Problem 1

Known:

Diffusivity of a chemical into a fossil and the concentration at a particular depth.

Find:

Time needed for diffusion and the total amount diffused.

Schematic and Given Data:

\[ D = 10^{-20} \, m^2/s \]
\[ c(x = 70 \times 10^{-6} \, m) = 0.01c_s \]

Strategy:

This is a transient problem and the two solution possibilities are the semi-infinite (error function) and finite geometries (slab/cylinder/sphere). The total thickness \( L \) is not provided and, instead, it is mentioned that "trace element enters only a small distance from the surface? This leaves us with no choice other than to think of a semi-infinite region and error function solution.

Assumptions:

Error function for time in part a). We are measuring far enough from the core.

Solution:

a.

\[ \frac{c - c_i}{c_s - c_i} = 1 - \text{erf} \left( \frac{x}{2\sqrt{Dt}} \right) \]
\[ \frac{0.01c_s}{c_s} = 0.01 = 1 - \text{erf} \left( \frac{70 \times 10^{-6}}{2\sqrt{10^{-20} \, t}} \right) \]
\[ 0.99 = \text{erf} \left( \frac{350,000}{\sqrt{t}} \right) \]
\[ 1.825 = \frac{350,000}{\sqrt{t}} \]
\[ t = 1166 \, \text{years} \]

b.
If there were consumption of the trace element, concentration everywhere would be lower than without reaction. Thus, the 0.01\(c_s\) value would have been higher for our model and would have lead to a longer time. Therefore, our calculation would underestimate the real age if there were reactions involved (but we are using a model without reaction).

c.

Flux is given by

\[
\frac{g}{m^2 s} = \sqrt{\frac{D}{\pi t}} (c_s - c_i)
\]

Total amount picked up (g/m\(^2\))

\[
\int n_s dt \left[ \frac{g}{m^2} \right] = \int_0^t \sqrt{\frac{D}{\pi t}} (c_s - c_i) dt
\]

\[
= \sqrt{\frac{D}{\pi}} (c_s - c_i) \frac{1}{\sqrt{t}}
\]

\[
= \sqrt{\frac{D}{\pi}} (c_s - c_i) \frac{t^{1/2}}{1/2}
\]

\[
= 2 \sqrt{\frac{D}{\pi}} (c_s - c_i) t^{1/2}
\]

Substituting values

\[
= 2 \sqrt{\frac{10^{-20}}{\pi}} (c_s - 0) \sqrt{t}
\]

\[
= 1.128 \times 10^{-10} c_s \sqrt{t}
\]

d.

\[
\frac{n_{2D}}{n_D} = \frac{2 \sqrt{\frac{2D}{\pi}} (c_s - c_i) t^{1/2}}{2 \sqrt{\frac{D}{\pi}} (c_s - c_i) t^{1/2}} = \sqrt{2}
\]
Problem 2

Known:

Properties of the construct along with boundary conditions.

Find:

Governing equation and solution (for concentration). The maximum cell density corresponding to the location of lowest glucose concentration.

Schematic and given data:

\[ c_s = 5.56 \times 10^{-6} \text{ mol/ml} \]
\[ c_{\text{min}} = 0.2 \times 10^{-6} \text{ mol/ml} \]
\[ D = 7.78 \times 10^{-10} \text{ m}^2/\text{s} \]
\[ R = -3.61 \times 10^{-11} \text{ mol/10}^6 \text{ cell} \cdot \text{s} \]

Strategy:

The problem involves diffusion with a zeroth order reaction. We have not done this in lecture so we do not already have a solution. We have to start from governing equation, drop the appropriate terms and obtain a solution for concentration as a function of position for the boundary conditions provided. We only have diffusion and reaction term in this steady state problem. Once we obtain the concentration profile (the solution), we know where the minimum concentration is and thus we can compute minimum cell density at this location.

Assumptions:

None

Solution:

a.

\[ 0 = D \frac{\partial^2 c}{\partial x^2} + RN \]

b.

