Transient mass diffusion

1 Errata

- Slide 10 places the transformed finite-wall boundary condition at infinity. Apply it at the wall surface

$$\Theta(L, t) = 0$$

  The finite wall ends at $x = L$.

- Slide 11 gives $c_A - c_{A0}$ as the normalized numerator and includes a stray x in the exponential decay factor. Use $c_A - c_{As}$ in the numerator. With the slide's full wall thickness L, use the decay factor

$$\exp\left(-\frac{n^2\pi^2 D_{AB}t}{L^2}\right)$$

- Slide 22 incorrectly groups the large-argument approximation. Use

$$\operatorname{erf}(\eta) \simeq 1 - \frac{e^{-\eta^2}}{\eta\sqrt{\pi}}$$

  The printed grouping incorrectly divides the whole expression by η.

- The deposition diagrams on slides 24 to 26 show a reaction that does not conserve oxygen. The printed reactants contain six oxygen atoms, while the products contain two. Use the balanced oxide-reduction step in the physical setup. The diffusion calculation starts with the maintained phosphorus surface concentration and does not use the erroneous reaction.

2 Reading list

- Bird et al. (2006), chapter 18.
- Geankoplis (2003), chapter 6.
- Welty et al. (2001), chapter 25.

Use molar flux in $\mathrm{mol\,m^{-2}\,s^{-1}}$ and concentration in $\mathrm{mol\,m^{-3}}$, unless an example specifies mass or atomic concentration.

3 Choose a time-dependent diffusion model

Given conditions	Model and checks
Slowly shrinking reacting body	Use a pseudo-steady surrounding profile with a moving-boundary inventory, Eq. 8.
Finite body, nearly uniform interior	Test $k_c(V/A_s)/D_{AB} \leq 0.1$ on a common concentration basis before using a lumped balance.
Finite body with internal gradients	Use half-thickness or radius in the Fourier and Biot numbers, Eq. 14; select the matching geometry and surface condition.
Early diffusion into a deep medium	Use the semi-infinite step solution; check penetration depth against the actual body dimension.
Reaction distributed within the body	Add a volume reaction term; the source-free diffusion solutions here no longer apply unchanged.

4 Pseudo steady state analysis

DEFINITION
Pseudo steady state

An approximation that neglects accumulation in a rapidly adjusting transport region while a slower boundary or system state changes with time. Its validity requires separated transport and system time scales.

4.1 Coal particle burning

A spherical carbon particle of current radius R burns in an effectively infinite gas. Oxygen diffuses inward, and carbon monoxide and carbon dioxide diffuse outward. The source assumes the product split

$$3\mathrm{C(s)} + 2.5\mathrm{O_2(g)} \rightarrow 2\mathrm{CO_2(g)} + \mathrm{CO(g)} \tag{1}$$

The atomic balance is correct. This particular split is an input to the model, not a universal combustion law. We assume instantaneous surface reaction, no homogeneous reaction in the gas, constant temperature, total molar concentration c and effective oxygen-mixture diffusivity D. The actual four-species problem generally requires multicomponent diffusion. Replacing it with one effective D is an additional approximation.

The gas establishes its profile on a time scale R^2/D. Treating that profile as steady at each instant is justified only when this time is much shorter than the particle shrinkage time. For a radius of 100 micrometres and $D = 10^{-4}$ m² s⁻¹ the relaxation scale is 10^{-4} s. This estimate

alone does not determine burnout time; density, gas concentration and kinetics also matter. Fast kinetics must be checked independently.

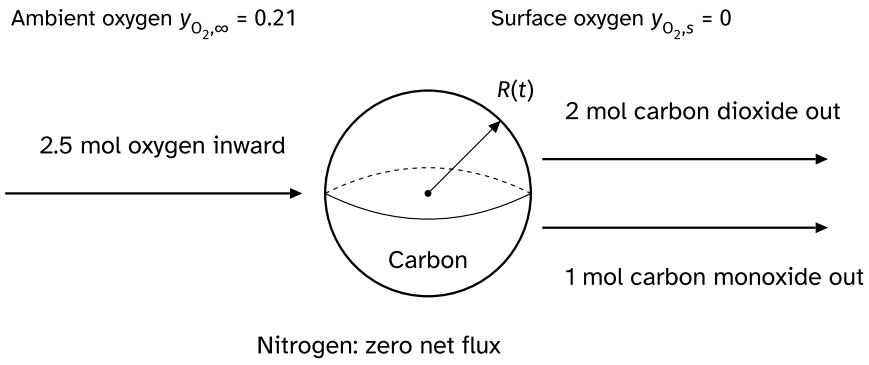


Figure 1: Oxygen diffuses inward while gaseous products diffuse outward. Positive radial flux points outward.

Spherical symmetry removes angular derivatives. No gas-phase reaction removes the source term. Pseudo steady state removes gas accumulation, so continuity reduces to

$$\frac{1}{r^2}\frac{d}{dr}(r^2 N_{O_2,r}) = 0, \qquad r^2 N_{O_2,r} = C \tag{2}$$

The integration constant C has units mol s^{-1}. It is $r^2 N$, rather than flux itself, that is constant. The molar rate crossing a sphere is $4\pi C$. Oxygen flux is negative because the positive coordinate points outward. Surface stoichiometry and stagnant nitrogen give

$$\begin{aligned} N_{CO_2,r} &= -0.8 N_{O_2,r} \\ N_{CO,r} &= -0.4 N_{O_2,r} \\ N_{N_2,r} &= 0 \\ N_{\mathrm{tot},r} &= -0.2 N_{O_2,r} \end{aligned} \tag{3}$$

Three moles of gas leave for every 2.5 moles of oxygen consumed. Consequently the total molar flux points outward and opposes inward oxygen diffusion. Nitrogen has zero total flux, although its diffusion and mixture transport need not separately vanish.

The effective mixture flux law and Eq. 3 yield

$$\begin{aligned} N_{O_2,r} &= -cD\frac{dy}{dr} + yN_{\mathrm{tot},r} \\ N_{O_2,r} &= -\frac{cD}{1+0.2y}\frac{dy}{dr} \\ C &= -\frac{cDr^2}{1+0.2y}\frac{dy}{dr} \end{aligned} \tag{4}$$

Here $y = y_{O_2}$. The boundary conditions are $y(R) = 0$, from instantaneous reaction, and $y(\infty) = y_\infty = 0.21$, from ambient air. Separating Eq. 4 gives

$$
\begin{aligned}
C\int_R^\infty \frac{dr}{r^2} &= -cD\int_0^{y_\infty}\frac{dy}{1+0.2y}\\
\frac{C}{R} &= -5cD\ln(1+0.2y_\infty)\\
N_{O_2,r}(R) &= -\frac{5cD}{R}\ln(1.042)
\end{aligned}
\tag{5}
$$

The logarithm is dimensionless. Its coefficient $5\ln(1.042) = 0.20571$ replaces the pure-diffusion coefficient 0.21. The outward mixture motion lowers the inward flux magnitude by about 2.04 percent.

The remaining concentration profile follows by integrating only to radius r:

$$
\ln(1+0.2y(r)) = \ln(1.042)\left(1-\frac{R}{r}\right) \tag{6}
$$

It satisfies both endpoints, and differentiating it recovers Eq. 4. Carbon consumption rate, written $\dot{n}_C$ in mol s^{-1}, is positive:

$$
\dot{n}_C = \frac{3}{2.5}\,4\pi R^2|N_{O_2,r}(R)| = 24\pi cD\ln(1.042)R \tag{7}
$$

With carbon density ρ_C in kg m^{-3} and molar mass M_C in kg mol^{-1}, the shrinking solid balance is

$$
\begin{aligned}
\frac{\rho_C}{M_C}4\pi R^2\frac{dR}{dt} &= -\dot{n}_C\\
R\frac{dR}{dt} &= -\frac{6cDM_C}{\rho_C}\ln(1.042)\\
R^2(t) &= R_0^2 - Kt\\
K &= \frac{12cDM_C}{\rho_C}\ln(1.042)
\end{aligned}
\tag{8}
$$

The coefficient K has units m² s^{-1}. Burnout occurs at $t_b = R_0^2/K$. This is a radius-squared law, and doubling the initial radius quadruples the model burnout time. Its use ends if surface kinetics, gas reaction, changing composition or temperature invalidates the assumptions.

EXERCISE

Exercise 1. Worked coal burnout model

For the reaction and air composition above, find the particle radius and burnout time in terms of R_0, c, D, ρ_C and M_C. Quantify the flux correction relative to pure diffusion.

See solution for Exercise 1

QUIZ

1. Pseudo steady state

A coal particle shrinks while its surrounding gas concentration field adjusts rapidly. When is a pseudo steady gas model justified?

