

CHAPTER 7 DIFFUSION

PROBLEM SOLUTIONS

7.6 The purification of hydrogen gas by diffusion through a palladium sheet was discussed in Section 7.3. Compute the number of kilograms of hydrogen that pass per hour through a 5-mm-thick sheet of palladium having an area of 0.25 m² at 500°C. Assume a diffusion coefficient of 1.0×10^{-8} m²/s, that the concentrations at the high- and low-pressure sides of the plate are 2.4 and 0.6 kg of hydrogen per cubic meter of palladium, and that steady-state conditions have been attained.

Solution

This problem calls for the mass of hydrogen, per hour, that diffuses through a Pd sheet. It first becomes necessary to employ both Equations 7.1a and 7.2. Combining these expressions and solving for the mass yields

$$\begin{aligned} M &= JAt = -DA \frac{\Delta C}{\Delta x} \\ &= - (1.0 \times 10^{-8} \text{ m}^2/\text{s}) (0.25 \text{ m}^2) (3600 \text{ s/h}) \left[\frac{0.6 - 2.4 \text{ kg/m}^3}{5 \times 10^{-3} \text{ m}} \right] \\ &= 3.2 \times 10^{-3} \text{ kg/h} \end{aligned}$$

7.8 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 1.5×10^{-8} kg/m²·s. Hint: Use Equation 6.10 to convert the concentrations from weight percent to kilograms of carbon per cubic meter of iron.

Solution

Let us first convert the carbon concentrations from weight percent to kilograms carbon per meter cubed using Equation 6.10a. For 0.012 wt% C

$$C_C'' = \frac{C_C}{\frac{C_C}{r_C} + \frac{C_{Fe}}{r_{Fe}}} \times 10^3$$

$$= \frac{0.012}{\frac{0.012}{2.25 \text{ g/cm}^3} + \frac{99.988}{7.87 \text{ g/cm}^3}} \times 10^3$$

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

Similarly, for 0.0075 wt% C

$$C_C'' = \frac{0.0075}{\frac{0.0075}{2.25 \text{ g/cm}^3} + \frac{99.9925}{7.87 \text{ g/cm}^3}} \times 10^3$$

$$= 0.590 \text{ kg C/m}^3$$

Now, using a rearranged form of Equation 7.2

$$D = -J \frac{\hat{e}_x x_A - x_B}{\hat{e}_x C_A - C_B}$$

$$= - (1.5 \times 10^{-8} \text{ kg/m}^2 \cdot \text{s}) \left[\frac{-10^{-3} \text{ m}}{0.944 \text{ kg/m}^3 - 0.590 \text{ kg/m}^3} \right]$$

$$= 4.23 \times 10^{-11} \text{ m}^2 / \text{s}$$

7.10 Show that

$$C_x = \frac{B}{\sqrt{Dt}} \exp\left(-\frac{x^2}{4Dt}\right)$$

is also a solution to Equation 7.4b. The parameter B is a constant, being independent of both x and t .

Solution

It can be shown that

$$C_x = \frac{B}{\sqrt{Dt}} \exp\left(-\frac{x^2}{4Dt}\right)$$

is a solution to

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

simply by taking appropriate derivatives of the C_x expression. When this is carried out,

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} = \frac{B}{2D^{1/2}t^{3/2}} \exp\left(-\frac{x^2}{4Dt}\right) - \frac{1}{2t} \exp\left(-\frac{x^2}{4Dt}\right)$$

7.11 Determine the carburizing time necessary to achieve a carbon concentration of 0.45 wt% at a position 2 mm into an iron–carbon alloy that initially contains 0.20 wt% C. The surface concentration is to be maintained at 1.30 wt% C, and the treatment is to be conducted at 1000°C. Use the diffusion data for γ -Fe in Table 7.2.

