CHAPTER 5

DIFFUSION

PROBLEM SOLUTIONS

Introduction

5.1 Self-diffusion is atomic migration in pure metals--i.e., when all atoms exchanging positions are of the same type. Interdiffusion is diffusion of atoms of one metal into another metal.

5.2 Self-diffusion may be monitored by using radioactive isotopes of the metal being studied. The motion of these isotopic atoms may be monitored by measurement of radioactivity level.

Diffusion Mechanisms

5.3 (a) With vacancy diffusion, atomic motion is from one lattice site to an adjacent vacancy. Self-diffusion and the diffusion of substitutional impurities proceed via this mechanism. On the other hand, atomic motion is from interstitial site to adjacent interstitial site for the interstitial diffusion mechanism.

(b) Interstitial diffusion is normally more rapid than vacancy diffusion because: (1) interstitial atoms, being smaller, are more mobile; and (2) the probability of an empty adjacent interstitial site is greater than for a vacancy adjacent to a host (or substitutional impurity) atom.

Steady-State Diffusion

5.4 Steady-state diffusion is the situation wherein the rate of diffusion into a given system is just equal to the rate of diffusion out, such that there is no net accumulation or depletion of diffusing species--i.e., the diffusion flux is independent of time.

5.5 (a) The driving force is that which compels a reaction to occur.

(b) The driving force for steady-state diffusion is the concentration gradient.

5.6 This problem calls for the mass of hydrogen, per hour, that diffuses through a Pd sheet. It first becomes necessary to employ both Equations 5.1a and 5.3. Combining these expressions and solving for the mass yields

$$M = JAt = -DAt\frac{\Delta C}{\Delta x}$$

$$= -\left(1.7 \times 10^{-8}\ \mathrm{m^2/s}\right)\left(0.25\ \mathrm{m^2}\right)(3600\ \mathrm{s/h})\left[\frac{0.4 - 2.0\ \mathrm{kg/m^3}}{6 \times 10^{-3}\ \mathrm{m}}\right]$$

$$= 4.1 \times 10^{-3}\ \mathrm{kg/h}$$

5.7 We are asked to determine the position at which the nitrogen concentration is 0.5 kg/m^3. This problem is solved by using Equation 5.3 in the form

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

If we take C_A to be the point at which the concentration of nitrogen is 2 kg/m^3, then it becomes necessary to solve for x_B, as

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

Assume x_A is zero at the surface, in which case

$$x_B = 0 + (1.2 \times 10^{-10}\ \mathrm{m^2/s})\left[\frac{2\ \mathrm{kg/m^3} - 0.5\ \mathrm{kg/m^3}}{1.0 \times 10^{-7}\ \mathrm{kg/m^2\text{-}s}}\right]$$

$$= 1.8 \text{ x } 10^{-3} \text{ m} = 1.8 \text{ mm}$$

5.8 This problem calls for computation of the diffusion coefficient for a steady-state diffusion situation. Let us first convert the carbon concentrations from weight percent to kilograms carbon per meter cubed using Equation 4.9a. For 0.015 wt% C

$$C''_\mathrm{C} = \frac{C_\mathrm{C}}{\dfrac{C_\mathrm{C}}{\rho_\mathrm{C}} + \dfrac{C_\mathrm{Fe}}{\rho_\mathrm{Fe}}} \times 10^3$$

$$= \frac{0.015}{\dfrac{0.015}{2.25\ \mathrm{g/cm^3}} + \dfrac{99.985}{7.87\ \mathrm{g/cm^3}}} \times 10^3$$

$$1.18\ \mathrm{kg\ C/m^3}$$

Similarly, for 0.0068 wt% C

$$C''_\mathrm{C} = \frac{0.0068}{\dfrac{0.0068}{2.25\ \mathrm{g/cm^3}} + \dfrac{99.9932}{7.87\ \mathrm{g/cm^3}}} \times 10^3$$

$$= 0.535\ \mathrm{kg\ C/m^3}$$

Now, using a rearranged form of Equation 5.3

$$D = -J\left[\frac{x_\mathrm{A} - x_\mathrm{B}}{C_\mathrm{A} - C_\mathrm{B}}\right]$$

$$= -\left(7.36 \times 10^{-9}\ \mathrm{kg/m^2\text{-}s}\right)\left[\frac{-2 \times 10^{-3}\ \mathrm{m}}{1.18\ \mathrm{kg/m^3} - 0.535\ \mathrm{kg/m^3}}\right]$$

$$= 2.3 \times 10^{-11}\ \mathrm{m^2/s}$$

5.9 This problems asks for us to compute the diffusion flux of nitrogen gas through a 1.5-mm thick plate of iron at 300°C when the pressures on the two sides are 0.10 and 5.0 MPa. Ultimately we will employ Equation 5.3 to solve this problem. However, it first becomes necessary to determine the concentration of hydrogen at each face using Equation 5.11. At the low pressure (or B) side

$$C_{\mathrm{N(B)}} = \left(4.90 \times 10^{-3}\right)\sqrt{0.10 \text{ MPa}} \exp\left[-\frac{37{,}600 \text{ J/mol}}{(8.31 \text{ J/mol-K})(300 + 273 \text{ K})}\right]$$

$$5.77 \text{ x } 10^{-7} \text{ wt\%}$$

Whereas, for the high pressure (or A) side

$$C_{\mathrm{N(A)}} = \left(4.90 \times 10^{-3}\right)\sqrt{5.0 \text{ MPa}} \exp\left[-\frac{37{,}600 \text{ J/mol}}{(8.31 \text{ J/mol-K})(300 + 273 \text{ K})}\right]$$

$$4.08 \text{ x } 10^{-6} \text{ wt\%}$$

We now convert concentrations in weight percent to mass of nitrogen per unit volume of solid. At face B there are $5.77 \text{ x } 10^{-7}$ g (or $5.77 \text{ x } 10^{-10}$ kg) of hydrogen in 100 g of Fe, which is virtually pure iron. From the density of iron (7.87 g/cm^3), the volume iron in 100 g (V_{B}) is just

$$V_{\mathrm{B}} = \frac{100 \text{ g}}{7.87 \text{ g/cm}^3} = 12.7 \text{ cm}^3 = 1.27 \times 10^{-5} \text{ m}^3$$

