Workshop 10: Transient mass diffusion

Attempt these problems before opening the worked solutions.

1 Carbon diffusion into steel

EXERCISE
Exercise 1. Time for case hardening

The surface of a mild steel component is commonly hardened by packing the component in a carbonaceous material in a furnace at a high temperature for a predetermined time. Consider such a component with a uniform initial carbon concentration of 0.15% by mass. The component is packed in a carbonaceous material and is placed in a high-temperature furnace. The diffusion coefficient of carbon in steel at the furnace temperature is given to be $4.8 \times 10^{-10}\ \mathrm{m}^2/\mathrm{s}$, and the equilibrium concentration of carbon in the iron at the interface is determined from equilibrium data to be 1.2% by mass. Determine how long the component should be kept in the furnace for the mass concentration of carbon 0.5 mm below the surface to reach 1%.

See solution for Exercise 1

2 Hydrogen leaving a sheet

EXERCISE
Exercise 2. Centre concentration in a finite slab

A large sheet of material 40 mm thick contains dissolved hydrogen at a uniform concentration of 3 $\mathrm{kmol}/\mathrm{m}^3$. The sheet is exposed to a fluid stream, causing the concentration of the dissolved hydrogen to be reduced suddenly to zero at both surfaces. This surface condition is maintained constant thereafter. If the mass diffusivity of hydrogen is $9 \times 10^{-7}\ \mathrm{m}^2/\mathrm{s}$, how much time is required to bring the density of dissolved hydrogen to 1.2 kg/m^3 at the centre of the sheet?

See solution for Exercise 2

3 Drug release from a bead

EXERCISE
Exercise 3. Drug release from a spherical bead

Consider a small spherical bead (D = 0.1 cm) that initially contains 0.2 mmol/L of the drug griseofulvin (species A). Determine the time it will take for the concentration of

griseofulvin to reach 10% of its initial value, if its diffusivity within the bead material is $1.5 \times 10^{-7}\ \mathrm{cm}^2/\mathrm{s}$. Upon release from the bead, the drug is immediately consumed so that the surface concentration can be assumed to be zero.

See solution for Exercise 3

Solutions

Exercise solutions

Exercise 1. Time for case hardening

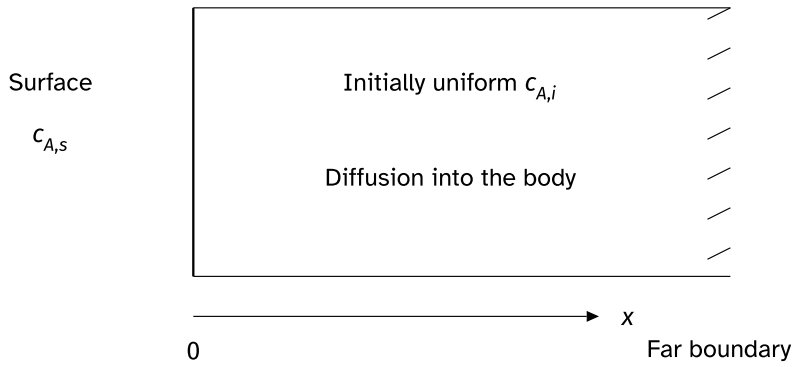


Figure 1: Carbon enters the steel through a maintained surface concentration. The target is at a depth measured inward from that surface; the far boundary remains unaffected.

Data

Quantity	Symbol	Value
Initial, surface and target mass fractions	w_i, w_s, w	$0.0015, 0.012, 0.010$
Target depth	x	$0.00050\ \mathrm{m}$
Diffusivity at furnace temperature	D	$4.8 \times 10^{-10}\ \mathrm{m^2\,s^{-1}}$

Assumptions

Assume constant diffusivity, no bulk motion or reaction inside each solid, uniform initial concentration and a maintained surface concentration. The surface condition changes at $t = 0$. For constant density, carbon mass fraction obeys the same diffusion equation as concentration.

Calculations

Define the normalised concentration

$$\Theta = \frac{C - C_s}{C_i - C_s}. \tag{1}$$

Use the same ratio with mass fraction w replacing C in problem 1. The error function is

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-u^2}\, du.$$

For interpolation, $\operatorname{erf}(0.170) = 0.189992$ and $\operatorname{erf}(0.171) = 0.191088$. A calculator with an inverse error function can also be used.

Treat the solid as a semi-infinite medium with a planar surface at $x = 0$, where x increases into the steel. Other surfaces are far beyond the diffusion penetration depth during the treatment. Assume no external transport resistance and constant steel density. Use fractions 0.0015, 0.012 and 0.010, or use percentages consistently. The semi-infinite solution is

$$\frac{w - w_i}{w_s - w_i} = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right). \tag{2}$$

The steel treatment time follows from the inverse error function at the specified depth.