Solution

In order to solve this problem it is first necessary to use Equation 7.5:

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

wherein, $C_x = 0.45$, $C_0 = 0.20$, $C_s = 1.30$, and $x = 2 \text{ mm} = 2 \times 10^{-3} \text{ m}$. Thus,

$$\frac{C_x - C_0}{C_s - C_0} = \frac{0.45 - 0.20}{1.30 - 0.20} = 0.2273 = 1 - \operatorname{erf} \frac{x}{2\sqrt{Dt}}$$

or

$$\operatorname{erf} \frac{x}{2\sqrt{Dt}} = 1 - 0.2273 = 0.7727$$

By linear interpolation using data from Table 7.1

z	$\operatorname{erf}(z)$
0.85	0.7707
z	0.7727
0.90	0.7970

$$\frac{z - 0.850}{0.900 - 0.850} = \frac{0.7727 - 0.7707}{0.7970 - 0.7707}$$

From which

$$z = 0.854 = \frac{x}{2\sqrt{Dt}}$$

Now, from Table 7.2, at 1000°C (1273 K)

$$D = (2.3 \times 10^{-5} \text{ m}^2/\text{s}) \exp \left[- \frac{148,000 \text{ J/mol}}{(8.31 \text{ J/mol}\cdot\text{K})(1273 \text{ K})} \right]$$

$$= 1.93 \times 10^{-11} \text{ m}^2/\text{s}$$

Thus,

$$0.854 = \frac{2 \times 10^{-3} \text{ m}}{(2)\sqrt{(1.93 \times 10^{-11} \text{ m}^2/\text{s})(t)}}$$

Solving for t yields

$$t = 7.1 \times 10^4 \text{ s} = 19.7 \text{ h}$$

7.12 An FCC iron–carbon alloy initially containing 0.35 wt% C is exposed to an oxygen-rich and virtually carbon-free atmosphere at 1400 K (1127°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 0.15 wt% after a 10-h treatment? The value of D at 1400 K is $6.9 \times 10^{-11} \text{ m}^2/\text{s}$.

Solution

This problem asks that we determine the position at which the carbon concentration is 0.15 wt% after a 10-h heat treatment at 1325 K when $C_0 = 0.35 \text{ wt\% C}$. From Equation 7.5

$$\frac{C_x - C_0}{C_s - C_0} = \frac{0.15 - 0.35}{0 - 0.35} = 0.5714 = 1 - \operatorname{erf} \left(\frac{x}{2\sqrt{Dt}} \right)$$

Thus,

$$\operatorname{erf} \left(\frac{x}{2\sqrt{Dt}} \right) = 0.4286$$

Using data in Table 7.1 and linear interpolation

z	$\operatorname{erf}(z)$
0.40	0.4284
z	0.4286
0.45	0.4755

$$\frac{z - 0.40}{0.45 - 0.40} = \frac{0.4286 - 0.4284}{0.4755 - 0.4284}$$

And,

$$z = 0.4002$$

Which means that

$$\frac{x}{2\sqrt{Dt}} = 0.4002$$

And, finally

$$x = 2(0.4002)\sqrt{Dt} = (0.8004)\sqrt{(6.9 \times 10^{-11} \text{ m}^2/\text{s})(3.6 \times 10^4 \text{ s})}$$

$$= 1.26 \times 10^{-3} \text{ m} = 1.26 \text{ mm}$$

Note: this problem may also be solved using the “Diffusion” module in the *VMSE* software. Open the “Diffusion” module, click on the “Diffusion Design” submodule, and then do the following:

1. Enter the given data in left-hand window that appears. In the window below the label “D Value” enter the value of the diffusion coefficient—viz. “6.9e-11”.
2. In the window just below the label “Initial, C0” enter the initial concentration—viz. “0.35”.
3. In the window the lies below “Surface, Cs” enter the surface concentration—viz. “0”.
4. Then in the “Diffusion Time t” window enter the time in seconds; in 10 h there are (60 s/min)(60 min/h)(10 h) = 36,000 s—so enter the value “3.6e4”.
5. Next, at the bottom of this window click on the button labeled “Add curve”.
6. On the right portion of the screen will appear a concentration profile for this particular diffusion situation. A diamond-shaped cursor will appear at the upper left-hand corner of the resulting curve. Click and drag this cursor down the curve to the point at which the number below “Concentration:” reads “0.15 wt%”. Then read the value under the “Distance:”. For this problem, this value (the solution to the problem) ranges between 1.24 and 1.30 mm.