Therefore, the concentration of hydrogen at the B face in kilograms of N per cubic meter of alloy [$C''_{\mathrm{N(B)}}$] is just

$$C''_{\mathrm{N(B)}} = \frac{C_{\mathrm{N(B)}}}{V_{\mathrm{B}}}$$

$$= \frac{5.77 \times 10^{-10} \text{ kg}}{1.27 \times 10^{-5} \text{ m}^3} = 4.54 \text{ x } 10^{-5} \text{ kg/m}^3$$

At the A face the volume of iron in 100 g (V_{A}) will also be $1.27 \text{ x } 10^{-5}$ m^3, and

$$C''_{\mathrm{N(A)}} = \frac{C_{\mathrm{N(A)}}}{V_{\mathrm{A}}}$$

$$= \frac{4.08 \times 10^{-9}\ \text{kg}}{1.27 \times 10^{-5}\ \text{m}^3} = 3.21 \text{ x } 10^{-4}\ \text{kg/m}^3$$

Thus, the concentration gradient is just the difference between these concentrations of nitrogen divided by the thickness of the iron membrane; that is

$$\frac{\Delta C}{\Delta x} = \frac{C^{\tilde{\text{Ő}}}_{\text{N(B)}} - C^{\tilde{\text{Ő}}}_{\text{N(A)}}}{x_{\text{B}} - x_{\text{A}}}$$

$$= \frac{4.54 \text{ x } 10^{-5}\ \text{kg/m}^3 - 3.21 \text{ x } 10^{-4}\ \text{kg/m}^3}{1.5 \times 10^{-3}\ \text{m}} = -\ 0.184\ \text{kg/m}^4$$

At this time it becomes necessary to calculate the value of the diffusion coefficient at 300°C using Equation 5.8. Thus,

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

$$= \left(3.0 \times 10^{-7}\ \text{m}^2/\text{s}\right) \exp\left(-\frac{76{,}150\ \text{J/mol}}{(8.31\ \text{J/mol}-\text{K})(300 + 273\ \text{K})}\right)$$

$$= 3.40 \text{ x } 10^{-14}\ \text{m}^2/\text{s}$$

And, finally, the diffusion flux is computed using Equation 5.3 by taking the negative product of this diffusion coefficient and the concentration gradient, as

$$J = -D\frac{\Delta C}{\Delta x}$$

$$= -\left(3.40 \times 10^{-14}\ \text{m}^2/\text{s}\right)\left(-\ 0.184\ \text{kg/m}^4\right) = 6.26 \times 10^{-15}\ \text{kg/m}^2\text{-s}$$

Nonsteady-State Diffusion

5.10 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,

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

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 $x = 4$ mm $= 4 \times 10^{-3}$ 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	erf(z)
0.80	0.7421
z	0.7500
0.85	0.7707

$$\frac{z - 0.800}{0.850 - 0.800} = \frac{0.7500 - 0.7421}{0.7707 - 0.7421}$$

From which

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

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

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

$$= 5.35 \times 10^{-11}\ \mathrm{m^2/s}$$

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

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

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	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

$$x = 2(0.4277)\sqrt{Dt} = (0.8554)\sqrt{(4.3 \times 10^{-11}\ \text{m}^2/\text{s})(3.6 \times 10^4\ \text{s})}$$

$$= 1.06 \text{ x } 10^{-3}\ \text{m} = 1.06\ \text{mm}$$

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. "4.3e-11".

2. In the window just below the label "Initial, C0" enter the initial concentration—viz. "0.55".

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 "0.25 wt%". Then read the value under the "Distance:". For this problem, this value (the solution to the problem) is 1.05 mm.

5.13 This problem asks us to compute the nitrogen concentration (C_x) at the 2 mm position after a 25 h diffusion time, when diffusion is nonsteady-state. From Equation 5.5

$$\frac{C_x - C_0}{C_s - C_0} = \frac{C_x - 0}{0.2 - 0} = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

$$= 1 - \operatorname{erf}\left[\frac{2 \times 10^{-3} \text{ m}}{(2)\sqrt{(1.9 \times 10^{-11} \text{ m}^2/\text{s})(25 \text{ h})(3600 \text{ s/h})}}\right]$$

$$= 1 - \operatorname{erf}(0.765)$$

Using data in Table 5.1 and linear interpolation

z	erf (z)
0.750	0.7112
0.765	y
0.800	0.7421

$$\frac{0.765 - 0.750}{0.800 - 0.750} = \frac{y - 0.7112}{0.7421 - 0.7112}$$

from which

$$y = \operatorname{erf}(0.765) = 0.7205$$

Thus,

$$\frac{C_x - 0}{0.2 - 0} = 1.0 - 0.7205$$

This expression gives

$$C_x = 0.056 \text{ wt\% N}$$

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. “1.9e-11”.

2. In the window just below the label “Initial, C0” enter the initial concentration—viz. “0”.

3. In the window the lies below “Surface, Cs” enter the surface concentration—viz. “0.2”.

4. Then in the “Diffusion Time t” window enter the time in seconds; in 25 h there are (60 s/min)(60 min/h)(25 h) = 90,000 s—so enter the value “9e4”.

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 “Distance:” reads “2.00 mm”. Then read the value under the “Concentration:”. For this problem, this value (the solution to the problem) is 0.06 wt%.

