1. (a) In the α-phase region the boundary conditions are:

$$c_\alpha(-\infty, t) = c_{\alpha\infty} \quad ; \quad \text{and} \quad c_\alpha(h_1, t) = c_{\alpha\beta}$$

Applying these boundary conditions we find:

$$\begin{aligned} c_{\alpha\infty} &= A_\alpha - B_\alpha \\ c_{\alpha\beta} &= A_\alpha + B_\alpha \text{erf}\left(\frac{h_1}{\sqrt{4D_\alpha t}}\right) \end{aligned}$$

Solving for B_α we find:

$$B_\alpha = \frac{-\left(c_{\alpha\infty} - c_{\alpha\beta}\right)}{1 + \text{erf}\left(h_1/\sqrt{4D_\alpha t}\right)}$$

In the β-phase region the boundary conditions are:

$$c_\beta(h_1, t) = c_{\beta\alpha} \quad ; \quad \text{and} \quad c_\beta(h_2, t) = c_{\beta\epsilon}$$

Applying these we find:

$$\begin{aligned} c_{\beta\alpha} &= A_\beta + B_\beta \text{erf}\left(\frac{h_1}{\sqrt{4D_\beta t}}\right) \\ c_{\beta\epsilon} &= A_\beta + B_\beta \text{erf}\left(\frac{h_2}{\sqrt{4D_\beta t}}\right) \end{aligned}$$

Solving these we find:

$$B_\beta = \frac{c_{\beta\alpha} - c_{\beta\epsilon}}{\text{erf}\left(h_1/\sqrt{4D_\beta t}\right) - \text{erf}\left(h_2/\sqrt{4D_\beta t}\right)}$$

And finally in the ϵ-phase region the boundary conditions are:

$$c_\epsilon(h_2, t) = c_{\epsilon\beta} \quad ; \quad \text{and} \quad c_\epsilon(\infty, t) = c_{\epsilon\infty}$$

Which yield:

$$\begin{aligned} c_{\epsilon\beta} &= A_\epsilon + B_\epsilon \text{erf}\left(\frac{h_2}{\sqrt{4D_\epsilon t}}\right) \\ c_{\epsilon\infty} &= A_\epsilon + B_\epsilon \end{aligned}$$

Solving for B_ϵ we find:

$$B_\epsilon = \frac{c_{\epsilon\beta} - c_{\epsilon\infty}}{\text{erf}\left(h_2/\sqrt{4D_\epsilon t}\right) - 1}$$

(b) The mass conservation equations at the interfaces are:

$$\frac{dh_1}{dt} = \frac{J_{\alpha\beta} - J_{\beta\alpha}}{c_{\alpha\beta} - c_{\beta\alpha}} \; ; \quad \text{and} \quad \frac{dh_2}{dt} = \frac{J_{\beta\epsilon} - J_{\epsilon\beta}}{c_{\beta\epsilon} - c_{\epsilon\beta}}$$

where the fluxes are given by Fick's first law.

(c) To find the width of the interface region as a function of time, we would use the composition profiles with the appropriate coefficients and Fick's first law to find the fluxes to insert into the right hand side of the mass conservation equations. We would then use the given expressions to find dh_1/dt and dh_2/dt to insert into the left hand side of the equation. This would give us two equations with two unknowns γ_1 and γ_2, which could be solved numerically. Given these constants, we could find the width of the β-phase region given by:

$$w = h_2 - h_1$$

(d) If $D_\alpha = D_\epsilon = 0$ there will be no diffusion in the α-phase or ϵ-phase regions, so the fluxes $J_{\alpha\beta}$ and $J_{\epsilon\beta}$ will be zero. In this case the mass conservation equations become:

$$\frac{dh_1}{dt} = \frac{-J_{\beta\alpha}}{c_{\alpha\infty} - c_{\beta\alpha}} \; ; \quad \text{and} \quad \frac{dh_2}{dt} = \frac{J_{\beta\epsilon}}{c_{\beta\epsilon} - c_{\epsilon\infty}}$$

With a linear composition profile in the β-phase region, the fluxes are given by:

$$J_{\beta\alpha} = J_{\beta\epsilon} = D_\beta \frac{c_{\beta\alpha} - c_{\beta\epsilon}}{h_2 - h_1} = D_\beta \frac{c_{\beta\alpha} - c_{\beta\epsilon}}{w}$$

So we find:

$$\begin{aligned} \frac{dw}{dt} = \frac{dh_2}{dt} - \frac{dh_1}{dt} &= \frac{J_{\beta\epsilon}}{c_{\beta\epsilon} - c_{\epsilon\infty}} + \frac{J_{\beta\alpha}}{c_{\alpha\infty} - c_{\beta\alpha}} \\ &= D_\beta \frac{c_{\beta\alpha} - c_{\beta\epsilon}}{w} \left(\frac{1}{c_{\beta\epsilon} - c_{\epsilon\infty}} + \frac{1}{c_{\alpha\infty} - c_{\beta\alpha}} \right) \end{aligned}$$