7.14 Consider a diffusion couple composed of two semi-infinite solids of the same metal, and that each side of the diffusion couple has a different concentration of the same elemental impurity; furthermore, assume each impurity level is constant throughout its side of the diffusion couple. For this situation, the solution to Fick's second law (assuming that the diffusion coefficient for the impurity is independent of concentration), is as follows:

$$C_x = \frac{C_1 + C_2}{2} - \frac{C_1 - C_2}{2} \operatorname{erf} \frac{x}{2\sqrt{Dt}} \quad (7.15)$$

In this expression, when the $x = 0$ position is taken as the initial diffusion couple interface, then C_1 is the impurity concentration for $x < 0$; likewise, C_2 is the impurity content for $x > 0$.

A diffusion couple composed of two silver-gold alloys is formed; these alloys have compositions of 98 wt% Ag-2 wt% Au and 95 wt% Ag-5 wt% Au. Determine the time this diffusion couple must be heated at 750°C (1023 K) in order for the composition to be 2.5 wt% Au at the 50 μm position into the 2 wt% Au side of the diffusion couple. Preexponential and activation energy values for Au diffusion in Ag are $8.5 \times 10^{-5} \text{ m}^2/\text{s}$ and 202,100 J/mol, respectively.

Solution

For this platinum-gold diffusion couple for which $C_1 = 5 \text{ wt\% Au}$ and $C_2 = 2 \text{ wt\% Au}$, we are asked to determine the diffusion time at 750°C that will give a composition of 2.5 wt% Au at the 50 μm position. Thus, for this problem, Equation 7.15 takes the form

$$2.5 = \frac{5 + 2}{2} - \frac{5 - 2}{2} \operatorname{erf} \frac{50 \times 10^{-6} \text{ m}}{2\sqrt{Dt}}$$

It now becomes necessary to compute the diffusion coefficient at 750°C (1023 K) given that $D_0 = 8.5 \times 10^{-5} \text{ m}^2/\text{s}$ and $Q_d = 202,100 \text{ J/mol}$. From Equation 7.8 we have

$$\begin{aligned} D &= D_0 \exp \left(-\frac{Q_d}{RT} \right) \\ &= (8.5 \times 10^{-5} \text{ m}^2/\text{s}) \exp \left(-\frac{202,100 \text{ J/mol}}{(8.31 \text{ J/mol}\cdot\text{K})(1023 \text{ K})} \right) \\ &= 4.03 \times 10^{-15} \text{ m}^2/\text{s} \end{aligned}$$

Substitution of this value into the above equation leads to

$$2.5 = \frac{5 + 20}{2} - \frac{5 - 20}{2} \operatorname{erf} \frac{50 \times 10^{-6} \text{ m}}{2\sqrt{(4.03 \times 10^{-15} \text{ m}^2/\text{s})(t)}}$$

This expression reduces to the following form:

$$0.6667 = \operatorname{erf} \frac{393.8\sqrt{s}}{\sqrt{t}}$$

Using data in Table 7.1, it is necessary to determine the value of z for which the error function is 0.6667. We use linear interpolation as follows:

z	$\operatorname{erf}(z)$
0.650	0.6420
y	0.6667
0.700	0.6778

$$\frac{y - 0.650}{0.700 - 0.650} = \frac{0.6667 - 0.6420}{0.6778 - 0.6420}$$

from which

$$y = 0.6844 = \frac{393.8\sqrt{s}}{\sqrt{t}}$$

And, solving for t gives

$$t = 3.31 \times 10^5 \text{ s} = 92 \text{ h}$$

7.15 For a steel alloy it has been determined that a carburizing heat treatment of 10-h duration will raise the carbon concentration to 0.45 wt% at a point 2.5 mm from the surface. Estimate the time necessary to achieve the same concentration at a 5.0-mm position for an identical steel and at the same carburizing temperature.

Solution

This problem calls for an estimate of the time necessary to achieve a carbon concentration of 0.45 wt% at a point 5.0 mm from the surface. From Equation 7.6b,

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

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

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

or

$$\frac{x_1^2}{t_1} = \frac{x_2^2}{t_2}$$

Thus,

$$\frac{(2.5 \text{ mm})^2}{10 \text{ h}} = \frac{(5.0 \text{ mm})^2}{t_2}$$

from which

$$t_2 = 40 \text{ h}$$

7.19 The preexponential and activation energy for the diffusion of iron in cobalt are $1.1 \times 10^{-5} \text{ m}^2/\text{s}$ and $253,300 \text{ J/mol}$, respectively. At what temperature will the diffusion coefficient have a value of $2.1 \times 10^{-14} \text{ m}^2/\text{s}$?