1. Whenever the particle radius is changing.
2. Only when the particle radius is exactly constant.
3. When gas diffusion adjusts much faster than the particle shrinks.
4. Whenever surface reaction is fast, regardless of gas diffusion time.

See solution for Quiz 1

5 Unsteady-state diffusion in a finite medium

5.1 Equation and boundary conditions

For a stationary medium, negligible bulk transport, no reaction and one-dimensional constant-property diffusion, species continuity becomes Fick's second law:

$$\frac{\partial c_A}{\partial t} = D_{AB}\frac{\partial^2 c_A}{\partial x^2} \tag{9}$$

Stationary solids and dilute solutes in stationary liquids can meet these assumptions. Equimolar counter-diffusion also removes total molar transport when the corresponding total-concentration model applies. Dilution alone does not remove imposed convection. These are reductions of continuity, not properties of every transient mixture.

The source begins with a wall of full thickness H, exposed at both faces to the same prescribed surface concentration c_{As}. Its initial concentration is uniformly c_{Ai}. The conditions are

$$c_A(x,0) = c_{Ai}$$

for $0 < x < H$ and

$$c_A(0,t) = c_A(H,t) = c_{As}$$

for $t > 0$. The initially discontinuous face value represents an ideal step. Define

$$\Theta = \frac{c_A - c_{As}}{c_{Ai} - c_{As}} \tag{10}$$

The symbol Θ denotes a dimensionless concentration departure. Lower-case θ is reserved for a dimensional temperature excess in the heat notes. The departure ratio in Eq. 10 goes from one initially to zero at equilibrium. Because the transformation is linear, Eq. 9 holds with Θ replacing c_A. Its conditions are $\Theta(x,0) = 1$, $\Theta(0,t) = 0$, and $\Theta(H,t) = 0$.

5.2 Series solution and symmetry

Separation of variables sets $\Theta = X(x)T(t)$. Division by $D_{AB}XT$ gives

$$\frac{X''}{X} = \frac{T'}{D_{AB}T} = -\mu^2.$$

Homogeneous face conditions select

$$X_n = \sin\left(\frac{n\pi x}{H}\right)$$

and temporal factors

$$\exp\left(-\frac{n^2\pi^2 D_{AB}t}{H^2}\right).$$

Expanding the initial value one in a sine series gives coefficient $4/(n\pi)$ for odd n and zero for even n. Thus

$$\begin{aligned} \Theta(x,t) &= \frac{4}{\pi}\sum_{n=1,3,5,\ldots}\frac{\sin\left(\frac{n\pi x}{H}\right)}{n}E_n \\ E_n &= \exp\left(-\frac{n^2\pi^2 D_{AB}t}{H^2}\right) \end{aligned} \tag{11}$$

Differentiating the series gives the molar flux

$$\begin{aligned} N_{A,x} &= \frac{4D_{AB}}{H}(c_{As}-c_{Ai})S \\ S &= \sum_{n=1,3,5,\ldots}\cos\left(\frac{n\pi x}{H}\right)E_n \end{aligned} \tag{12}$$

At $x = H/2$ every cosine is zero, so there is no flux through the symmetry plane. Higher modes decay faster than the first. The series represents the initial interior value in its limit at $t = 0$; at the stepped faces it follows the imposed condition.

DEFINITION

Mass Fourier number

The dimensionless time $\mathrm{Fo}_m = D_{AB}t/L^2$, elapsed time divided by the species-diffusion time L^2/D_{AB}. Use wall half-thickness or cylinder or sphere radius for the finite-body solutions here. It corresponds to the thermal Fourier number with D_{AB} replacing α.

The mass Fourier number indicates how far diffusion has progressed:

- For $\mathrm{Fo}_m \ll 1$, the diffusion distance $\sqrt{D_{AB}t}$ is small compared with L. A semi-infinite model can describe early changes near an exposed surface if distant boundaries have little influence.
- For $\mathrm{Fo}_m \sim 1$, diffusion has reached distances comparable to the body length. Finite geometry and the other boundaries matter.
- For $\mathrm{Fo}_m \gg 1$, diffusion has had time to redistribute species throughout the body. A small external transfer coefficient can still delay equilibration with the surroundings.

The boundary condition and any external resistance determine how far equilibration has progressed. The wall example below gives 0.25 using half-thickness and 0.0625 using full thickness. That factor of four changes whether the stated one-term approximation is justified.

For charts and the following formulas, use half-thickness $L = H/2$, centre coordinate

$$\xi = \frac{x - \frac{H}{2}}{L}$$

and Fourier number $\mathrm{Fo}_m = D_{AB}t/L^2$. Confusing full and half thickness changes the Fourier number by a factor of four. For a prescribed surface concentration the centre and spatial one-term solution is

$$\begin{aligned} \Theta_0 &\simeq \frac{4}{\pi} e^{-\frac{\pi^2 \mathrm{Fo}_m}{4}} \\ \frac{\Theta}{\Theta_0} &\simeq \cos\left(\frac{\pi\xi}{2}\right) \end{aligned} \tag{13}$$

Here subscript zero means the centre value, not initial time. The omitted second mode decays nine times as fast. A one-term approximation is useful for $\mathrm{Fo}_m \gtrsim 0.2$ using this half-thickness convention; it is an approximation, not an exact formula for all finite times.

QUIZ

2. The finite-wall length

A wall has full thickness $H = 4$ mm and equal exposure at both faces. For its half-thickness Fourier number, use $D = 10^{-9}\ \mathrm{m^2\,s^{-1}}$ and $t = 1000$ s. What is Fo_m?

1. 0.25.
2. 0.0625.
3. 0.50.
4. 4.0.

See solution for Quiz 2

5.3 Groups used in the finite-body examples

DEFINITION

Mass Biot number

The dimensionless resistance ratio $\mathrm{Bi}_m = k_c L/D_{AB}$, comparing internal species-diffusion resistance with external film resistance on the same concentration basis. Here k_c is expressed on the interior basis. It is the species counterpart of the thermal Biot number.

Although its algebra resembles Sherwood number, mass Biot uses the body's internal diffusivity and length, while Sherwood uses the fluid diffusivity and transfer length.

- For $\mathrm{Bi}_m \ll 1$, the external film offers most of the resistance. Internal diffusion keeps the concentration nearly uniform, so a lumped species balance may be appropriate.
- For $\mathrm{Bi}_m \sim 1$, internal diffusion and external film transfer both matter. Retain the spatial diffusion equation and the film boundary condition.

- For $\mathrm{Bi}_m \gg 1$, internal diffusion limits the response and large concentration gradients can develop. The surface is close to equilibrium with the external fluid, so a prescribed surface concentration can be a useful approximation.

For a lumped-model test, use $L_c = V/A_s$, with exposed area A_s, and check $k_c L_c / D_{AB} \leq 0.1$. The half-thickness or radius used by finite-body solutions gives a different numerical value for cylinders and spheres.

For $k_c = 10^{-5}\ \mathrm{m\,s^{-1}}$, $L = 10^{-3}\ \mathrm{m}$ and $D_{AB} = 10^{-9}\ \mathrm{m^2\,s^{-1}}$, $\mathrm{Bi}_m = 10$; a uniform interior is unjustified. Convert phase concentrations before comparing resistances, and retain half-thickness or radius for the stated solutions.

DEFINITION
Partition coefficient

An equilibrium ratio of concentrations in two phases, for example

$$K = \frac{c^*_{A,\mathrm{inside}}}{c^*_{A,\mathrm{outside}}}.$$

It is dimensionless only when numerator and denominator use the same concentration units and basis. Its direction must be specified before converting a film coefficient.

With this convention, an outside-basis film coefficient becomes $k_{c,\mathrm{inside}} = k_{c,\mathrm{outside}}/K$. Reversing the definition of K reverses the conversion. A mole-fraction equilibrium slope cannot be substituted for a concentration ratio without the corresponding conversion.

For finite-body solutions define a geometry length L_g: wall half-thickness L for a two-sided wall, or radius R_b for a long cylinder or sphere. Reserve $L_c = V/A_s$ for the lumped-model test. The two lengths are related by

Geometry	L_g for the finite-body solution	$L_c = V/A_s$ for the lumped test
Two-sided wall of thickness $2L$	L	L
Long cylinder, with end transfer neglected	R_b	$R_b/2$
Sphere	R_b	$R_b/3$

Use the geometry length consistently in both groups:

$$\mathrm{Fo}_m = \frac{D_{AB} t}{L_g^2}$$

$$\mathrm{Bi}_m = \frac{k_c L_g}{D_{AB}} \tag{14}$$

Here Bi_m is based on L_g, not V/A_s. A sphere with $k_c R_b/D_{AB} = 0.30$ has a lumped-test value of 0.10. Do not use 0.10 in a sphere eigenvalue equation that expects the radius-based value 0.30. Here k_c is on the interior concentration basis. Convert an external-phase concentration using the partition relation before imposing its boundary condition. Prescribed surface concentration corresponds to infinite Bi. Use the matching heat-equation solution with α replaced by D_{AB} and temperature departure replaced by concentration departure.