5.14 For this platinum-gold diffusion couple for which C_1 = 1 wt% Au and C_2 = 4 wt% Au, we are asked to determine the diffusion time at 1000°C that will give a composition of 2.8 wt% Au at the 10 μm position. Thus, for this problem, Equation 5.12 takes the form

$$2.8 = \left(\frac{1 + 4}{2}\right) - \left(\frac{1 - 4}{2}\right) \mathrm{erf}\left(\frac{10 \times 10^{-6}\ \mathrm{m}}{2\sqrt{Dt}}\right)$$

It now becomes necessary to compute the diffusion coefficient at 1000°C (1273 K) given that $D_0 = 1.3 \times 10^{-5}\ \mathrm{m^2/s}$ and Q_d = 252,000 J/mol. From Equation 5.8 we have

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

$$= \left(1.3 \times 10^{-5}\ \mathrm{m^2/s}\right) \exp\left[-\frac{252{,}000\ \mathrm{J/mol}}{(8.31\ \mathrm{J/mol-K})(1273\ \mathrm{K})}\right]$$

$$= 5.87 \times 10^{-16}\ \mathrm{m^2/s}$$

Substitution of this value into the above equation leads to

$$2.8 = \left(\frac{1 + 4}{2}\right) - \left(\frac{1 - 4}{2}\right) \mathrm{erf}\left[\frac{10 \times 10^{-6}\ \mathrm{m}}{2\sqrt{(5.87 \times 10^{-16}\ \mathrm{m^2/s})\,(t)}}\right]$$

This expression reduces to the following form:

$$0.2000 = \mathrm{erf}\left[\frac{206.4\sqrt{\mathrm{s}}}{\sqrt{t}}\right]$$

Using data in Table 5.1, it is necessary to determine the value of z for which the error function is 0.2000. We use linear interpolation as follows:

z	erf (z)
0.150	0.1680
y	0.2000
0.200	0.2227

$$\frac{y - 0.150}{0.200 - 0.150} = \frac{0.2000 - 0.1680}{0.2227 - 0.1680}$$

from which

$$y = 0.1793 = \frac{206.4\sqrt{\mathrm{s}}}{\sqrt{t}}$$

And, solving for *t* gives

$$t = 1.33 \text{ x } 10^{6} \text{ s} = 368 \text{ h} = 15.3 \text{ days}$$

5.15 This problem calls for an estimate of the time necessary to achieve a carbon concentration of 0.35 wt% at a point 6.0 mm from the surface. From Equation 5.6b,

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

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

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

or

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

Thus,

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

from which

$$t_2 = 135\ \text{h}$$

Factors That Influence Diffusion

5.16 We are asked to compute the diffusion coefficients of C in both α and γ iron at 900°C. Using the data in Table 5.2,

$$D_\alpha = \left(6.2 \times 10^{-7} \text{ m}^2/\text{s}\right) \exp\left[-\frac{80{,}000 \text{ J/mol}}{(8.31 \text{ J/mol-K})(1173 \text{ K})}\right]$$

$$= 1.69 \text{ x } 10^{-10} \text{ m}^2/\text{s}$$

$$D_\gamma = \left(2.3 \times 10^{-5} \text{ m}^2/\text{s}\right) \exp\left[-\frac{148{,}000 \text{ J/mol}}{(8.31 \text{ J/mol-K})(1173 \text{ K})}\right]$$

$$= 5.86 \text{ x } 10^{-12} \text{ m}^2/\text{s}$$

The *D* for diffusion of C in BCC α iron is larger, the reason being that the atomic packing factor is smaller than for FCC γ iron (0.68 versus 0.74—Section 3.4); this means that there is slightly more interstitial void space in the BCC Fe, and, therefore, the motion of the interstitial carbon atoms occurs more easily.

5.17 This problem asks us to compute the magnitude of *D* for the diffusion of Mg in Al at 400°C (673 K). Incorporating the appropriate data from Table 5.2 into Equation 5.8 leads to

$$D = \left(1.2 \times 10^{-4} \text{ m}^2/\text{s}\right) \exp\left[-\frac{131{,}000 \text{ J/mol}}{(8.31 \text{ J/mol-K})(673 \text{ K})}\right]$$

$$= 8.1 \times 10^{-15} \text{ m}^2/\text{s}$$

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

1. In the left-hand window that appears, click on the “Mg-Al” pair under the “Diffusing Species”-“Host Metal” headings.

2. Next, at the bottom of this window, click the “Add Curve” button.

3. A log D versus 1/T plot then appears, with a line for the temperature dependence of the diffusion coefficient for Mg in Al. 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 “Temperature (T):” label reads 673 K (inasmuch as this is the Kelvin equivalent of 400ºC). Finally, the diffusion coefficient value at this temperature is given under the label “Diff Coeff (D):”. For this problem, the value is 7.8 x 10^{-15} m^2/s.

5.18 We are asked to calculate the temperature at which the diffusion coefficient for the diffusion of Zn in Cu has a value of 2.6 x 10^{-16} m^2/s. Solving for *T* from Equation 5.9a

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

and using the data from Table 5.2 for the diffusion of Zn in Cu (i.e., D_0 = 2.4 x 10^{-5} m^2/s and Q_d = 189,000 J/mol) , we get

$$T = -\frac{189,000 \text{ J/mol}}{(8.31 \text{ J/mol-K})\left[\ln\left(2.6 \times 10^{-16} \text{ m}^2/\text{s}\right) - \ln\left(2.4 \times 10^{-5} \text{ m}^2/\text{s}\right)\right]}$$

$$= 901 \text{ K} = 628°\text{C}$$

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, there is a preset set of data for the diffusion of Zn in Cu system. However, the temperature range does not extend to conditions specified in the problem statement. Thus, this requires us specify our settings by clicking 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 from Table 5.2—viz. "2.4e-5". Next just below the "Qd" window enter the activation energy value—viz. "189". 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 500ºC and 1000ºC, so enter "500" in the "T Min" box that is beside "C"; and similarly for the maximum temperature—enter "1000" 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 Zn in Cu. 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 2.6 x 10^{-16} m^2/s. The temperature at which the diffusion coefficient has this value is given under the label "Temperature (T):". For this problem, the value is 903 K.