This can be integrated to find:

$$w = \sqrt{2 D_\beta t \left(c_{\beta\alpha} - c_{\beta\epsilon} \right) \left(\frac{1}{c_{\beta\epsilon} - c_{\epsilon\infty}} + \frac{1}{c_{\alpha\infty} - c_{\beta\alpha}} \right)}$$

2. (a) The initial and boundary conditions for the solution in the slab $0 \le z \le d$ are

$$c(z,0) = c_0 \ , \quad c(0,t) = 0 \ \text{ and } \quad c(d,t) = 0$$

This is almost exactly the same as that for the square wave problem worked in the text. If we denote that solution as $c^{sq}(z,t)$ we can see that in square wave case the initial and boundary conditions for the solution in the region $0 \le z \le L$ were

$$c^{sq}(z,0) = c_0 \ , \quad c^{sq}(0,t) = \frac{c_0}{2} \ \text{ and } \quad c^{sq}(L,t) = \frac{c_0}{2}$$

Hence if we let $L \to d$ we see that a solution

$$c(z,t) = 2\left[c^{sq}(z,t) - \frac{c_0}{2}\right]$$

will solve the differential equation and match the initial and boundary conditions. Hence our solution is

$$c(z,t) = \frac{4c_0}{\pi}\sum_{j=0}^{\infty}\left(\frac{1}{2j+1}\right)\sin\frac{(2j+1)\pi z}{d}\exp\left\{-\left[\frac{(2j+1)\pi}{d}\right]^2 Dt\right\}$$

(b) The average composition in the slab is found by

$$\begin{aligned}\langle c(t)\rangle &= \frac{1}{d}\int_0^d c(z,t)\ dz \\ &= \frac{8c_0}{\pi^2}\sum_{j=0}^{\infty}\left(\frac{1}{2j+1}\right)^2\exp\left\{-\left[\frac{(2j+1)\pi}{d}\right]^2 Dt\right\}\end{aligned}$$

Interestingly, since $\langle c(0)\rangle = c_0$, we can find the sum

$$\sum_{j=0}^{\infty}\left(\frac{1}{2j+1}\right)^2 = \frac{\pi^2}{8}$$

(c) The ratio of the magnitudes of the $(j+1)^{\text{th}}$ term to the jth term is

$$R_{j,j+1} = \left(\frac{2j+1}{2j+3}\right)^2\exp\left[\frac{-(j+1)8\pi^2 Dt}{d^2}\right]$$

This is nearly the same as that for the concentration at a point found in the text; the difference is just an additional factor of $(2j+1)/(2j+3)$, which is important only for small j. The ratio of the first two terms is then

$$R_{0,1} = \frac{1}{9} \exp\left(\frac{-8\pi^2 Dt}{d^2}\right)$$

This ratio is 1/100 at a time $t_{0.01}$ found by

$$\frac{1}{100} = \frac{1}{9} \exp\left(\frac{-8\pi^2 Dt_{0.01}}{d^2}\right)$$

Solving yields

$$\begin{aligned} t_{0.01} &= \frac{d^2}{8\pi^2 D} \ln\left(\frac{100}{9}\right) \\ &= \frac{0.03\ d^2}{D} \end{aligned}$$

The average concentration at this time is

$$\begin{aligned} \langle c(t_{0.01})\rangle &= \frac{8c_0}{\pi^2} \sum_{j=0}^{\infty} \left(\frac{1}{2j+1}\right)^2 \exp\left\{-\left[\frac{(2j+1)\pi}{d}\right]^2 Dt_{0.01}\right\} \\ &= \frac{8c_0}{\pi^2} \sum_{j=0}^{\infty} \left(\frac{1}{2j+1}\right)^2 \exp\left[-\frac{(2j+1)^2}{8} \ln\frac{100}{9}\right] \\ &= \frac{8c_0}{\pi^2} (0.74 + 0.0074 + ...) \\ &\approx 0.6\ c_0 \end{aligned}$$

(d) Considering only the first term, the average composition is given by

$$\langle c(t)\rangle \approx \frac{8c_0}{\pi^2} \exp\left[-\left(\frac{\pi}{d}\right)^2 Dt\right]$$

This has an exponential decay with characteristic time

$$\tau = \frac{d^2}{\pi^2 D}$$

3. (a) The approach for this problem is the same as the cylindrical example worked in Section 1.2.4 in this chapter. We rate of radioactive material escaping (in atoms per time) is given by

$$\dot{m} = 2\pi h D(c_i - c_o)\frac{1}{\ln(r_o/r_i)}$$

(b) Poor Matt's approach to this problem is to solve the steady-state problem in one-dimensional, flat-plate geometry. In this case, the diffusion equation becomes

