

**Series 5 Solution**

**17 October 2025**

**Exercise 1 Steel carburizing**

We use the equation defining the diffusion from the surface at a constant concentration (eq. 5.7 of the text).

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

$$\frac{C(x) - C_0}{C_s - C_0} = \frac{0.5 - 0.02}{1 - 0.02} = 0.49 = \left( 1 - \operatorname{erf} \left( \frac{x}{2\sqrt{Dt}} \right) \right)$$

Thus:

$$\operatorname{erf} \left( \frac{x}{2\sqrt{Dt}} \right) = 0.51$$

Looking up the *erf* function table, we get the following:

$$\frac{0.51 - 0.4755}{0.5205 - 0.4755} = \frac{z - 0.45}{0.5 - 0.45}$$

$$z = \frac{x}{2\sqrt{Dt}} = 0.483$$

From this, we get the following:

$$t = \frac{(10^{-3} [m])^2}{4(0.483)^2 (20 \cdot 10^{-6} [m^2 / s] \cdot \exp((-142 [kJ / mol]) / 1273 [K] \cdot 8.314 [J / mol / K]))^2} = 9.96h$$

The diffusion coefficient used is for the face-centered cubic (f.c.c.) phase and a temperature of 1000°C. The surface carburizing of steels is classically performed at a rate of about 1/10th of a millimeter per hour. The process is thus more precise but slow and, therefore, expensive.

## Exercise 2: Conduction in an ionic crystal

All calculations are made in one dimension. For example, the electrical conductivity  $\sigma$  related to the electron flux is given by :

$$J_{el} = \sigma E$$

Let's calculate electron flux  $J_{el}$  :

$$J_{el} = \underbrace{C_i v_i}_{J_i} q$$

where  $J_i$  is the flux of the ions.

Now, 
$$v_i = \frac{D_i F}{kT} = \frac{D_i q_i E}{kT}$$

Therefore:  $J_i = \frac{C_i D_i q_i^2 E}{kT}$  and the electrical conductivity is:

$$\sigma = \frac{C_i D_i q_i^2}{kT} = \frac{C_i q_i^2}{kT} D_{i0} \exp\left(\frac{-Q_i}{kT}\right)$$

If a concentration gradient is present, then:

$$J_{el} = J_i q_i = q_i \left( \frac{C_i D_i q_i E}{kT} - D_i \frac{\partial C_i}{\partial x} \right)$$

## Exercise 3: Conduction in a two-component ionic crystal

An example of such a crystal is a diffusion couple, such as NaCl-KCl, where only metal ions diffuse and the underlying Cl lattice remains steady.

Without any electrical field:

$$J_A = -D_A^* \frac{\partial C_A}{\partial x}$$

$$J_B = -D_B^* \frac{\partial C_B}{\partial x}$$

and

$$C_A + C_B = \text{constant} \Rightarrow \frac{\partial C_A}{\partial x} = -\frac{\partial C_B}{\partial x}$$

Since  $D_A^* \neq D_B^*$  then  $J_A \neq J_B$  , which would produce a total flux:

$$J = J_A + J_B = (D_A^* - D_B^*) \frac{\partial C_A}{\partial x} \tag{5.3.1}$$

However, electrical neutrality implies that the total flux is zero, resulting in an electric field  $E$ . As calculated in exercise 2 above, the flux equations for ions A and B become:

$$\begin{aligned} J_A &= -D_A^* \frac{\partial C_A}{\partial x} + q_i E \frac{D_A^* C_A}{kT} \\ J_B &= -D_B^* \frac{\partial C_B}{\partial x} + q_i E \frac{D_B^* C_B}{kT} \end{aligned} \quad (5.3.2)$$

In this case,  $J = J_A + J_B = 0$ , which allows the calculation of  $E$ :

$$E = \frac{kT}{q_i} \frac{D_A^* - D_B^*}{C_A D_A^* + C_B D_B^*} \frac{\partial C_A}{\partial x} \quad (5.3.3)$$

By inserting (5.3.3) in (5.3.2), the fluxes can be expressed as a function of concentration gradients:

$$\begin{aligned} J_A &= -\bar{D}_A \frac{\partial C_A}{\partial x} \\ J_B &= -\bar{D}_B \frac{\partial C_B}{\partial x} \end{aligned} \quad (5.3.4)$$

with

$$\bar{D} = \frac{D_A^* \cdot D_B^*}{X_A D_A^* + X_B D_B^*}$$

Beware not to confuse this coefficient of ionic interdiffusion with that of chemical interdiffusion  $\tilde{D} = X_B D_A^* + X_A D_B^*$  obtained by the Boltzmann-Matano method.