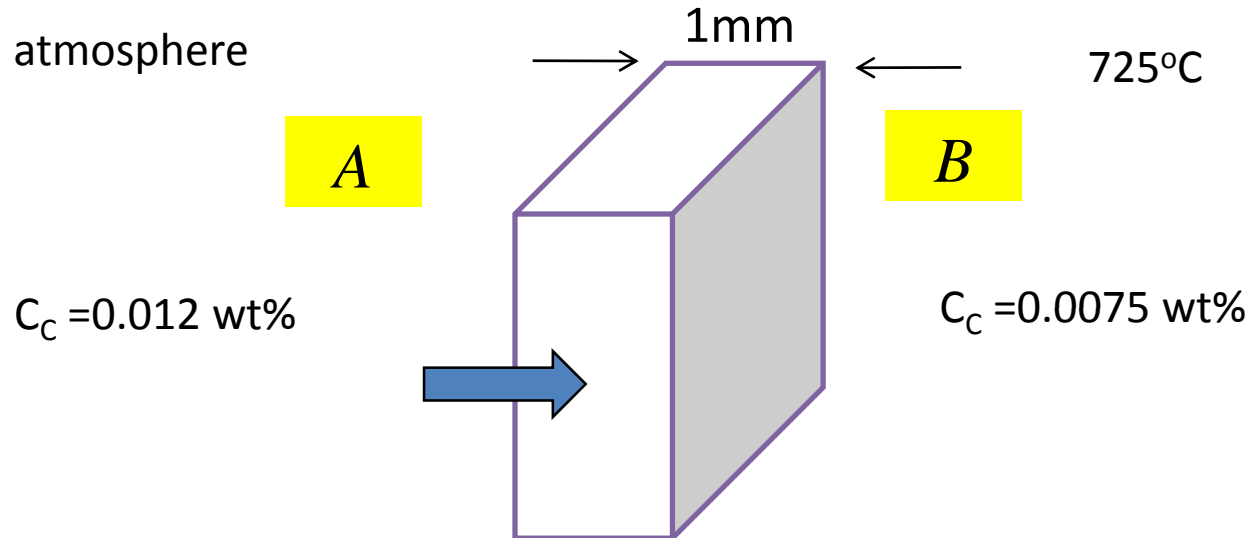
Fick's first law of diffusion

$$J = -D \frac{dC}{dx}$$

if linear $\frac{dC}{dx} \cong \frac{\Delta C}{\Delta x} = \frac{C_2 - C_1}{x_2 - x_1}$

$D \equiv$ diffusion coefficient m^2/s

Similar to 5.8: A sheet of BCC iron 1 mm thick was exposed to a carburizing gas atmosphere on one side and a decarburizing atmosphere on the other side at 725°C. After having reached steady state, the iron was quickly cooled to room temperature. The carbon concentrations at the two surfaces of the sheet were determined to be 0.012 and 0.0075 wt%. Compute the diffusion coefficient if the diffusion flux is $1.4 \times 10^{-8} \text{ kg/m}^2\text{-s}$?



$$J = 1.4 \times 10^{-8} \text{ kg/m}^2\text{-s}, D = ?$$

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Dr.Waleed Khalil Ahmed CRU-COE-UAEU

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convert the carbon concentrations from wt% to kg /m³ (**composition conversion,Ch.4-4.4p.86**)

1. Concentration 0.012 wt%

$$C_C'' = \left(\frac{C_C}{\frac{C_C}{\rho_C} + \frac{C_{Fe}}{\rho_{Fe}}} \right) \times 10^3$$
$$= \left(\frac{0.012}{\frac{0.012}{2.25 \text{ g/cm}^3} + \frac{99.988}{7.87 \text{ g/cm}^3}} \right) \times 10^3$$

$$C_A = 0.944 \text{ kg /m}^3$$

2. Concentration 0.0075 wt%

$$C_C'' = \left(\frac{C_C}{\frac{C_C}{\rho_C} + \frac{C_{Fe}}{\rho_{Fe}}} \right) \times 10^3$$
$$= \left(\frac{0.0075}{\frac{0.0075}{2.25 \text{ g/cm}^3} + \frac{99.9925}{7.87 \text{ g/cm}^3}} \right) \times 10^3$$

$C_B = 0.59 \text{ kg /m}^3$

$$\therefore J = -D \frac{dC}{dx}$$

$$\therefore D = -J \left[\frac{x_A - x_B}{C_A - C_B} \right]$$

$$= - (1.40 \times 10^{-8} \text{ kg/m}^2\text{-s}) \left[\frac{-10^{-3} \text{ m}}{0.944 \text{ kg/m}^3 - 0.590 \text{ kg/m}^3} \right]$$

$$= 3.95 \times 10^{-11} \text{ m}^2/\text{s}$$

5.25:The steady-state diffusion flux through a metal plate is $7.8 \times 10^{-8} \text{ kg/m}^2\text{-s}$ at a temperature of 1200°C and when the concentration gradient is -500 kg/m^4 . Calculate the diffusion flux at 1000°C for the same concentration gradient and assuming activation energy for diffusion of $145,000 \text{ J/mol}$.