QUIZ

3. Internal versus external resistance

Using the same concentration basis inside and outside a body, $\mathrm{Bi}_m = k_c L/D_{AB} \gg 1$. Which interpretation is correct?

1. The interior concentration must be uniform.
2. Internal diffusion is instantaneous.
3. The external film supplies most of the resistance.
4. Diffusion inside the body offers much more resistance than the outside film.

See solution for Quiz 3

5.4 Application of Heisler charts

The following eigenvalue formulas supply the centre ratio, position correction and volume average needed for the classroom example (Çengel and Ghajar 2015).

For a plane wall measured from its centre, the convective boundary gives $\lambda \tan \lambda = \mathrm{Bi}_m$. The lowest positive eigenvalue λ_1 and its amplitude are

$$\begin{aligned} A_1 &= \frac{4 \sin \lambda_1}{2\lambda_1 + \sin(2\lambda_1)} \\ \Theta_0 &\simeq A_1 e^{-\lambda_1^2 \mathrm{Fo}_m} \\ \frac{\Theta}{\Theta_0} &\simeq \cos(\lambda_1 \xi) \\ \bar{\Theta} &\simeq \Theta_0 \frac{\sin \lambda_1}{\lambda_1} \end{aligned} \tag{15}$$

The overbar means volume average. $F = 1 - \bar{\Theta}$ is the fraction of the eventual total exchange completed, for either uptake or release. The original total-transfer charts use

$$\mathrm{Bi}_m^2 \mathrm{Fo}_m = \frac{k_c^2 t}{D_{AB}}.$$

At infinite Bi this coordinate diverges, so the finite one-term average is easier to use directly.

For an infinitely long cylinder of radius R_b, radial diffusion has Bessel functions J_0 and J_1. These are mathematical functions, not the diffusive flux symbol J_A. With $\zeta = r/R_b$, the eigenvalue condition and solution are

$$
\begin{aligned}
\lambda_1 J_1(\lambda_1) &= \mathrm{Bi}_m J_0(\lambda_1) \\
A_1 &= \frac{2J_1(\lambda_1)}{\lambda_1[J_0^2(\lambda_1)+J_1^2(\lambda_1)]} \\
\Theta_0 &\simeq A_1 e^{-\lambda_1^2 \mathrm{Fo}_m} \\
\frac{\Theta}{\Theta_0} &\simeq J_0(\lambda_1 \zeta) \\
\bar{\Theta} &\simeq \Theta_0 \frac{2J_1(\lambda_1)}{\lambda_1}
\end{aligned}
\tag{16}
$$

For infinite Bi, $\lambda_1 = 2.40483$ and $A_1 = 1.60197$. A short cylinder also diffuses axially. Under separable initial and boundary conditions its solution is the product of a radial cylinder solution and an axial plane-wall solution. Whether end effects can be ignored depends on time and position as well as aspect ratio. The source's length rule is a practical estimate, not a universal exact threshold.

For a sphere of radius R_b, define $\zeta = r/R_b$. The eigenvalue condition is $1 - \lambda_1 \cot \lambda_1 = \mathrm{Bi}_m$, and

$$
\begin{aligned}
A_1 &= \frac{4(\sin\lambda_1 - \lambda_1 \cos\lambda_1)}{2\lambda_1 - \sin(2\lambda_1)} \\
\Theta_0 &\simeq A_1 e^{-\lambda_1^2 \mathrm{Fo}_m} \\
\frac{\Theta}{\Theta_0} &\simeq \frac{\sin(\lambda_1 \zeta)}{\lambda_1 \zeta} \\
\bar{\Theta} &\simeq 3\Theta_0 \frac{\sin\lambda_1 - \lambda_1 \cos\lambda_1}{\lambda_1^3}
\end{aligned}
\tag{17}
$$

At the centre the position ratio has limiting value one. At infinite Bi, $\lambda_1 = \pi$, $A_1 = 2$, and

$$
\Theta_0 \simeq 2e^{-\pi^2 \mathrm{Fo}_m}, \qquad F \simeq 1 - \frac{3\Theta_0}{\pi^2} \tag{18}
$$

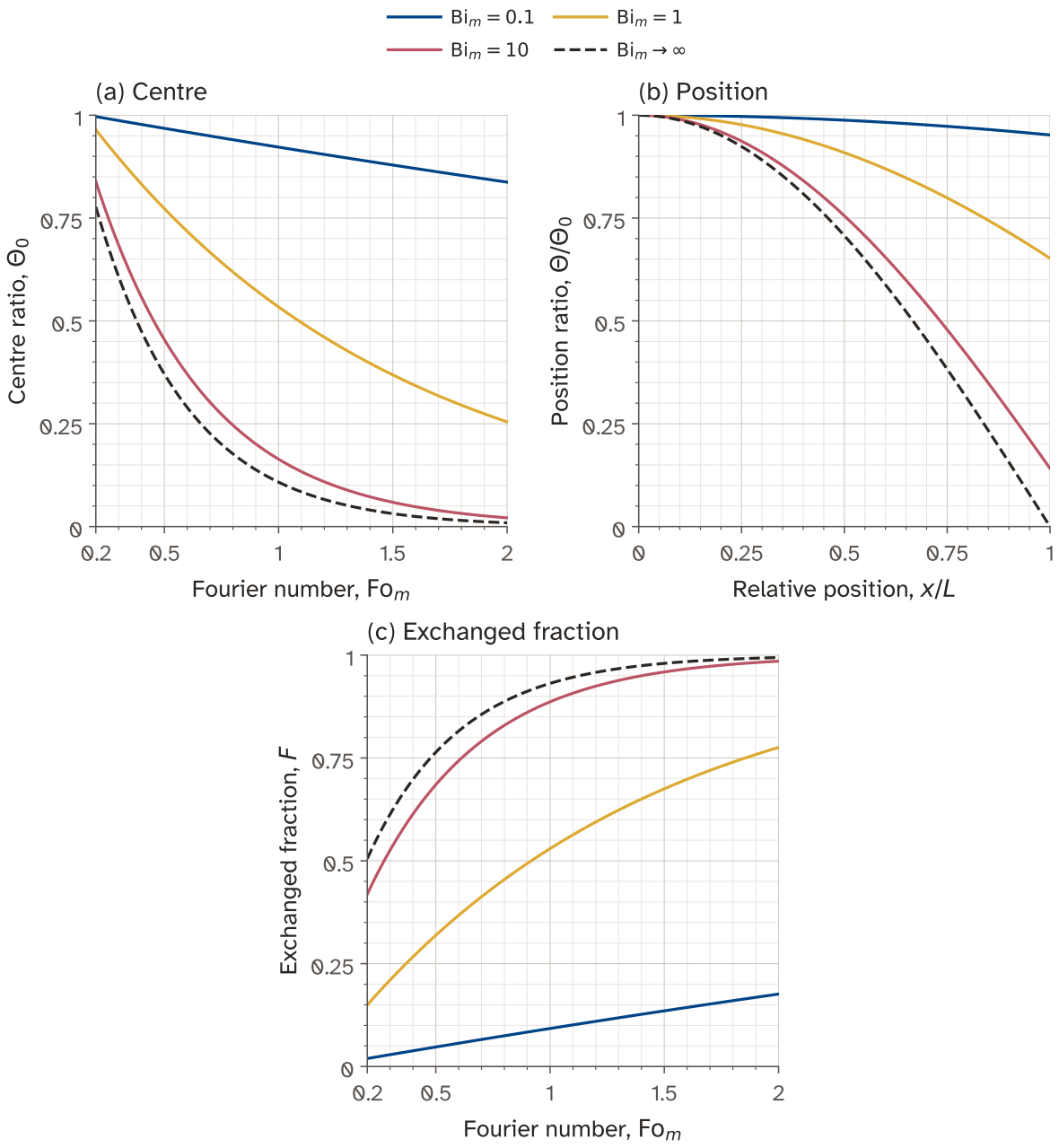


Figure 2: One-term plane-wall diffusion solutions for the centre, position ratio and exchanged fraction.