Solution

For this problem we are given D_0 (1.1×10^{-5}) and Q_d ($253,300 \text{ J/mol}$) for the diffusion of Fe in Co, and asked to compute the temperature at which $D = 2.1 \times 10^{-14} \text{ m}^2/\text{s}$. Solving for T from Equation 7.9a yields

$$T = \frac{Q_d}{R(\ln D_0 - \ln D)}$$

$$= \frac{253,300 \text{ J/mol}}{(8.31 \text{ J/mol} \cdot \text{K}) [\ln (1.1 \times 10^{-5} \text{ m}^2/\text{s}) - \ln (2.1 \times 10^{-14} \text{ m}^2/\text{s})]}$$

$$= 1518 \text{ K} = 1245^\circ\text{C}$$

Note: this problem may also be solved using the “Diffusion” module in the *VMSE* software. Open the “Diffusion” module, click on the “D vs 1/T Plot” submodule, and then do the following:

1. In the left-hand window that appears, click on the “Custom1” box.
2. In the column on the right-hand side of this window enter the data for this problem. In the window under “D0” enter preexponential value—viz. “1.1e-5”. Next just below the “Qd” window enter the activation energy value—viz. “253.3”. It is next necessary to specify a temperature range over which the data is to be plotted. The temperature at which D has the stipulated value is probably between 1000°C and 1500°C , so enter “1000” in the “T Min” box that is beside “C”; and similarly for the maximum temperature—enter “1500” in the box below “T Max”.
3. Next, at the bottom of this window, click the “Add Curve” button.
4. A log D versus $1/T$ plot then appears, with a line for the temperature dependence of the diffusion coefficient for Fe in Co. At the top of this curve is a diamond-shaped cursor. Click-and-drag this cursor down the line to the point at which the entry under the “Diff Coeff (D):” label reads $2.1 \times 10^{-14} \text{ m}^2/\text{s}$. The temperature at which the diffusion coefficient has this value is given under the label “Temperature (T):”. For this problem, the value is 1519 K.

7.22 The diffusion coefficients for silver in copper are given at two temperatures:

T ($^{\circ}\text{C}$)	D (m^2/s)
650	5.5×10^{-16}
900	1.3×10^{-13}

- (a) Determine the values of D_0 and Q_d .
 (b) What is the magnitude of D at 875°C ?

Solution

(a) Using Equation 7.9a, we set up two simultaneous equations with Q_d and D_0 as unknowns as follows:

$$\ln D_1 = \ln D_0 - \frac{Q_d}{R} \frac{1}{T_1}$$

$$\ln D_2 = \ln D_0 - \frac{Q_d}{R} \frac{1}{T_2}$$

Solving for Q_d in terms of temperatures T_1 and T_2 (923 K [650°C] and 1173 K [900°C]) and D_1 and D_2 (5.5×10^{-16} and 1.3×10^{-13} m^2/s), we get

$$\begin{aligned} Q_d &= -R \frac{\ln D_1 - \ln D_2}{\frac{1}{T_1} - \frac{1}{T_2}} \\ &= - \frac{(8.31 \text{ J/mol}\cdot\text{K}) [\ln (5.5 \times 10^{-16}) - \ln (1.3 \times 10^{-13})]}{\frac{1}{923 \text{ K}} - \frac{1}{1173 \text{ K}}} \\ &= 196,700 \text{ J/mol} \end{aligned}$$

Now, solving for D_0 from Equation 7.8 (and using the 650°C value of D)

$$\begin{aligned} D_0 &= D_1 \exp \left[\frac{Q_d}{RT_1} \right] \\ &= (5.5 \times 10^{-16} \text{ m}^2/\text{s}) \exp \left[\frac{196,700 \text{ J/mol}}{(8.31 \text{ J/mol}\cdot\text{K})(923 \text{ K})} \right] \\ &= 7.5 \times 10^{-5} \text{ m}^2/\text{s} \end{aligned}$$

Excerpts from this work may be reproduced by instructors for distribution on a not-for-profit basis for testing or instructional purposes only to students enrolled in courses for which the textbook has been adopted. Any other reproduction or translation of this work beyond that permitted by Sections 107 or 108 of the 1976 United States Copyright Act without the permission of the copyright owner is unlawful.