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial z^2} = 0$$

Hence $\partial c/\partial z$ = constant, which means that the concentration profile is linear. The rate of material escaping is then

$$\dot{m} = 2\pi h D(c_i - c_0)\frac{r_o}{r_o - r_1}$$

This is always greater than the correct answer of part a). The difference is

$$\text{error} = 2\pi h D(c_i - c_o)\left[\frac{r_o}{r_o - r_i} - \frac{1}{\ln(r_o/r_i)}\right]$$

This varies between $\pi h D(c_i - c_o)$ and $2\pi h D(c_i - c_o)$ as the pipe wall thickness goes from 0 to r_o.

Interestingly if Matt had taken the area of the pipe to be $2\pi h r_i$ his estimate would have been

$$\dot{m} = 2\pi h D(c_i - c_0)\frac{r_i}{r_o - r_1}$$

which is always *less* than the actual value by an amount which varies from $\pi h D(c_i - c_o)$ to 0 as the pipe wall thickness goes from 0 to r_o.

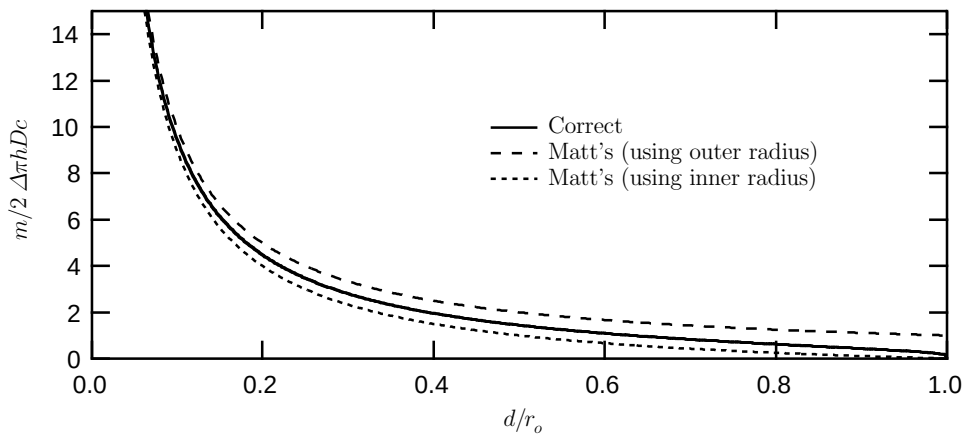

Figure 1.4: Rate of material escaping from a pipe of length h as a function of wall thickness d relative to outer diameter.

(c) The plots are shown in Figure 1.4. The error for the plate assumption using the outer diameter of the pipe for the area is smallest for thin pipes.

4. (a) The concentration of the isotopic tracer is given by the thin film solution

$$c(z,t) = \frac{m}{\sqrt{4\pi Dt}} \exp\left(\frac{-z^2}{4Dt}\right)$$

(b) Taking the definition used in the notes for the width as the distance between inflection points we find

$$w = 2\sqrt{2Dt}$$

(c) The temperature dependence in the above expression for width will be in the diffusivity, which takes the form

$$D = D_0 \; e^{-Q/RT}$$

Solving our expression for the width for D we find

$$D = \frac{1}{2t_A}\left(\frac{w}{2}\right)^2$$

Inserting the temperature-dependence of D we find and solving for T

$$T = \frac{Q}{R\ln\left(8D_0 t_A/w^2\right)}$$

(d) The diffusivity has the form

$$D = D_0 \; e^{-Q/RT}$$

From the Table 1 in the paper by Brown and Ashby we find that for Ge, the parameters D_0 and Q are given by

$$D_0 = 4.4 \times 10^{-3} \text{ m}^2/\text{sec.} \quad \text{and} \quad \frac{Q}{RT_m} = 32.25$$

where T_m is the melting point of Ge, which is $T_m = 1211$ K. Hence the diffusivity is given by

$$D(\text{m}^2/\text{sec.}) = 4.4 \times 10^{-3} \; \exp\left(-32.25\frac{T_m}{T}\right)$$

The diffusion coefficient for isotopic Ge is the tracer diffusion coefficient.

(e) Using numbers from above we find

$$\begin{aligned} T &= \frac{Q}{RT_m}\frac{T_m}{\ln\left(8D_0t_A/w^2\right)} \\ &= 32.25\frac{1211\text{ K}}{\ln\left[8\cdot 4.4\times 10^{-3}/(0.1\times 10^{-6})^2\right]} \\ &= 1053\text{ K} \end{aligned}$$

The diffusivity at this temperature is found to be

$$D = 3.5\times 10^{-19}\text{ m}^2/\text{s}$$