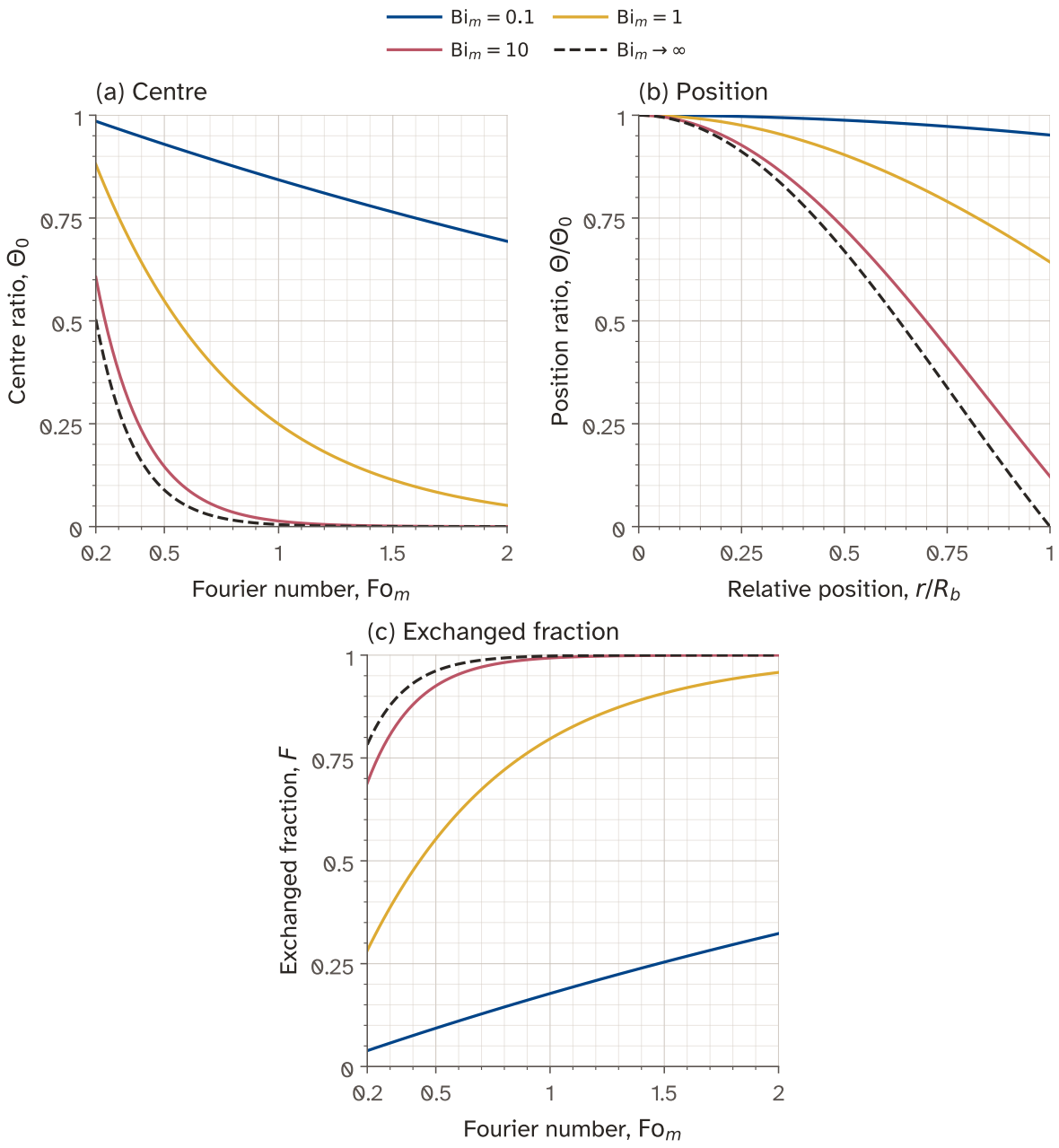


Figure 3: One-term long-cylinder diffusion solutions for the centre, position ratio and exchanged fraction.

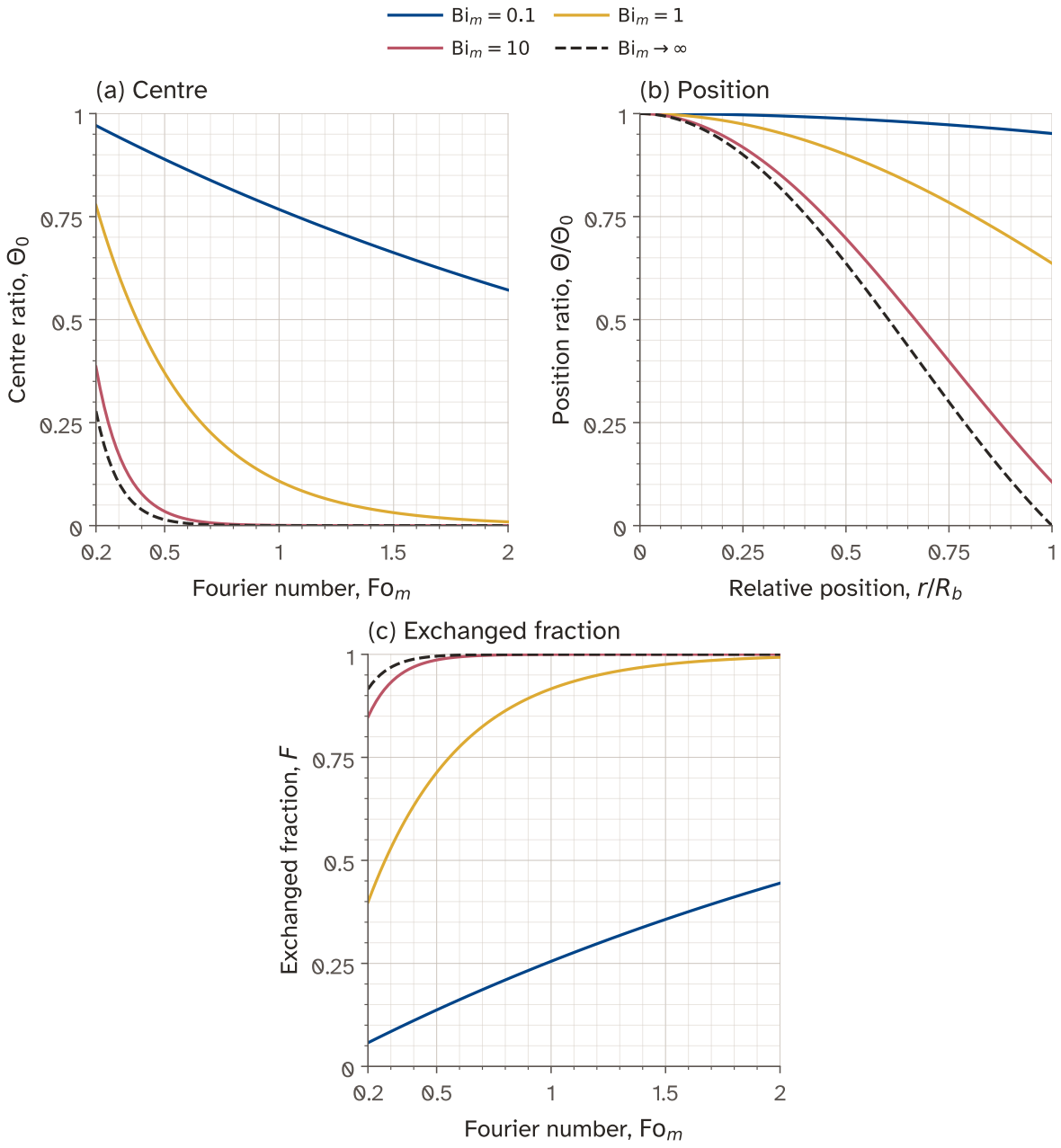


Figure 4: One-term spherical diffusion solutions for the centre, position ratio and exchanged fraction.

EXERCISE
Exercise 2. Drug capsule

A spherical drug capsule (0.652 cm diameter) has an initial concentration of 68.9 mg/cm ^{3} Dramamine.

- What is the residual concentration of Dramamine at the centre of the spherical bead after 48 hours?

The capsule is intended to release the drug in the gastrointestinal system. Its nontoxic gelatinous material allows the drug to diffuse out gradually. The drug within the bead is the source of A; the surrounding fluid is the sink.

Data: D_{AB} (Dramamine in the gel matrix of the capsule) = $3 \times 10^{-7}\ \mathrm{cm}^2/\mathrm{s}$ at body temperature of $37\ ^\circ\mathrm{C}$.

See solution for Exercise 2

QUIZ
4. Released fraction versus centre concentration
A finite sphere releases solute to a sink. Which quantity determines the fraction of the eventual total release completed?

1. One minus the centre concentration ratio.
2. One minus the concentration departure ratio averaged over the whole sphere.
3. The surface concentration alone.
4. The concentration at any arbitrarily chosen radius.