$J = 7.8 \times 10^{-8} \text{ kg/m}^2\text{-s}$ at 1200°C

$$\frac{\Delta C}{\Delta x} = \frac{C_2 - C_1}{x_2 - x_1} = -500 \text{ kg/m}^4 \text{ assumed constant}$$

Find J at 1000°C

Diffusion and Temperature

$$D = D_0 \exp\left(-\frac{Q_d}{RT}\right)$$

D = diffusion coefficient [m^2/s]

D_0 = pre-exponential (time independent coefficient)[m^2/s](fixed)

Q_d = activation energy [J/mol or cal/mol or eV/atom]

R = gas constant [8.314 J/mol-K or 1.987 cal/mol-K or $8.62 \cdot 10^{-5}$ eV/atom-K]

T = absolute temperature [K]

Note: D as a function of Temperature is used for steady and non-steady state cases.

$$J = -D \frac{\Delta C}{\Delta x} = -D_0 \frac{\Delta C}{\Delta x} \exp\left(-\frac{Q_d}{RT}\right) \quad \rightarrow$$

$$\begin{aligned} D_0 &= -\frac{J}{\frac{\Delta C}{\Delta x}} \exp\left(\frac{Q_d}{RT}\right) \\ &= -\left(\frac{7.8 \times 10^{-8} \text{ kg/m}^2 \cdot \text{s}}{-500 \text{ kg/m}^4}\right) \exp\left[\frac{145,000 \text{ J/mol}}{(8.31 \text{ J/mol} \cdot \text{K})(1200 + 273 \text{ K})}\right] \\ &= 2.18 \times 10^{-5} \text{ m}^2/\text{s} \end{aligned}$$

At 1000°C

$$J = -D_0 \left(\frac{\Delta C}{\Delta x} \right) \exp \left(-\frac{Q_d}{RT} \right)$$
$$= -(2.18 \times 10^{-5} \text{ m}^2/\text{s})(-500 \text{ kg/m}^4) \exp \left[-\frac{145,000 \text{ J/mol}}{(8.31 \text{ J/mol} \cdot \text{K})(1273 \text{ K})} \right]$$
$$= 1.21 \times 10^{-8} \text{ kg/m}^2\text{-s}$$

Non-steady State Diffusion

- The concentration of diffusing species is a function of both time and position $C = C(x,t)$
- In this case [Fick's Second Law](#) is used

Fick's Second Law

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

(concentration in terms of both position and time)

5.4 Nonsteady-State Diffusion

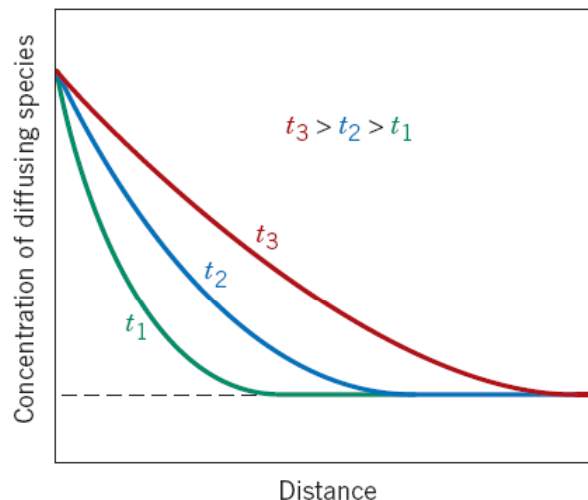


Figure 5.5 Concentration profiles for nonsteady-state diffusion taken at three different times, t_1 , t_2 , and t_3 .

Assumptions

1. Before diffusion, any of the diffusing solute atoms in the solid are uniformly distributed with concentration of C_0 .
2. The value of x at the surface is zero and increases with distance into the solid.
3. The time is taken to be zero the instant before the diffusion process begins.