The required fraction of the surface concentration change is

$$\frac{0.010 - 0.0015}{0.012 - 0.0015} = 0.809524.$$

Hence Eq. 2 gives $\operatorname{erf}(z) = 0.190476$, where

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

Inversion gives $z = 0.170441$.

Using $x = 5.0 \times 10^{-4}\,\mathrm{m}$,

$$t = \frac{x^2}{4Dz^2} = 4482.18\,\mathrm{s} = 74.703\,\mathrm{min}.$$

Interpolation of the supplied table gives about $4482\,\mathrm{s}$.

The source's rounded $z = 0.17$ gives about $4505\,\mathrm{s}$.

The characteristic penetration distance $2\sqrt{Dt} = 2.93\,\mathrm{mm}$ must be small relative to the component dimensions for this planar semi-infinite model to apply.

The answer excludes furnace heating time.

Answer

The required diffusion time at furnace temperature is $4.48 \times 10^3\,\mathrm{s}$, approximately $74.7\,\mathrm{min}$. Furnace warm-up time is additional.

Back to Exercise 1

Exercise 2. Centre concentration in a finite slab

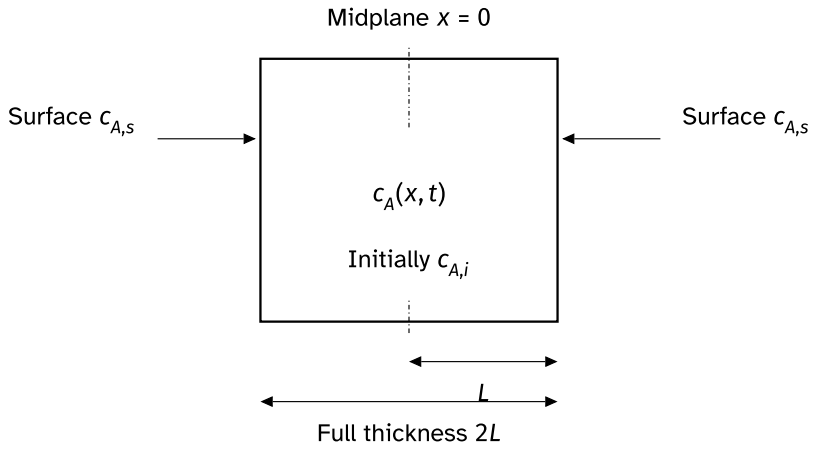


Figure 2: Hydrogen leaves both faces of the sheet under equal surface conditions. Use half-thickness L between the centre plane and either face.

Data

Quantity	Symbol	Value
Sheet thickness and half-thickness	$2L, L$	$0.040, 0.020\ \mathrm{m}$
Initial molar concentration	C_i	$3.0\ \mathrm{kmol\,m^{-3}}$
Target centre mass concentration	$\rho_{H_2,0}$	$1.2\ \mathrm{kg\,m^{-3}}$
Surface concentration	C_s	0
Diffusivity	D	$9.0 \times 10^{-7}\ \mathrm{m^2\,s^{-1}}$
Molecular hydrogen molar mass	M_{H_2}	$2.0\ \mathrm{kg\,kmol^{-1}}$

The worked solution uses molecular hydrogen molar mass $M_{H_2} = 2.0\,\mathrm{kg\,kmol^{-1}}$.

Assumptions

Assume one-dimensional diffusion normal to the faces, negligible edge effects and no external transport resistance. Set $x = 0$ at the centre, with faces at $x = \pm L$ and half-thickness $L = 20\,\mathrm{mm}$. Define $Fo = Dt/L^2$.

Calculations

The exact centre concentration ratio is

$$\Theta_0 = \frac{4}{\pi}\sum_{n=0}^{\infty}\frac{(-1)^n}{2n+1}\exp\left[-\frac{(2n+1)^2\pi^2 Fo}{4}\right].$$

For $Fo \gtrsim 0.2$, use the first-term approximation

$$\Theta_0 \simeq \frac{4}{\pi}\exp\left(-\frac{\pi^2 Fo}{4}\right). \tag{3}$$

Use Eq. 1 with $C_s = 0$. Convert the target mass concentration to molar concentration before forming the ratio. Check that the calculated Fo is consistent with the approximation.

The sheet target is one fifth of its initial hydrogen concentration after unit conversion.