See solution for Quiz 4

6 Unsteady-state diffusion in a semi-infinite medium

6.1 Conditions and similarity reduction

A stationary body occupies $x > 0$ and starts uniformly at c_{Ai}. At $t = 0$ its surface is set to c_{As} and held there. With no reaction, no convection and constant diffusivity, Eq. 9 applies with

$$c_A(x, 0) = c_{Ai},$$
$$c_A(0, t) = c_{As},$$
$$c_A(\infty, t) = c_{Ai}.$$

A finite body approximates this model while the disturbance is shallow relative to its depth. An engineering depth estimate is $4\sqrt{D_{AB}t}$, corresponding to less than 0.5 percent of the surface concentration change remaining. The condition $4\sqrt{D_{AB}t} < L_c$ is $\mathrm{Fo}_m < 1/16$, consistent with the earlier rough 0.05 threshold.

There is no imposed length in the infinite-depth problem. Diffusion supplies $\sqrt{D_{AB}t}$, so set

$$\eta = \frac{x}{2\sqrt{D_{AB}t}}, \qquad c_A(x,t) = f(\eta) \tag{20}$$

The factor two is a convention for the standard error function. The chain rule gives

$$\begin{aligned} \partial_t c_A &= -\frac{\eta}{2t} f' \\ \partial_x^2 c_A &= \frac{1}{4D_{AB}t} f'' \\ f'' + 2\eta f' &= 0 \end{aligned} \tag{21}$$

Set $g = f'$. Then $g'/g = -2\eta$ gives $g = Be^{-\eta^2}$, and a second integration gives

$$f = A + B\int_0^\eta e^{-u^2}\, du.$$

Surface and far-field conditions determine $A = c_{As}$ and

$$B = \frac{2(c_{Ai} - c_{As})}{\sqrt{\pi}}.$$

Initial and far-field conditions both become the same $\eta \to \infty$ limit. Thus three original conditions become two conditions for this second-order ODE.

$$\begin{aligned} \operatorname{erf}(\eta) &= \frac{2}{\sqrt{\pi}}\int_0^\eta e^{-u^2}\, du \\ \frac{c_A - c_{Ai}}{c_{As} - c_{Ai}} &= \operatorname{erfc}(\eta) = 1 - \operatorname{erf}(\eta) \end{aligned} \tag{22}$$

At $\eta = 0$ the ratio is one and the surface concentration is correct; at infinity the ratio is zero and the initial concentration is recovered. Differentiating and integrating the resulting surface flux give

$$\begin{aligned} N_{A,x}(0,t) &= (c_{As} - c_{Ai})\sqrt{\frac{D_{AB}}{\pi t}} \\ q_A(t) &= 2(c_{As} - c_{Ai})\sqrt{\frac{D_{AB}t}{\pi}} \end{aligned} \tag{23}$$

Here q_A is net uptake per unit area in mol m^{-2}, positive when $c_{As} > c_{Ai}$. The ideal flux diverges as $t \to 0^+$ because of the instantaneous step; its time integral stays finite. Finite external transfer smooths this singularity. Uptake scaling with $\sqrt{t}$ is consistent with diffusion control under these conditions, but does not by itself prove this model uniquely.

6.2 Examples: estimating penetration depth

At $x = 4\sqrt{D_{AB}t}$, the similarity argument is two and $\operatorname{erfc}(2) = 0.004678$. Only 0.468 percent of the surface concentration change remains there. Use a table or numerical error function when converting a concentration ratio to depth.

Oxygen diffusing into still water with $D = 2 \times 10^{-9}$ m² s⁻¹ for an hour has the estimated depth 10.73 mm. Carbon entering steel with $D = 10^{-11}$ m² s⁻¹ for eight hours has depth 2.147 mm. These source examples show how one equation applies to liquid absorption, case hardening and semiconductor doping.

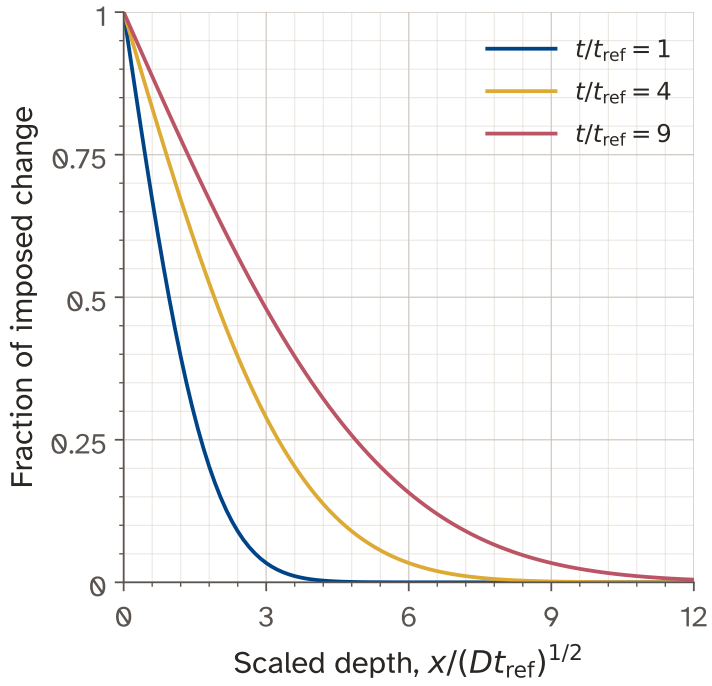


Figure 6: Concentration profiles in a semi-infinite medium after a step in surface concentration.

QUIZ

5. Semi-infinite diffusion scaling

In the fixed-surface-concentration semi-infinite model, how long does it take for the same fractional concentration change to reach twice the depth, with diffusivity unchanged?

1. Half as long.
2. Twice as long.
3. Four times as long.
4. The same time.

See solution for Quiz 5

7 Case study 2: chemical vapour deposition

7.1 Physical setup and assumptions

Phosphorus oxychloride supplies phosphorus-containing oxide at the hot silicon surface. A balanced reduction step between that oxide and silicon is

$$2\mathrm{P_2O_5} + 5\mathrm{Si} \rightarrow 5\mathrm{SiO_2} + 4\mathrm{P} \tag{24}$$

The University of Illinois predeposition description gives this oxide-reduction step and the resulting constant-source diffusion model. This equation describes the reduction step, rather than the full chemistry of the deposition furnace.

The phosphorus-rich coating supplies phosphorus, which then diffuses into the silicon. The present calculation models diffusion only. Assume isothermal silicon, a coating large enough to maintain constant surface concentration, no reaction in the solid, a stationary lattice and constant diffusivity. The wafer is much thicker than the penetration depth, so it is semi-infinite on this time scale. A finite source would instead deplete and produce a different boundary condition and profile.

At $1100\,^{\circ}\mathrm{C}$ the supplied surface atomic concentration is $C_{ns} = 2.5 \times 10^{20}$ atoms cm^{-3}, the initial concentration is $C_{ni} = 0$, and $D = 6.5 \times 10^{-13}$ cm^2 s^{-1}. We write C_n for atomic concentration to distinguish it from c_A in molar units. The linear diffusion equation and dimensionless ratios are unchanged by this unit choice. The source's silicon atomic density 5×10^{22} atoms cm^{-3} makes the surface atomic fraction 0.005. A dilute fixed-lattice approximation is reasonable here; dilution is not a general justification for neglecting flow in other media.

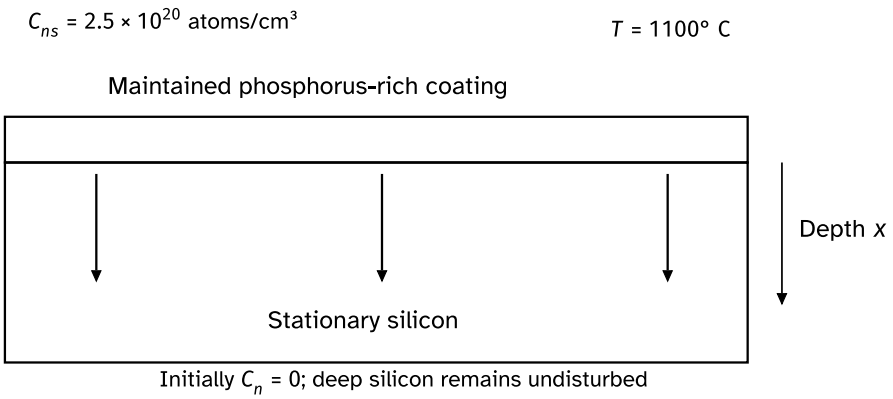


Figure 7: Phosphorus diffuses from a maintained coating into stationary silicon.