These boundary conditions are simply stated as

$$\text{For } t = 0, C = C_0 \text{ at } 0 \leq x \leq \infty$$

$$\text{For } t > 0, C = C_s \text{ (the constant surface concentration) at } x = 0$$

$$C = C_0 \text{ at } x = \infty$$

Application of these boundary conditions to Equation 5.4b yields the solution

$$\frac{C_x - C_0}{C_s - C_0} = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \quad (5.5)$$

where C_x represents the concentration at depth x after time t .

^{7/15/} $\operatorname{erf}(x/2\sqrt{Dt})$ is the Gaussian error function,

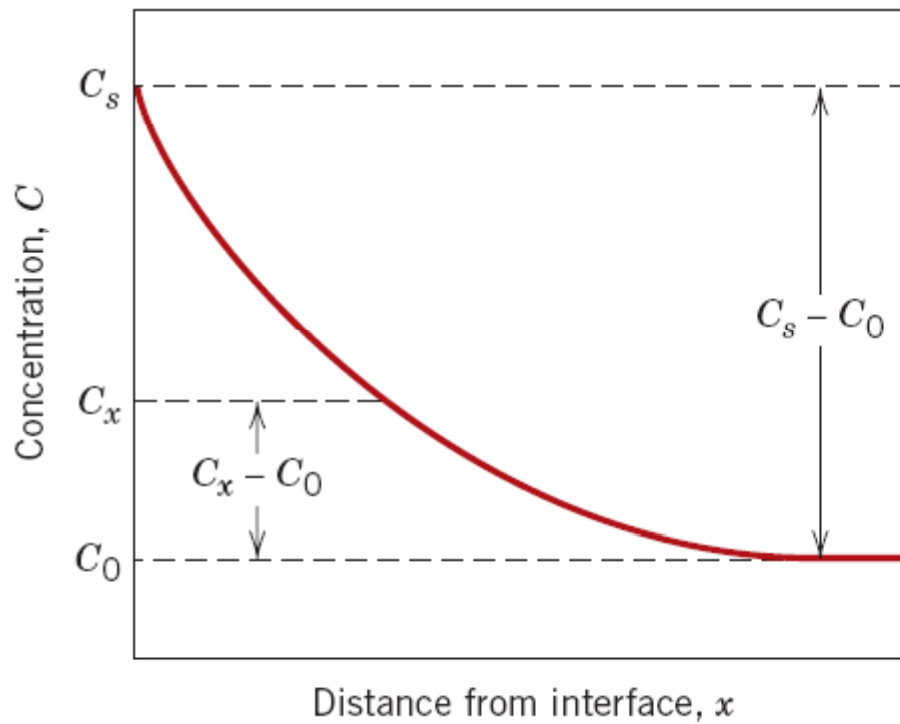


Figure 5.6 Concentration profile for nonsteady-state diffusion; concentration parameters relate to Equation 5.5.

³ This Gaussian error function is defined by

$$\text{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-y^2} dy$$

where $x/2\sqrt{Dt}$ has been replaced by the variable z .

Table 5.1 Tabulation of Error Function Values

z	$erf(z)$	z	$erf(z)$	z	$erf(z)$
0	0	0.55	0.5633	1.3	0.9340
0.025	0.0282	0.60	0.6039	1.4	0.9523
0.05	0.0564	0.65	0.6420	1.5	0.9661
0.10	0.1125	0.70	0.6778	1.6	0.9763
0.15	0.1680	0.75	0.7112	1.7	0.9838
0.20	0.2227	0.80	0.7421	1.8	0.9891
0.25	0.2763	0.85	0.7707	1.9	0.9928
0.30	0.3286	0.90	0.7970	2.0	0.9953
0.35	0.3794	0.95	0.8209	2.2	0.9981
0.40	0.4284	1.0	0.8427	2.4	0.9993
0.45	0.4755	1.1	0.8802	2.6	0.9998
0.50	0.5205	1.2	0.9103	2.8	0.9999

5.15 For a steel alloy it has been determined that a carburizing heat treatment of 15 h duration will raise the carbon concentration to 0.35 wt% at a point 2.0 mm from the surface. Estimate the time necessary to achieve the same concentration at a 6.0-mm position for an identical steel and at the same carburizing temperature.