5.19 For this problem we are given D_0 (1.1 x 10^{-4}) and Q_d (272,000 J/mol) for the diffusion of Cr in Ni, and asked to compute the temperature at which D = 1.2 x 10^{-14} $\mathrm{m^2/s}$. Solving for T from Equation 5.9a yields

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

$$= \frac{272{,}000\ \mathrm{J/mol}}{(8.31\ \mathrm{J/mol\text{-}K})\left[\ln\left(1.1 \times 10^{-4}\ \mathrm{m^2/s}\right) - \ln\left(1.2 \times 10^{-14}\ \mathrm{m^2/s}\right)\right]}$$

$$= 1427\ \mathrm{K} = 1154°\mathrm{C}$$

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-4”. Next just below the “Qd” window enter the activation energy value—viz. “272”. 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 1000ºC and 1500ºC, 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 Cr in Ni. 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 1.2 x 10^{-14} $\mathrm{m^2/s}$. The temperature at which the diffusion coefficient has this value is given under the label “Temperature (T):”. For this problem, the value is 1430 K.

5.20 In this problem we are given Q_d for the diffusion of Cu in Ag (i.e., 193,000 J/mol) and asked to compute D at 1200 K given that the value of D at 1000 K is 1.0×10^{-14} m^2/s. It first becomes necessary to solve for D_0 from Equation 5.8 as

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

$$= \left(1.0 \times 10^{-14}\ \text{m}^2/\text{s}\right) \exp\left[\frac{193{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(1000\ \text{K})}\right]$$

$$= 1.22 \times 10^{-4}\ \text{m}^2/\text{s}$$

Now, solving for D at 1200 K (again using Equation 5.8) gives

$$D = \left(1.22 \times 10^{-4}\ \text{m}^2/\text{s}\right) \exp\left[-\frac{193{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(1200\ \text{K})}\right]$$

$$= 4.8 \times 10^{-13}\ \text{m}^2/\text{s}$$

5.21 (a) Using Equation 5.9a, we set up two simultaneous equations with Q_d and D_0 as unknowns as follows:

$$\ln D_1 = \ln D_0 - \frac{Q_d}{R}\left(\frac{1}{T_1}\right)$$

$$\ln D_2 = \ln D_0 - \frac{Q_d}{R}\left(\frac{1}{T_2}\right)$$

Now, solving for Q_d in terms of temperatures T_1 and T_2 (1473 K and 1673 K) and D_1 and D_2 (2.2 x 10^{-15} and 4.8 x 10^{-14} $\mathrm{m^2/s}$), we get

$$Q_d = -R\,\frac{\ln D_1 - \ln D_2}{\dfrac{1}{T_1} - \dfrac{1}{T_2}}$$

$$= -(8.31\ \mathrm{J/mol\text{-}K})\,\frac{\left[\ln\left(2.2 \times 10^{-15}\right) - \ln\left(4.8 \times 10^{-14}\right)\right]}{\dfrac{1}{1473\ \mathrm{K}} - \dfrac{1}{1673\ \mathrm{K}}}$$

$$= 315{,}700\ \mathrm{J/mol}$$

Now, solving for D_0 from Equation 5.8 (and using the 1473 K value of D)

$$D_0 = D_1 \exp\left(\frac{Q_d}{RT_1}\right)$$

$$= \left(2.2 \times 10^{-15}\ \mathrm{m^2/s}\right)\exp\left[\frac{315{,}700\ \mathrm{J/mol}}{(8.31\ \mathrm{J/mol\text{-}K})(1473\ \mathrm{K})}\right]$$

$$= 3.5 \times 10^{-4}\ \mathrm{m^2/s}$$

(b) Using these values of D_0 and Q_d, D at 1573 K is just

$$D = \left(3.5 \times 10^{-4}\ \mathrm{m^2/s}\right)\exp\left[-\frac{315{,}700\ \mathrm{J/mol}}{(8.31\ \mathrm{J/mol\text{-}K})(1573\ \mathrm{K})}\right]$$

$$= 1.1 \times 10^{-14} \text{ m}^2/\text{s}$$

Note: this problem may also be solved using the "Diffusion" module in the *VMSE* software. Open the "Diffusion" module, click on the "D0 and Qd 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 (viz. "1473" and "1673", in the first two boxes under the column labeled "T (K)". Next, enter the corresponding diffusion coefficient values (viz. "2.2e-15" and "4.8e-14").

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 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 3.49 x 10^{-4} m^2/s and 315 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 "1573". The value of the diffusion coefficient at this temperature is given under the label "Diff Coeff (D):". For our problem, this value is 1.2 x 10^{-14} m^2/s.

5.22 (a) Using Equation 5.9a, we set up two simultaneous equations with Q_d and D_0 as unknowns as follows:

$$\ln D_1 = \ln D_0 - \frac{Q_d}{R}\left(\frac{1}{T_1}\right)$$

$$\ln D_2 = \ln D_0 - \frac{Q_d}{R}\left(\frac{1}{T_2}\right)$$

Solving for Q_d in terms of temperatures T_1 and T_2 (873 K [600°C] and 973 K [700°C]) and D_1 and D_2 ($5.5 \text{ x } 10^{-14}$ and $3.9 \text{ x } 10^{-13}$ m^2/s), we get

$$Q_d = -R \frac{\ln D_1 - \ln D_2}{\dfrac{1}{T_1} - \dfrac{1}{T_2}}$$

$$= -\frac{(8.31 \text{ J/mol-K})\left[\ln\left(5.5 \times 10^{-14}\right) - \ln\left(3.9 \times 10^{-13}\right)\right]}{\dfrac{1}{873 \text{ K}} - \dfrac{1}{973 \text{ K}}}$$