7.2 Mathematical statement and depth calculation

The initial condition is $C_n(x, 0) = 0$. The two boundary conditions are $C_n(0, t) = C_{ns}$ and $C_n(\infty, t) = 0$. The solution of Eq. 9 on this number-density basis is

$$C_n(x, t) = C_{ns}\ \mathrm{erfc}\left(\frac{x}{2\sqrt{Dt}}\right) \tag{25}$$

EXERCISE

Exercise 3. Case study 2: phosphorus in silicon

Chemical vapour deposition takes place at $1100\,^{\circ}\mathrm{C}$, where phosphorus diffuses into silicon. The surface concentration is maintained at $C_{AS} = 2.5 \times 10^{20}$ phosphorus atoms per cm^3 of solid silicon. For comparison, pure silicon contains about 5×10^{22} silicon atoms per cm^3, so the phosphorus concentration is dilute.

Treat the phosphorus-rich coating as an effectively infinite source relative to the amount transferred. Predict the depth at which the phosphorus concentration reaches one percent of the surface value after one hour, 2.5×10^{18} phosphorus atoms per cm^3. Also predict the concentration profile after one hour.

See solution for Exercise 3

7.3 Calculated concentration profile

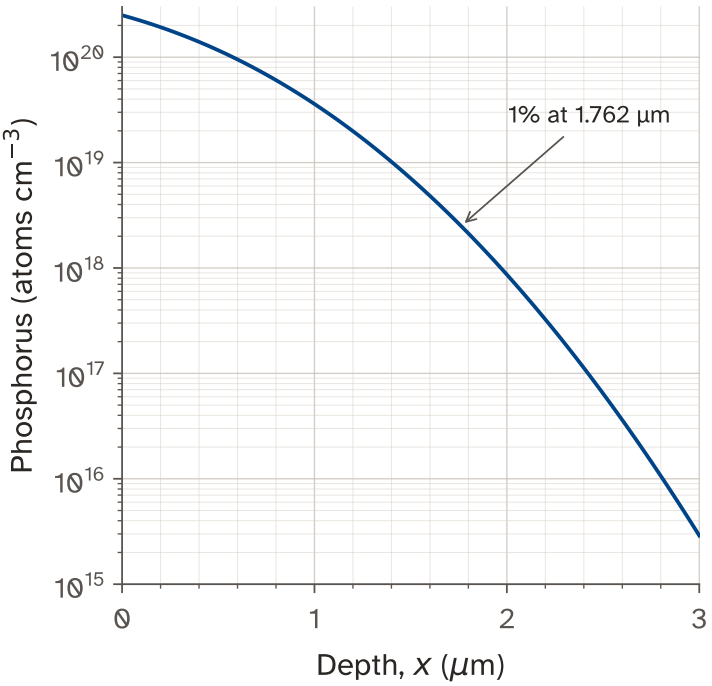


Figure 8: Calculated one-hour phosphorus concentration profile, with the one-percent depth marked.

The plotted one-hour solution uses Eq. 25. Its depth scales with $\sqrt{Dt}$, so doubling a specified concentration depth requires four times the duration at unchanged diffusivity. An electrical junction depth also needs the wafer's background dopant concentration.

QUIZ

6. Transferring a heat-equation solution

You want to reuse a transient heat-conduction solution for solute uptake. What must match as well as the geometry and differential equation?

1. The initial conditions and the conditions at every boundary, including how concentrations on opposite sides of an interface are related.
2. Only the numerical value of thermal conductivity.
3. Only the external fluid velocity.
4. Nothing, because every diffusion problem has the same solution.

See solution for Quiz 6

8 Additional examples

EXERCISE

Exercise 4. Concentration, instantaneous flux and total uptake

A stationary polymer initially contains a uniform solute concentration of 0.20 mol m⁻³. At $t = 0$ one face is held at 2.0 mol m⁻³ by a maintained reservoir. Use constant diffusivity $D_{AB} = 1.0 \times 10^{-10}$ m² s⁻¹, negligible external resistance and no reaction. The polymer is 0.020 m thick and transport is normal to the exposed face; neglect edges.

After one hour, find the concentration 0.60 mm below the surface, the instantaneous surface flux and the cumulative uptake per unit exposed area. Check the semi-infinite approximation, and describe the effect of increasing the duration to four hours.

See solution for Exercise 4

EXERCISE

Exercise 5. Use Henry's law to set a transient diffusion boundary

A 0.10 m deep layer of still water at 298 K initially contains dissolved molecular oxygen uniformly at 10 g m⁻³. At $t = 0$ a regulated pure-oxygen headspace maintains an oxygen partial pressure of 2.0 atm above the water. Use Henry's law in the form $p_A = Hc_{As}$ with $H = 0.80$ atm m³ mol⁻¹, and $D_{AB} = 2.1 \times 10^{-9}$ m² s⁻¹. The molar mass of molecular oxygen is 32.0 g mol⁻¹.

How long does the concentration 5.0 mm below the interface take to reach 20 g m⁻³? Assume negligible gas-side resistance, rapid interfacial equilibration, constant properties, no reaction and no liquid motion. Check whether a semi-infinite approximation is consistent with the result. For the calculation,

$$\operatorname{erf}(1.03608) = 0.857143.$$

See solution for Exercise 5

9 What you should now be able to calculate

Choose finite-body or semi-infinite diffusion, distinguish centre from average concentration, and find concentration profiles, uptake or a target time.

Practice: Workshop 10 for hydrogen uptake and drug release.

10 Report an error

Email Ranjeet Utikar with the title Transient mass diffusion, the URL `/mass-transport/transient-diffusion/`, and the equation or passage to check.

References

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Shah, Milinkumar. n.d. "CHEN3001-TP: Mass Transport 3." Curtin University. Unpublished.

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Solutions

Quiz solutions

Quiz 1. Pseudo steady state

Correct choice: 3.

The gas diffusion time is of order

$$t_{\text{gas}} \sim \frac{R^2}{D}$$

It must be much shorter than the time over which the particle radius changes appreciably. Then the gas field can be treated as steady at each slowly changing radius. A fast surface reaction alone does not establish this separation of times.

Back to Quiz 1

Quiz 2. The finite-wall length

Correct choice: 1.

For equal exposure on both faces, use the half-thickness:

$$L = \frac{H}{2} = 0.002\ \text{m}$$

Thus,

$$\text{Fo}_m = \frac{Dt}{L^2} = \frac{10^{-9}(1000)}{(0.002)^2} = 0.25$$

Using the full thickness would give a Fourier number four times smaller.

Back to Quiz 2

Quiz 3. Internal versus external resistance

Correct choice: 4.

On the same concentration basis, the ratio of internal to external resistance is of order

$$\frac{\frac{L}{D_{AB}}}{\frac{1}{k_c}} = \frac{k_c L}{D_{AB}} = \text{Bi}_m$$

A large mass Biot number means that internal diffusion offers much more resistance than the external film. Concentration can vary substantially inside the body; a uniform interior is not justified.

Back to Quiz 3

Quiz 4. Released fraction versus centre concentration

Correct choice: 2.

Find how much solute remains by averaging concentration over the whole sphere. With the normalized departure used here,

$$F = 1 - \bar{\Theta}$$

The centre concentration describes only one position. It cannot be used in place of the volume average when calculating the amount released.

Back to Quiz 4

Quiz 5. Semi-infinite diffusion scaling

Correct choice: 3.

The same fractional concentration change occurs at the same similarity variable:

$$\eta = \frac{x}{2\sqrt{D_{AB}t}}$$

With diffusivity unchanged,

$$\frac{t_2}{t_1} = \left(\frac{x_2}{x_1}\right)^2 = 2^2 = 4$$

It takes four times as long to reach twice the depth. Check that the far boundary is still unaffected.

Back to Quiz 5

Quiz 6. Transferring a heat-equation solution

Correct choice: 1.

Replacing temperature by concentration and thermal diffusivity by species diffusivity transfers a solution only when the initial and boundary conditions also correspond. A prescribed surface concentration and a finite transfer coefficient are different problems. Across phases, concentration may jump according to equilibrium.

Back to Quiz 6

Exercise solutions

Exercise 1. Worked coal burnout model

Calculation and answer

Data

Quantity	Value
Initial particle radius	R_0
Gas total molar concentration	c
Effective oxygen diffusivity	D
Carbon density	ρ_C
Carbon molar mass	M_C
Ambient oxygen mole fraction	$y_{O_2,\infty} = 0.21$
Reaction stoichiometry	2.5 mol oxygen consumed per 3 mol carbon

Assumptions

- Spherical particle with uniform solid density.
- Pseudo steady diffusion in the surrounding gas.
- Instantaneous surface reaction and no gas-phase reaction.
- Constant temperature, total concentration and effective diffusivity.