5.15:Solution

After 15h , $C_c = 0.35$ wt% at 2mm from surface

What would be time necessary for the **same concentration** by at 6mm from the surface ?

$$\frac{C_1 - C_0}{C_s - C_0} = \text{constant} \qquad \frac{x}{2\sqrt{Dt}} = \text{constant}$$

From Equation 5.6b,

$$\frac{x^2}{Dt} = \text{constant}$$

But since the temperature is constant, so also is D constant, and

$$\frac{x^2}{t} = \text{constant} \quad \longrightarrow \quad \frac{x_1^2}{t_1} = \frac{x_2^2}{t_2}$$

$$\frac{(2.0 \text{ mm})^2}{15 \text{ h}} = \frac{(6.0 \text{ mm})^2}{t_2} \quad \longrightarrow \quad t_2 = 135 \text{ h}$$

5.11 Determine the carburizing time necessary to achieve a carbon concentration of 0.30 wt% at a position 4 mm into an iron–carbon alloy that initially contains 0.10 wt% C. The surface concentration is to be maintained at 0.90 wt% C, and the treatment is to be conducted at 1100°C. Use the diffusion data for γ -Fe in Table 5.2.

Time $t=?$

$C_1=0.3$ wt% at $X=4$ mm

$C_0=0.1$ wt%

$C_s=0.9$ wt%

$T=1100$ °C

5.11 We are asked to compute the carburizing (i.e., diffusion) time required for a specific nonsteady-state diffusion situation. It is first necessary to use Equation 5.5:

$$\frac{C_x - C_0}{C_s - C_0} = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

wherein, $C_x = 0.30$, $C_0 = 0.10$, $C_s = 0.90$, and $x = 4 \text{ mm} = 4 \times 10^{-3} \text{ m}$. Thus,

$$\frac{C_x - C_0}{C_s - C_0} = \frac{0.30 - 0.10}{0.90 - 0.10} = 0.2500 = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

or

$$\operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) = 1 - 0.2500 = 0.7500$$

By linear interpolation using data from Table 5.1

z	$\text{erf}(z)$
0.80	0.7421
z	0.7500
0.85	0.7707

$$\frac{z - 0.80}{0.85 - 0.80} = \frac{0.7500 - 0.7421}{0.7707 - 0.7421}$$

From which

$$z = 0.814 = \frac{x}{2\sqrt{Dt}}$$

Now, from Table 5.2, at 1100°C (1373 K)

$$D = D_0 \exp\left(-\frac{Q_d}{RT}\right)$$

$$D = (2.3 \times 10^{-5} \text{ m}^2/\text{s}) \exp\left[-\frac{148,000 \text{ J/mol}}{(8.31 \text{ J/mol}\cdot\text{K})(1373 \text{ K})}\right]$$

Thus,

$$0.814 = \frac{4 \times 10^{-3} \text{ m}}{(2)\sqrt{(5.35 \times 10^{-11} \text{ m}^2/\text{s})(t)}}$$

Solving for t yields

$$t = 1.13 \times 10^5 \text{ s} = 31.3 \text{ h}$$

5-12

An FCC iron–carbon alloy initially containing 0.55 wt% C is exposed to an oxygen-rich and virtually carbon-free atmosphere at 1325 K (1052°C). Under these circumstances the carbon diffuses from the alloy and reacts at the surface with the oxygen in the atmosphere; that is, the carbon concentration at the surface position is maintained essentially at 0 wt% C. (This process of carbon depletion is termed *decarburization*.) At what position will the carbon concentration be 0.25 wt% after a 10-h treatment? The value of D at 1325 K is $4.3 \times 10^{-11} \text{ m}^2/\text{s}$.

5.12 This problem asks that we determine the position at which the carbon concentration is 0.25 wt% after a 10-h heat treatment at 1325 K when $C_0 = 0.55$ wt% C. From Equation 5.5

$$\frac{C_x - C_0}{C_s - C_0} = \frac{0.25 - 0.55}{0 - 0.55} = 0.5455 = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

Thus,

$$\operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) = 0.4545$$

Using data in Table 5.1 and linear interpolation

z	$\text{erf}(z)$
0.40	0.4284
z	0.4545
0.45	0.4755

$$\frac{z - 0.40}{0.45 - 0.40} = \frac{0.4545 - 0.4284}{0.4755 - 0.4284}$$

And,

$$z = 0.4277$$

Which means that

$$\frac{x}{2\sqrt{Dt}} = 0.4277$$

And, finally

$$\begin{aligned}x &= 2(0.4277)\sqrt{Dt} = (0.8554)\sqrt{(4.3 \times 10^{-11} \text{ m}^2/\text{s})(3.6 \times 10^4 \text{ s})} \\ &= 1.06 \times 10^{-3} \text{ m} = 1.06 \text{ mm}\end{aligned}$$