Convert the centre target to

$$C_0 = \frac{1.2}{2.0} = 0.60\,\mathrm{kmol\,m^{-3}}.$$

Then

$$\Theta_0 = \frac{0.60}{3.0} = 0.20.$$

Solving Eq. 3 gives

$$Fo = \frac{4}{\pi^2}\ln\left(\frac{\frac{4}{\pi}}{0.20}\right) = 0.750183.$$

The time uses the half-thickness, not the total thickness:

$$t = Fo\frac{L^2}{D} = 333.415\,\mathrm{s} = 5.55691\,\mathrm{min}.$$

Since $Fo > 0.2$, the first-term approximation is appropriate.

The next term at this time is about -2.47×10^{-8} in Θ_0, so retaining it does not change the reported time.

The source chart gives $Fo \approx 0.75$ and $t \approx 333\,\mathrm{s}$.

Using the full 40 mm thickness in place of L would overestimate time by a factor of four.

Answer

The centre reaches $1.2\,\mathrm{kg\,m^{-3}}$ of molecular hydrogen after $333\,\mathrm{s}$, or $5.56\,\mathrm{min}$. The resulting Fourier number supports the first-term approximation.

Back to Exercise 2

Exercise 3. Drug release from a spherical bead

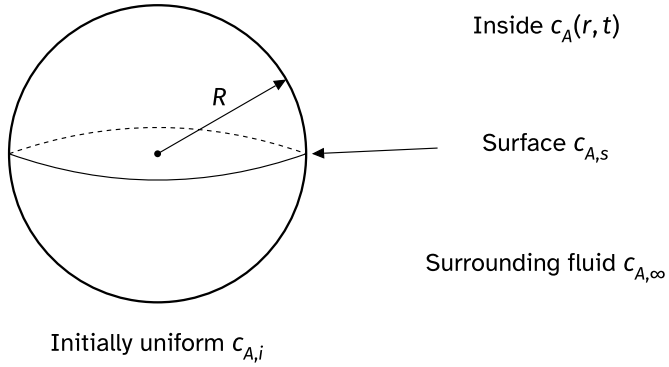


Figure 3: Drug diffuses radially from an initially uniform spherical bead to a sink. The centre concentration and total amount remaining are different measures.

Data

Quantity	Symbol	Value
Diameter and radius	d, a	$0.10, 0.050\ \mathrm{cm}$
Initial concentration	C_i	$0.20\ \mathrm{mmol\,L^{-1}}$
Target centre concentration	C_0	$0.020\ \mathrm{mmol\,L^{-1}}$
Surface concentration	C_s	0
Diffusivity	D	$1.5 \times 10^{-7}\ \mathrm{cm^2\,s^{-1}}$

The source question does not specify the location of the target concentration. This worked solution uses the centre, following the supplied solution.

Assumptions

Assume spherical symmetry, a fixed bead radius $a = d/2$, constant temperature and no reaction inside the bead. The centre has zero radial concentration gradient; the surface at $r = a$ has $C_s = 0$. Define $Fo = Dt/a^2$.

Calculations

The exact centre concentration ratio is

$$\Theta_0 = 2\sum_{n=1}^{\infty}(-1)^{n+1}\exp(-n^2\pi^2 Fo).$$

For $Fo \gtrsim 0.2$, use

$$\Theta_0 \simeq 2\exp(-\pi^2 Fo). \tag{4}$$

Check the approximation after computing Fo. Centre concentration differs from the volume-averaged concentration. This question uses the centre, matching the coordinator's worked solution.

The bead centre reaches the specified fraction when its Fourier number is about 0.304.

The target is $C_0 = 0.020\,\mathrm{mmol\,L^{-1}}$, giving $\Theta_0 = 0.10$.

Using Eq. 4 yields

$$Fo = \frac{\ln\left(\frac{2}{0.10}\right)}{\pi^2} = 0.303531.$$

Use

$$a = 0.050\,\mathrm{cm} = 5.0 \times 10^{-4}\,\mathrm{m}$$

and $D = 1.5 \times 10^{-11}\,\mathrm{m^2\,s^{-1}}$.

Then

$$t = Fo\frac{a^2}{D} = 5058.85\,\mathrm{s} = 84.3142\,\mathrm{min} = 1.40524\,\mathrm{h}.$$

The Fourier number exceeds 0.2.

At this time the second term of the exact centre series is -1.25×10^{-5}, so the first-term ratio is accurate to about 0.013%.

The exact series gives about $5058.64\,\mathrm{s}$.

The source rounds Fo to 0.3 and obtains $5000\,\mathrm{s}$ or 1.39 hours.

The diameter must first be halved.

Initial concentration cancels from the ratio because this constant-property diffusion model is linear.

Answer

The bead centre reaches ten percent of its initial concentration after approximately 5.06×10^3 s, or $84.3\,\mathrm{min}$. This is a centre-concentration result, not a volume-average result.

Back to Exercise 3