Calculations

The steady gas calculation supplies the oxygen flux at each current radius. Writing Eq. 5 for the inward magnitude gives

$$|N_{O_2,r}(R)| = \frac{5cD}{R}\ln(1+0.2y_\infty)$$

Substituting the ambient mole fraction gives

$$|N_{O_2,r}(R)| = \frac{5cD}{R}\ln(1.042) = 0.20571\frac{cD}{R}$$

Multiply the oxygen rate by the stoichiometric carbon-to-oxygen ratio:

$$\dot{n}_C = \frac{3}{2.5}4\pi R^2|N_{O_2,r}(R)| = 24\pi cD\ln(1.042)R$$

The carbon inventory is

$$n_C = \left(\frac{\rho_C}{M_C}\right)\frac{4\pi R^3}{3}.$$

Its decrease equals the positive consumption rate:

$$\frac{\rho_C}{M_C} 4\pi R^2 \frac{dR}{dt} = -24\pi c D \ln(1.042) R$$

Cancel a factor of radius and integrate from R_0 at zero time to R at time t:

$$\int_{R_0}^{R} R\, dR = -\frac{6 c D M_C}{\rho_C} \ln(1.042) \int_0^t dt$$

Thus $R^2 = R_0^2 - Kt$, with

$$K = \frac{12 c D M_C \ln(1.042)}{\rho_C}.$$

The dimensions of K are $\mathrm{m^2\,s^{-1}}$, as required for a radius-squared decay law.

Without outward mixture flow, the oxygen flux magnitude would be $0.21 cD/R$. The relative reduction is

$$1 - \frac{0.20571}{0.21} = 0.02043$$

The outward product flow therefore reduces the oxygen supply by 2.04 percent. Doubling R_0 quadruples burnout time within this model.

Answer

The radius and burnout time are

$$R(t) = \sqrt{R_0^2 - Kt}, \qquad K = 0.49370 \frac{c D M_C}{\rho_C}$$

$$t_b = \frac{\rho_C R_0^2}{0.49370 c D M_C}$$

The radius expression applies for $0 \le t \le t_b$. The oxygen flux is 2.04 percent smaller than the pure-diffusion estimate. No numerical burnout time is determined without the carbon density and operating gas properties.

Back to Exercise 1

Exercise 2. Drug capsule

Calculation and answer

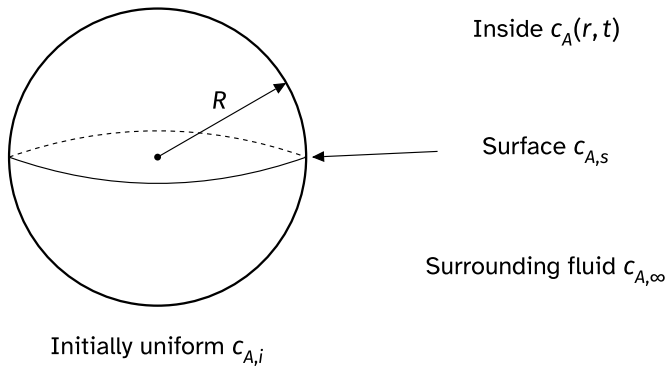


Figure 5: Drug initially fills the spherical bead uniformly. It diffuses radially to a sink at the surface. Total release requires the concentration averaged over the whole bead.

The spherical diffusion model is the one shown in Figure 4. The maintained sink fixes the surface concentration, while the centre concentration is the requested unknown.

Data

Quantity	Value
Bead diameter	$d = 0.652\ \mathrm{cm}$
Bead radius	$R_b = 0.326\ \mathrm{cm}$
Initial drug concentration	$C_{mi} = 68.9\ \mathrm{mg\,cm^{-3}}$
Drug diffusivity	$D = 3 \times 10^{-7}\ \mathrm{cm^2\,s^{-1}}$
Duration	$t = 48\ \mathrm{h} = 172800\ \mathrm{s}$
Body temperature	$T = 37\ ^\circ\mathrm{C}$

Assumptions

- Spherical, stationary gel with constant radius.
- Uniform initial drug concentration.
- Well-stirred sink maintains zero surface concentration.
- No drug reaction within the gel.
- Constant diffusivity.

Calculations

The sink removes drug from the bead surface while internal diffusion supplies it from the centre. A prescribed surface concentration corresponds to infinite mass Biot number. First calculate the Fourier number using the radius:

$$\mathrm{Fo}_m = \frac{Dt}{R_b^2} = \frac{3 \times 10^{-7}(172800)}{0.326^2} = 0.48779$$

The Fourier number exceeds 0.2, so the first spherical eigenmode is sufficient. For zero surface concentration the centre ratio is

$$\Theta_0 = \frac{C_{mc}}{C_{mi}} \simeq 2e^{-\pi^2 \mathrm{Fo}_m}$$

Substitution gives

$$\Theta_0 \simeq 2e^{-\pi^2(0.48779)} = 0.016226$$

Multiply this ratio by the initial concentration to recover the centre concentration:

$$C_{mc} = C_{mi}\Theta_0 = 68.9(0.016226) = 1.1180 \ \mathrm{mg\,cm^{-3}} \tag{19}$$

As an additional check on total release, the spherical volume-average ratio is $\bar{\Theta} \simeq 3\Theta_0/\pi^2$. Hence

$$F = 1 - \bar{\Theta} \simeq 1 - \frac{3(0.016226)}{\pi^2} = 0.99507$$

The centre retains 1.62 percent of its initial concentration while only 0.493 percent of the initial drug remains in the entire bead. The centre has the largest residual concentration, so these two results have the expected order. Finite external resistance or swelling-dependent diffusivity requires a different model.

Answer

After 48 hours, the concentration at the centre is approximately

$$C_{mc} = 1.12 \ \mathrm{mg\,cm^{-3}}$$

The corresponding additional estimate is 99.5 percent of the drug released.

Back to Exercise 2

Exercise 3. Case study 2: phosphorus in silicon

Calculation and answer

The coating and diffusion direction are shown in Figure 7. The calculated profile in Figure 8 can be used to check the recovered one-percent depth.

Data

- Surface phosphorus concentration $C_{ns} = 2.5 \times 10^{20} \ \mathrm{atoms\,cm^{-3}}$
- Initial phosphorus concentration $C_{ni} = 0$
- Diffusivity at 1100 degrees Celsius $D = 6.5 \times 10^{-13} \ \mathrm{cm^2\,s^{-1}}$
- Duration $t = 3600 \ \mathrm{s}$
- Target concentration

$$0.01C_{ns} = 2.5 \times 10^{18}\ \text{atoms}\,\text{cm}^{-3}$$

Assumptions

- One-dimensional diffusion into stationary silicon.
- Uniform temperature and constant diffusivity.
- No reaction in the silicon.
- An effectively infinite coating maintains the surface concentration.
- The wafer is sufficiently thick for the semi-infinite approximation.

Calculations

Phosphorus enters from the maintained coating and diffuses into the initially phosphorus-free silicon. The semi-infinite diffusion solution on an atomic-concentration basis is

$$C_n(x,t) = C_{ns}\ \text{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)$$

At the target concentration,

$$\text{erfc}(\eta) = \frac{2.5 \times 10^{18}}{2.5 \times 10^{20}} = 0.01$$

Therefore $\text{erf}(\eta) = 0.99$, and the inverse error function gives $\eta = 1.821386$. The source table reading of 1.82 gives the same depth to three significant figures.

The one-hour diffusion length is

$$2\sqrt{Dt} = 2\sqrt{6.5 \times 10^{-13}(3600)} = 9.67471 \times 10^{-5}\ \text{cm}$$

The requested depth follows from the definition of η:

$$\begin{aligned} x &= 2\eta\sqrt{Dt} = 1.821386(9.67471 \times 10^{-5}) \\ &= 1.76214 \times 10^{-4}\ \text{cm} = 1.76214\ \mu\text{m} \end{aligned} \tag{26}$$

Substituting the same diffusion length into the concentration solution gives the complete profile:

$$C_n(x) = 2.5 \times 10^{20}\ \text{erfc}\left(\frac{x}{0.967471\ \mu\text{m}}\right)\ \text{atoms}\,\text{cm}^{-3} \tag{27}$$

At $x = 0.967471\ \mu\text{m}$, the profile gives $3.93248 \times 10^{19}\ \text{atoms}\,\text{cm}^{-3}$. At $x = 2\ \mu\text{m}$ it gives $8.6523 \times 10^{17}\ \text{atoms}\,\text{cm}^{-3}$. Substitution of the calculated target depth recovers one percent of the surface concentration.

For an illustrative $300\ \mu\text{m}$ wafer, the disturbance-depth estimate is $4\sqrt{Dt} = 1.93494\ \mu\text{m}$ and the thickness-based Fourier number is 2.6×10^{-6}. The far boundary is therefore well beyond the diffusion region. The one-percent criterion defines a concentration depth; an electrical junction depth also requires the wafer's background dopant concentration.