(b) Using these values of D_0 and Q_d , D at 1148 K (875°C) is just

$$D = (7.5 \times 10^{-5} \text{ m}^2/\text{s}) \exp \left[- \frac{196,700 \text{ J/mol}}{(8.31 \text{ J/mol} \cdot \text{K})(1148 \text{ K})} \right]$$
$$= 8.3 \times 10^{-14} \text{ m}^2/\text{s}$$

Note: this problem may also be solved using the “Diffusion” module in the *VMSE* software. Open the “Diffusion” module, click on the “ D_0 and Q_d from Experimental Data” submodule, and then do the following:

1. In the left-hand window that appears, enter the two temperatures from the table in the book (converted from degrees Celsius to Kelvins) (viz. “923” (650°C) and “1173” (900°C), in the first two boxes under the column labeled “T (K)”. Next, enter the corresponding diffusion coefficient values (viz. “5.5e-16” and “1.3e-13”).
3. Next, at the bottom of this window, click the “Plot data” button.
4. A log D versus 1/T plot then appears, with a line for the temperature dependence for this diffusion system. At the top of this window are give values for D_0 and Q_d ; for this specific problem these values are $7.55 \times 10^{-5} \text{ m}^2/\text{s}$ and 196 kJ/mol, respectively
5. To solve the (b) part of the problem we utilize the diamond-shaped cursor that is located at the top of the line on this plot. Click-and-drag this cursor down the line to the point at which the entry under the “Temperature (T):” label reads “1148” (i.e., 875°C). The value of the diffusion coefficient at this temperature is given under the label “Diff Coeff (D):”. For our problem, this value is $8.9 \times 10^{-14} \text{ m}^2/\text{s}$.

7.28 A copper-nickel diffusion couple similar to that shown in Figure 7.1a is fashioned. After a 700-h heat treatment at 1100°C (1373 K) the concentration of Cu is 2.5 wt% at the 3.0-mm position within the nickel. At what temperature must the diffusion couple need to be heated to produce this same concentration (i.e., 2.5 wt% Cu) at a 2.0-mm position after 700 h? The preexponential and activation energy for the diffusion of Cu in Ni are given in Table 7.2.

Solution

In order to determine the temperature to which the diffusion couple must be heated so as to produce a concentration of 2.5 wt% Ni at the 2.0-mm position, we must first utilize Equation 7.6b with time t being a constant. That is

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

or

$$\frac{x_{1100}^2}{D_{1100}} = \frac{x_T^2}{D_T}$$

Now, solving for D_T from this equation, yields

$$D_T = \frac{x_T^2 D_{1100}}{x_{1100}^2}$$

and incorporating the temperature dependence of D_{1100} utilizing Equation (7.8), realizing that for the diffusion of Cu in Ni (Table 7.2)

$$D_0 = 2.7 \times 10^{-5} \text{ m}^2/\text{s}$$

$$Q_d = 256,000 \text{ J/mol}$$

then

$$D_T = \frac{(x_T)^2 D_0 \exp\left(-\frac{Q_d}{RT}\right)}{x_{1100}^2}$$

$$= \frac{(2 \text{ mm})^2 (2.7 \times 10^{-5} \text{ m}^2/\text{s}) \exp\left(-\frac{256,000 \text{ J/mol}}{(8.31 \text{ J/mol}\cdot\text{K})(1373 \text{ K})}\right)}{(3 \text{ mm})^2}$$

$$= 2.16 \times 10^{-15} \text{ m}^2/\text{s}$$

We now need to find the T at which D has this value. This is accomplished by rearranging Equation 7.9a and solving for T as

$$T = \frac{Q_d}{R (\ln D_0 - \ln D)}$$
$$= \frac{256,000 \text{ J/mol}}{(8.31 \text{ J/mol} \cdot \text{K}) [\ln (2.7 \times 10^{-5} \text{ m}^2/\text{s}) - \ln (2.16 \times 10^{-15} \text{ m}^2/\text{s})]}$$
$$= 1325 \text{ K} = 1052^\circ\text{C}$$