$$= 138{,}300 \text{ J/mol}$$

Now, solving for D_0 from Equation 5.8 (and using the 600°C value of D)

$$D_0 = D_1 \exp\left(\frac{Q_d}{RT_1}\right)$$

$$= \left(5.5 \times 10^{-14} \text{ m}^2/\text{s}\right)\exp\left[\frac{138{,}300 \text{ J/mol}}{(8.31 \text{ J/mol-K})(873 \text{ K})}\right]$$

$$= 1.05 \text{ x } 10^{-5} \text{ m}^2/\text{s}$$

(b) Using these values of D_0 and Q_d, D at 1123 K (850°C) is just

$$D = \left(1.05 \times 10^{-5} \text{ m}^2/\text{s}\right)\exp\left[-\frac{138{,}300 \text{ J/mol}}{(8.31 \text{ J/mol-K})(1123 \text{ K})}\right]$$

$$= 3.8 \times 10^{-12}\ \text{m}^2/\text{s}$$

Note: this problem may also be solved using the "Diffusion" module in the *VMSE* software. Open the "Diffusion" module, click on the "D0 and Qd 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. "873" (600ºC) and "973" (700ºC), in the first two boxes under the column labeled "T (K)". Next, enter the corresponding diffusion coefficient values (viz. "5.5e-14" and "3.9e-13").

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 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 1.04 x 10^{-5} m^2/s and 138 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 "1123" (i.e., 850ºC). The value of the diffusion coefficient at this temperature is given under the label "Diff Coeff (D):". For our problem, this value is 1.2 x 10^{-14} m^2/s.

5.23 This problem asks us to determine the values of Q_d and D_0 for the diffusion of Au in Ag from the plot of log D versus 1/T. According to Equation 5.9b the slope of this plot is equal to $-\frac{Q_d}{2.3R}$ (rather than $-\frac{Q_d}{R}$ since we are using log D rather than ln D) and the intercept at 1/T = 0 gives the value of log D_0. The slope is equal to

$$\text{slope} = \frac{\Delta(\log D)}{\Delta\left(\frac{1}{T}\right)} = \frac{\log D_1 - \log D_2}{\frac{1}{T_1} - \frac{1}{T_2}}$$

Taking 1/T_1 and 1/T_2 as 1.0 x 10^{-3} and 0.90 x 10^{-3} K^{-1}, respectively, then the corresponding values of log D_1 and log D_2 are –14.68 and –13.57. Therefore,

$$Q_d = -2.3\,R\,(\text{slope})$$

$$Q_d = -2.3\,R\,\frac{\log D_1 - \log D_2}{\frac{1}{T_1} - \frac{1}{T_2}}$$

$$= -(2.3)(8.31\ \text{J/mol-K})\left[\frac{-14.68 - (-13.57)}{\left(1.0 \times 10^{-3} - 0.90 \times 10^{-3}\right)\ \text{K}^{-1}}\right]$$

$$= 212{,}200\ \text{J/mol}$$

Rather than trying to make a graphical extrapolation to determine D_0, a more accurate value is obtained analytically using Equation 5.9b taking a specific value of both D and T (from 1/T) from the plot given in the problem; for example, D = 1.0 x 10^{-14} m^2/s at T = 1064 K (1/T = 0.94 x 10^{-3} K^{-1}). Therefore

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

$$= \left(1.0 \times 10^{-14}\ \text{m}^2/\text{s}\right)\exp\left[\frac{212{,}200\ \text{J/mol}}{(8.31\ \text{J/mol-K})(1064\ \text{K})}\right]$$

$$= 2.65 \times 10^{-4}\ \text{m}^2/\text{s}$$

5.24 This problem asks that we compute the temperature at which the diffusion flux is 6.3 x 10^{-10} kg/m^2-s. Combining Equations 5.3 and 5.8 yields

$$J = -D\,\frac{\Delta C}{\Delta x}$$

$$= -D_0\,\frac{\Delta C}{\Delta x}\exp\left(-\frac{Q_d}{RT}\right)$$

Solving for *T* from this expression leads to

$$T = \left(\frac{Q_d}{R}\right)\frac{1}{\ln\left(-\dfrac{D_0\Delta C}{J\,\Delta x}\right)}$$

$$= \left(\frac{80{,}000\ \text{J/mol}}{8.31\ \text{J/mol-K}}\right)\frac{1}{\ln\left[\dfrac{(6.2\times10^{-7}\ \text{m}^2/\text{s})(0.85\ \text{kg/m}^3 - 0.40\ \text{kg/m}^3)}{(6.3\times10^{-10}\ \text{kg/m}^2\text{-s})(10\times10^{-3}\ \text{m})}\right]}$$

$$= 900\ \text{K} = 627°\text{C}$$

5.25 In order to solve this problem, we must first compute the value of D_0 from the data given at 1200°C (1473 K); this requires the combining of both Equations 5.3 and 5.8 as

$$J = -D\,\frac{\Delta C}{\Delta x}$$

$$= -D_0\,\frac{\Delta C}{\Delta x}\exp\left(-\frac{Q_d}{RT}\right)$$

Solving for D_0 from the above expression gives

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

$$= -\left(\frac{7.8 \times 10^{-8}\ \text{kg/m}^2\text{-s}}{-500\ \text{kg/m}^4}\right)\exp\left[\frac{145{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(1200 + 273\ \text{K})}\right]$$

$$= 2.18 \text{ x } 10^{-5}\ \text{m}^2/\text{s}$$

The value of the diffusion flux at 1273 K may be computed using these same two equations as follows:

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

$$= -\left(2.18 \times 10^{-5}\ \text{m}^2/\text{s}\right)\left(-500\ \text{kg/m}^4\right)\exp\left[-\frac{145{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(1273\ \text{K})}\right]$$

$$= 1.21 \text{ x } 10^{-8}\ \text{kg/m}^2\text{-s}$$

5.26 To solve this problem it is necessary to employ Equation 5.7

$$Dt = \text{constant}$$

Which, for this problem, takes the form

$$D_{1000}t_{1000} = D_{\mathrm{T}}t_{\mathrm{T}}$$

At 1000°C, and using the data from Table 5.2, for the diffusion of carbon in γ-iron—i.e.,

$D_0 = 2.3 \text{ x } 10^{-5}$ m^2/s

$Q_d = 148{,}000$ J/mol

the diffusion coefficient is equal to

$$D_{1000} = \left(2.3 \text{ x } 10^{-5} \text{ m}^2\text{/s}\right) \exp\left[-\frac{148{,}000 \text{ J/mol}}{(8.31 \text{ J/mol-K})(1000 + 273 \text{ K})}\right]$$

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

Thus, from the above equation

$$\left(1.93 \times 10^{-11} \text{ m}^2\text{/s}\right)(12 \text{ h}) = D_{\mathrm{T}}(4 \text{ h})$$

And, solving for D_{T}

$$D_{\mathrm{T}} = \frac{\left(1.93 \times 10^{-11} \text{ m}^2\text{/s}\right)(12 \text{ h})}{4 \text{ h}} = 5.79 \text{ x } 10^{-11} \text{ m}^2\text{/s}$$

Now, solving for T from Equation 5.9a gives

$$T = -\frac{Q_d}{R\left(\ln D_{\mathrm{T}} - \ln D_0\right)}$$

$$= -\frac{148{,}000 \text{ J/mol}}{(8.31 \text{ J/mol-K})\left[\ln\left(5.79 \times 10^{-11} \text{ m}^2\text{/s}\right) - \ln\left(2.3 \text{ x } 10^{-5} \text{ m}^2\text{/s}\right)\right]}$$

$$= 1381 \text{ K} = 1108°\text{C}$$

5.27 (a) We are asked to calculate the diffusion coefficient for Mg in Al at 450°C. Using the data in Table 5.2 and Equation 5.8

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

$$= \left(1.2 \times 10^{-4}\ \text{m}^2/\text{s}\right)\exp\left[-\frac{131{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(450 + 273\ \text{K})}\right]$$

$$= 4.08 \text{ x } 10^{-14}\ \text{m}^2/\text{s}$$

(b) This portion of the problem calls for the time required at 550°C to produce the same diffusion result as for 15 h at 450°C. Equation 5.7 is employed as

$$D_{450}t_{450} = D_{550}t_{550}$$

Now, from Equation 5.8 the value of the diffusion coefficient at 550°C is calculated as

$$D_{550} = \left(1.2 \times 10^{-4}\ \text{m}^2/\text{s}\right)\exp\left[-\frac{131{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(550 + 273\ \text{K})}\right]$$

$$= 5.76 \text{ x } 10^{-13}\ \text{m}^2/\text{s}$$

Thus,

$$t_{550} = \frac{D_{450}t_{450}}{D_{550}}$$

$$= \frac{\left(4.08 \times 10^{-14}\ \text{m}^2/\text{s}\right)(15\ \text{h})}{\left(5.76 \times 10^{-13}\ \text{m}^2/\text{s}\right)} = 1.06\ \text{h}$$

5.28 In order to determine the temperature to which the diffusion couple must be heated so as to produce a concentration of 3.0 wt% Ni at the 2.0-mm position, we must first utilize Equation 5.6b with time *t* being a constant. That is

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

Or

$$\frac{x_{1000}^2}{D_{1000}} = \frac{x_{\mathrm{T}}^2}{D_{\mathrm{T}}}$$

Now, solving for D_{T} from this equation, yields

$$D_{\mathrm{T}} = \frac{x_{\mathrm{T}}^2 D_{1000}}{x_{1000}^2}$$

and incorporating the temperature dependence of D_{1000} utilizing Equation (5.8), yields

$$D_{\mathrm{T}} = \frac{\left(x_{\mathrm{T}}^2\right)\left[D_0 \exp\left(-\frac{Q_d}{RT}\right)\right]}{x_{1000}^2}$$

$$= \frac{(2\ \mathrm{mm})^2\left[\left(2.7 \times 10^{-4}\ \mathrm{m^2/s}\right)\exp\left(-\frac{236{,}000\ \ \mathrm{J/mol}}{(8.31\ \ \mathrm{J/mol\text{-}K})(1273\ \ \mathrm{K})}\right)\right]}{(1\ \mathrm{mm})^2}$$

$$= 2.21 \text{ x } 10^{-13}\ \mathrm{m^2/s}$$

We now need to find the *T* at which *D* has this value. This is accomplished by rearranging Equation 5.9a and solving for *T* as

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

$$= \frac{236{,}000\ \mathrm{J/mol}}{(8.31\ \mathrm{J/mol\text{-}K})\left[\ln\left(2.7 \times 10^{-4}\ \mathrm{m^2/s}\right) - \ln\left(2.21 \times 10^{-13}\ \mathrm{m^2/s}\right)\right]}$$

$$= 1357\ \mathrm{K} = 1084^\circ\mathrm{C}$$

5.29 In order to determine the position within the diffusion couple at which the concentration of A in B is 2.5 wt%, we must employ Equation 5.6b with *t* constant. That is