Answer

After one hour the one-percent concentration depth is $1.76\ \mu\text{m}$. The one-hour phosphorus concentration profile is given by Eq. 27.

Back to Exercise 3

Exercise 4. Concentration, instantaneous flux and total uptake

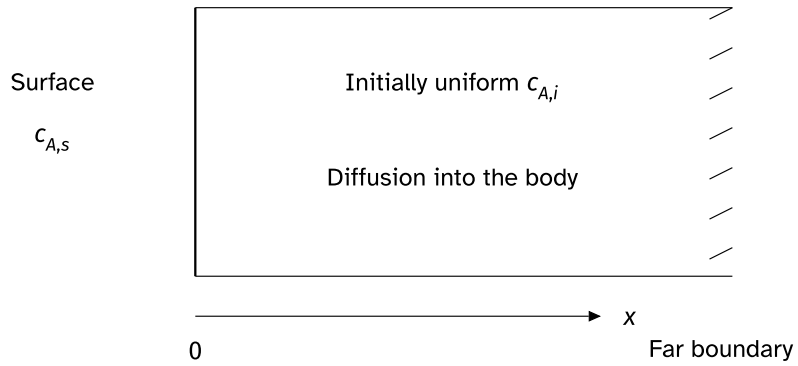


Figure 9: Solute enters an initially uniform body from a maintained surface concentration. Position is measured inward from the exposed face.

Data

Quantity	Value
Initial concentration	$c_{Ai} = 0.20\ \mathrm{mol\,m^{-3}}$
Surface concentration	$c_{As} = 2.0\ \mathrm{mol\,m^{-3}}$
Diffusivity	$D_{AB} = 10^{-10}\ \mathrm{m^2\,s^{-1}}$
Evaluation depth	$x = 0.000600\ \mathrm{m}$
Evaluation time	$t = 3600\ \mathrm{s}$
Body thickness	$H = 0.020\ \mathrm{m}$

Assumptions

- One-dimensional diffusion into a stationary polymer.
- Uniform initial concentration and maintained surface concentration.
- Negligible external resistance and edge effects.
- No reaction and constant diffusivity.

Calculations

At 3600 s, $\sqrt{D_{AB}t} = 0.000600$ m. The estimated disturbance depth is $4\sqrt{D_{AB}t} = 0.00240$ m, well short of the 0.020 m far boundary. The semi-infinite solution is appropriate on this scale.

At $x = 0.000600$ m,

$$\eta = \frac{x}{2\sqrt{D_{AB}t}} = 0.5.$$

The concentration relation is

$$c_A = c_{Ai} + (c_{As} - c_{Ai})\operatorname{erfc}(\eta)$$

Since $\operatorname{erfc}(0.5) = 0.479500$, substitution gives

$$c_A = 0.20 + (2.0 - 0.20)(0.479500) = 1.063\ \mathrm{mol\,m^{-3}}$$

The instantaneous surface flux follows from the surface gradient:

$$N_A(0,t) = (c_{As} - c_{Ai})\sqrt{\frac{D_{AB}}{\pi t}}$$

Substituting the concentration difference and elapsed time into Eq. 23 gives

$$N_A(0,t) = (2.0 - 0.20)\sqrt{\frac{10^{-10}}{\pi(3600)}} = 1.693 \times 10^{-7}\ \mathrm{mol\,m^{-2}\,s^{-1}}$$

The cumulative uptake is the time integral of surface flux:

$$q_A(t) = 2(c_{As} - c_{Ai})\sqrt{\frac{D_{AB}t}{\pi}}$$

Substituting the same data gives

$$q_A(t) = 2(2.0 - 0.20)\sqrt{\frac{10^{-10}(3600)}{\pi}} = 1.219 \times 10^{-3}\ \mathrm{mol\,m^{-2}}$$

Multiplying the final flux by the duration would give half this uptake. The surface flux was greater earlier and falls as $t^{-1/2}$.

After four hours, the disturbance depth and cumulative uptake both double, while instantaneous surface flux halves. The disturbance depth is then 0.00480 m, still below the far boundary. At a fixed depth the concentration also changes; only points at equal $x/\sqrt{t}$ have the same concentration ratio. These results require the maintained surface concentration and constant diffusivity specified in the problem.

Answer

After one hour, $c_A = 1.06\ \mathrm{mol\,m^{-3}}$ at 0.60 mm, $N_A(0,t) = 1.69 \times 10^{-7}\ \mathrm{mol\,m^{-2}\,s^{-1}}$ and $q_A = 1.22 \times 10^{-3}\ \mathrm{mol\,m^{-2}}$. At four hours the uptake and disturbance depth double and the surface flux halves.

Back to Exercise 4

Exercise 5. Use Henry’s law to set a transient diffusion boundary

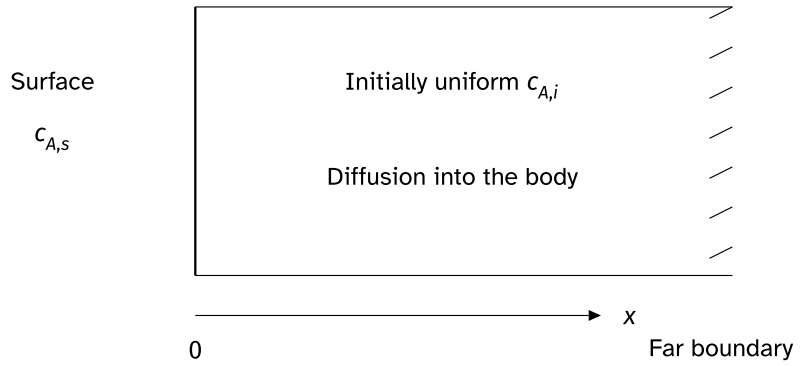


Figure 10: Oxygen enters water through the top surface. Henry's law sets the dissolved surface concentration; the target is at a specified depth below that surface.

Data

Quantity	Value
Water depth	$L = 0.10\ \mathrm{m}$
Oxygen diffusivity	$D_{AB} = 2.1 \times 10^{-9}\ \mathrm{m^2\,s^{-1}}$
Oxygen partial pressure	$p_A = 2.0\ \mathrm{atm}$
Henry’s constant	$H = 0.80\ \mathrm{atm\,m^3\,mol^{-1}}$
Initial mass concentration	$10\ \mathrm{g\,m^{-3}}$
Target mass concentration	$20\ \mathrm{g\,m^{-3}}$
Evaluation depth	$x = 0.0050\ \mathrm{m}$
Oxygen molar mass	$M_A = 32.0\ \mathrm{g\,mol^{-1}}$

Assumptions

- One-dimensional diffusion in stationary water.
- Uniform initial concentration.
- Maintained gas partial pressure and rapid interfacial equilibrium.
- Negligible gas-side resistance.
- Constant properties and no reaction.

Calculations

The initial concentration and the interfacial equilibrium concentration are different. Henry’s law fixes the latter on a molar basis:

$$c_{As} = \frac{p_A}{H} = \frac{2.0}{0.80} = 2.50\ \mathrm{mol\,m^{-3}} = 80.0\ \mathrm{g\,m^{-3}}$$

The regulated headspace makes this a maintained surface boundary, as required by Eq. 22. The surface value would change if gas were depleted from an unregulated finite headspace.

Using mass concentration C_m, which is proportional to molar concentration, the semi-infinite solution is

$$\frac{C_m - C_{mi}}{C_{ms} - C_{mi}} = \operatorname{erfc}\left(\frac{x}{2\sqrt{D_{AB}t}}\right)$$

At the target, this ratio is

$$\frac{20 - 10}{80 - 10} = \frac{1}{7}.$$

Thus $\operatorname{erf}(\eta) = 6/7$ and $\eta = 1.03608$. Solving for time,

$$\begin{aligned} t &= \frac{x^2}{4D_{AB}\eta^2} \\ &= \frac{(0.0050)^2}{4(2.1 \times 10^{-9})(1.03608)^2} \\ &= 2773\ \mathrm{s} = 46.2\ \mathrm{min} \end{aligned}$$

The disturbance-depth estimate is $4\sqrt{D_{AB}t} = 0.00965$ m, much less than the 0.10 m water depth. The far boundary is therefore unimportant on this time scale within the stated diffusion-only model.

At twice the target depth, reaching the same concentration requires four times the duration, about 3.08 hours. Using 16 g mol^{-1} would describe atomic oxygen and impose the wrong surface concentration for this problem. Natural convection, mixing or biological consumption would require revisiting the stated model rather than changing only the diffusion time.

Answer

The target concentration is reached after approximately 2.77×10^3 s $= 46.2$ min. The disturbance depth is about 9.65 mm, so the semi-infinite approximation is consistent with the 100 mm water depth.

Back to Exercise 5