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

Or

$$\frac{x_{800}^2}{D_{800}} = \frac{x_{1000}^2}{D_{1000}}$$

It is first necessary to compute values for both D_{800} and D_{1000}; this is accomplished using Equation 5.8 as follows:

$$D_{800} = \left(1.5 \times 10^{-4} \text{ m}^2\text{/s}\right) \exp\left[-\frac{125{,}000 \text{ J/mol}}{(8.31 \text{ J/mol-K})(800 + 273 \text{ K})}\right]$$

$$= 1.22 \text{ x } 10^{-10} \text{ m}^2\text{/s}$$

$$D_{1000} = \left(1.5 \times 10^{-4} \text{ m}^2\text{/s}\right) \exp\left[-\frac{125{,}000 \text{ J/mol}}{(8.31 \text{ J/mol-K})(1000 + 273 \text{ K})}\right]$$

$$= 1.11 \text{ x } 10^{-9} \text{ m}^2\text{/s}$$

Now, solving the above expression for x_{1000} yields

$$x_{1000} = x_{800}\sqrt{\frac{D_{1000}}{D_{800}}}$$

$$= (5 \text{ mm})\sqrt{\frac{1.11 \times 10^{-9} \text{ m}^2\text{/s}}{1.22 \times 10^{-10} \text{ m}^2\text{/s}}}$$

$$= 15.1 \text{ mm}$$

5.31 This problem asks us to compute the temperature at which a nonsteady-state 48 h diffusion anneal was carried out in order to give a carbon concentration of 0.30 wt% C in FCC Fe at a position 3.5 mm below the surface. From Equation 5.5

$$\frac{C_x - C_0}{C_s - C_0} = \frac{0.30 - 0.10}{1.10 - 0.10} = 0.2000 = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

Or

$$\operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) = 0.8000$$

Now it becomes necessary, using the data in Table 5.1 and linear interpolation, to determine the value of $\frac{x}{2\sqrt{Dt}}$.

Thus

$\underline{z}$	$\underline{\operatorname{erf}(z)}$
0.90	0.7970
y	0.8000
0.95	0.8209

$$\frac{y - 0.90}{0.95 - 0.90} = \frac{0.8000 - 0.7970}{0.8209 - 0.7970}$$

From which

$$y = 0.9063$$

Thus,

$$\frac{x}{2\sqrt{Dt}} = 0.9063$$

And since t = 48 h (172,800 s) and x = 3.5 mm (3.5 x 10^{-3} m), solving for D from the above equation yields

$$D = \frac{x^2}{(4t)(0.9063)^2}$$

$$= \frac{\left(3.5 \times 10^{-3}\ \text{m}\right)^2}{(4)(172{,}800\ \text{s})(0.821)} = 2.16 \times 10^{-11}\ \text{m}^2/\text{s}$$

Now, in order to determine the temperature at which D has the above value, we must employ Equation 5.9a; solving this equation for T yields

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

From Table 5.2, D_0 and Q_d for the diffusion of C in FCC Fe are 2.3 x 10^{-5} m^2/s and 148,000 J/mol, respectively. Therefore

$$T = \frac{148{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})\left[\ln\left(2.3 \times 10^{-5}\ \text{m}^2/\text{s}\right) - \ln\left(2.16 \times 10^{-11}\ \text{m}^2/\text{s}\right)\right]}$$

= 1283 K = 1010°C

5.30 In order to compute the diffusion time at 900°C to produce a carbon concentration of 0.75 wt% at a position 0.5 mm below the surface we must employ Equation 5.6b with position constant; that is

$$Dt = \text{constant}$$

Or

$$D_{600}t_{600} = D_{900}t_{900}$$

In addition, it is necessary to compute values for both D_{600} and D_{900} using Equation 5.8. From Table 5.2, for the diffusion of C in α-Fe, Q_d = 80,000 J/mol and D_0 = 6.2 x 10^{-7} m^2/s. Therefore,

$$D_{600} = \left(6.2 \times 10^{-7}\ \text{m}^2/\text{s}\right)\exp\left[-\frac{80{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(600 + 273\ \text{K})}\right]$$

$$= 1.01 \text{ x } 10^{-11}\ \text{m}^2/\text{s}$$

$$D_{900} = \left(6.2 \times 10^{-7}\ \text{m}^2/\text{s}\right)\exp\left[-\frac{80{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(900 + 273\ \text{K})}\right]$$

$$= 1.69 \text{ x } 10^{-10}\ \text{m}^2/\text{s}$$

Now, solving the original equation for t_{900} gives

$$t_{900} = \frac{D_{600}t_{600}}{D_{900}}$$

$$= \frac{\left(1.01 \times 10^{-11}\,\text{m}^2/\text{s}\right)(100\ \text{min})}{1.69 \times 10^{-10}\,\text{m}^2/\text{s}}$$

$$= 5.98\ \text{min}$$

DESIGN PROBLEMS

Steady-State Diffusion

5.D1 This problem calls for us to ascertain whether or not a hydrogen-nitrogen gas mixture may be enriched with respect to hydrogen partial pressure by allowing the gases to diffuse through an iron sheet at an elevated temperature. If this is possible, the temperature and sheet thickness are to be specified; if such is not possible, then we are to state the reasons why. Since this situation involves steady-state diffusion, we employ Fick's first law, Equation 5.3. Inasmuch as the partial pressures on the high-pressure side of the sheet are the same, and the pressure of hydrogen on the low pressure side is five times that of nitrogen, and concentrations are proportional to the square root of the partial pressure, the diffusion flux of hydrogen J_H is the square root of 5 times the diffusion flux of nitrogen J_N--i.e.

$$J_H = \sqrt{5}\, J_N$$

Thus, equating the Fick's law expressions incorporating the given equations for the diffusion coefficients and concentrations in terms of partial pressures leads to the following

$$J_H$$

$$= \frac{1}{\Delta x} \times$$

$$(2.5 \times 10^{-3})\left(\sqrt{0.1013\ \text{MPa}} - \sqrt{0.051\ \text{MPa}}\right)\exp\left(-\frac{27.8\ \text{kJ}}{RT}\right)(1.4 \times 10^{-7}\ \text{m}^2/\text{s})\exp\left(-\frac{13.4\ \text{kJ}}{RT}\right)$$

$$= \sqrt{5}\, J_N$$

$$= \frac{\sqrt{5}}{\Delta x} \times$$

$$(2.75 \times 10^{3})\left(\sqrt{0.1013\ \text{MPa}} - \sqrt{0.01013\ \text{MPa}}\right)\exp\left(-\frac{37.6\ \text{kJ}}{RT}\right)(3.0 \times 10^{-7}\ \text{m}^2/\text{s})\exp\left(-\frac{76.15\ \text{kJ}}{RT}\right)$$

The Δx's cancel out, which means that the process is independent of sheet thickness. Now solving the above expression for the absolute temperature T gives

$$T = 3467\ \text{K}$$

which value is extremely high (surely above the vaporization point of iron). Thus, such a diffusion process is *not possible*.

5.D2 This problem calls for us to ascertain whether or not an A_2-B_2 gas mixture may be enriched with respect to the A partial pressure by allowing the gases to diffuse through a metal sheet at an elevated temperature. If this is possible, the temperature and sheet thickness are to be specified; if such is not possible, then we are to state the reasons why. Since this situation involves steady-state diffusion, we employ Fick's first law, Equation 5.3. Inasmuch as the partial pressures on the high-pressure side of the sheet are the same, and the pressure of A_2 on the low pressure side is 2.5 times that of B_2, and concentrations are proportional to the square root of the partial pressure, the diffusion flux of A, J_A, is the square root of 2.5 times the diffusion flux of nitrogen J_B--i.e.

$$J_A = \sqrt{2.5}\, J_B$$

Thus, equating the Fick's law expressions incorporating the given equations for the diffusion coefficients and concentrations in terms of partial pressures leads to the following

$$J_A$$

$$= \frac{1}{\Delta x} \times$$

$$\left(1.5 \times 10^3\right)\left(\sqrt{0.1013 \text{ MPa}} - \sqrt{0.051 \text{ MPa}}\right) \exp\left(-\frac{20.0 \text{ kJ}}{RT}\right)\left(5.0 \times 10^{-7} \text{ m}^2/\text{s}\right) \exp\left(-\frac{13.0 \text{ kJ}}{RT}\right)$$

$$= \sqrt{2.5}\, J_B$$

$$= \frac{\sqrt{2.5}}{\Delta x} \times$$

$$\left(2.0 \times 10^3\right)\left(\sqrt{0.1013 \text{ MPa}} - \sqrt{0.0203 \text{ MPa}}\right) \exp\left(-\frac{27.0 \text{ kJ}}{RT}\right)\left(3.0 \times 10^{-6} \text{ m}^2/\text{s}\right) \exp\left(-\frac{21.0 \text{ kJ}}{RT}\right)$$

The Δx's cancel out, which means that the process is independent of sheet thickness. Now solving the above expression for the absolute temperature T gives

$$T = 568 \text{ K } (295°\text{C})$$

5.D4 This is a nonsteady-state diffusion situation; thus, it is necessary to employ Equation 5.5, utilizing values/value ranges for the following parameters:

$$C_0 = 0.15 \text{ wt\% C}$$

$$1.2 \text{ wt\% C} \leq C_s \leq 1.4 \text{ wt\% C}$$

$$C_x = 0.75 \text{ wt\% C}$$

$$x = 0.65 \text{ mm}$$

$$1000^\circ\text{C} \leq T \leq 1200^\circ\text{C}$$

Let us begin by assuming a specific value for the surface concentration within the specified range—say 1.2 wt% C. Therefore

$$\frac{C_x - C_0}{C_s - C_0} = \frac{0.75 - 0.15}{1.20 - 0.15}$$

$$= 0.5714 = 1 - \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

And thus

$$1 - 0.5714 = 0.4286 = \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

Using linear interpolation and the data presented in Table 5.1

z	erf (z)
0.4000	0.4284
y	0.4286
0.4500	0.4755

$$\frac{0.4286 - 0.4284}{0.4755 - 0.4284} = \frac{y - 0.4000}{0.4500 - 0.4000}$$

From which

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

The problem stipulates that x = 0.65 mm = 6.5 x 10^{-4} m. Therefore

$$\frac{6.5 \times 10^{-4}\ \text{m}}{2\sqrt{Dt}} = 0.4002$$

Which leads to

$$Dt = 6.59 \text{ x } 10^{-7}\ \text{m}^2$$

Furthermore, the diffusion coefficient depends on temperature according to Equation 5.8; and, as noted in Design Example 5.1, D_0 = 2.3 x 10^{-5} m^2/s and Q_d = 148,000 J/mol. Hence

$$Dt = D_0 \exp\left(-\frac{Q_d}{RT}\right)(t) = 6.59 \times 10^{-7}\ \text{m}^2$$

$$\left(2.3 \times 10^{-5}\ \text{m}^2/\text{s}\right)\exp\left[-\frac{148{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(T)}\right](t) = 6.59 \times 10^{-7}\ \text{m}^2$$

And solving for the time t

$$t\ (\text{in s}) = \frac{2.86 \times 10^{-2}}{\exp\left(-\dfrac{17{,}810}{T}\right)}$$

Thus, the required diffusion time may be computed for some specified temperature (in K). Below are tabulated t values for three different temperatures that lie within the range stipulated in the problem.

Temperature (°C)	Time	
	s	h
1000	34,100	9.5
1100	12,300	3.4
1200	5,100	1.4

Now, let us repeat the above procedure for two other values of the surface concentration, say 1.3 wt% C and 1.4 wt% C. Below is a tabulation of the results, again using temperatures of 1000°C, 1100°C, and 1200°C.

C_s (wt% C)	Temperature (°C)	Time s	Time h
1.3	1000	26,700	7.4
	1100	9,600	2.7
	1200	4,000	1.1
1.4	1000	21,100	6.1
	1100	7,900	2.2
	1200	1,500	0.9