\[ c(x = L) = c_s \]
\[ \frac{\partial c}{\partial x} (x = 0) = 0 \]

c.
\[ \frac{\partial c}{\partial x} = -\frac{RN}{D} x + k_1 \]
\[ \frac{\partial c}{\partial x} \bigg|_{x=0} = 0 = -\frac{RN}{D} 0 + k_1 \Rightarrow k_1 = 0 \]
\[ c = -\frac{RN}{2D} x^2 + k_2 \]
\[ c_s = -\frac{RN}{2D} L^2 + k_2 \]
\[ k_2 = c_s + \frac{RN}{2D} L^2 \]
\[ c = -\frac{RN}{2D} x^2 + \left( c_s + \frac{RNL^2}{2D} \right) = \frac{RN}{2D} (L^2 - x^2) + c_s \]

d.
The minimum concentration is at \( x = 0 \)
e.
\[ 0.2 \times 10^{-6} \left[ \frac{mol}{ml} \right] = \frac{-3.61 \times 10^{-6} \left[ \frac{mol}{cell \cdot s} \right] N \left[ cell \right]_{ml} - 2 \times 7.78 \times 10^{-10} \left[ \frac{m^2}{s} \right] \left( 0.002^2 - 0^2 \right) + 5.56 \times 10^{-6} \left[ \frac{mol}{ml} \right]}{2 \times 7.78 \times 10^{-10} \left[ \frac{m^2}{s} \right]} \]
\[ N = 5.78 \times 10^{-4} \left[ \frac{cell}{ml} \right] \]
f.
Change \( c_s \)
\[ 0.2 \times 10^{-6} \left[ \frac{mol}{ml} \right] = \frac{-3.61 \times 10^{-6} \left[ \frac{mol}{cell \cdot s} \right] \left( 2 \times 5.78 \times 10^{-4} \right) \left[ cell \right]_{ml} - 2 \times 7.78 \times 10^{-10} \left[ \frac{m^2}{s} \right] \left( 0.002^2 - 0^2 \right) + c_s \left[ \frac{mol}{ml} \right]}{2 \times 7.78 \times 10^{-10} \left[ \frac{m^2}{s} \right]} \]
\[ c_s = 1.09 \times 10^{-5} \left[ \frac{cell}{ml} \right] \]
Problem 3

Known:
Average velocity of stream, dispersion coefficient, first order decay

Find:
Distances downstream and upstream that have a particular concentration.

Schematic and Given Data:

\[ t_{\frac{1}{2}} = 8 \text{ days} = 691200 \text{s} \]

\[ m_{\text{water}} = 7000 \frac{\text{kg}}{\text{hr}} = 1.94 \frac{\text{kg}}{\text{s}} \]

Concentration in the dumped water = 300000 \( \frac{Bq}{cm^3} \)

\[ E = 10 \frac{m^2}{s} \]

\[ \rho_{\text{water}} = 1000 \frac{\text{kg}}{m^3} \]

\[ u = 3 \frac{km}{hr} = 0.833 \frac{m}{s} \]

\[ V = 280 \frac{m^3}{s} \]

\[ \rho_{w} = 1000 \frac{\text{kg}}{m^3} \]

Strategy:
This is a convection-dispersion problem in a stream and will directly use the solution that we have in the text. Calculate the rate constant from the given half life, for the first order reaction, to be used in the formula. The flux calculations (shown in the text) include both dispersive and convective flux.

Assumptions:
None

Solution:
The solutions follow from text. The only difficulty for this question is being consistent with units and first finding k". 
In the following equation, \( c \) is the concentration of radioactive water \( \text{Bq/cm}^3 \)

\[
c_i(z) = \begin{cases} 
\frac{\dot{m}_i}{A \nu} \exp \left[ \frac{u}{2E} \left( 1 + \psi \right) z \right] & \text{z} < 0 \\
\frac{\dot{m}_i}{A \nu} \exp \left[ \frac{u}{2E} \left( 1 - \psi \right) z \right] & \text{z} > 0 
\end{cases}
\]

\[
\psi = \sqrt{1 + \frac{4Ek''}{u^2}}
\]

In order to find \( k'' \), we use the fact about half life

\[
c = 0.5c_0 = c_0 \exp \left( -k'' t_{1/2} \right)
\]

\[
k'' = -\ln(0.5) \frac{t_{1/2}}{1.003 \times 10^{-6} \text{s}}
\]

Next we find \( \psi \) where all units are in meters and seconds. Note that it is important to keep several decimal places.

\[
\psi = \sqrt{1 + \frac{4Ek''}{u^2}} = \sqrt{1 + \frac{4(10)(1.003 \times 10^{-6})}{0.83^2}} = 1.00003
\]

\[
c_i(z) = \begin{cases} 
\frac{\dot{m}_i}{V \nu} \exp \left[ \frac{0.83}{2(10)} \left( 1 + 1.00003 \right) z \right] & \text{z} < 0 \\
\frac{\dot{m}_i}{V \nu} \exp \left[ \frac{0.83}{2(10)} \left( 1 - 1.00003 \right) z \right] & \text{z} > 0
\end{cases}
\]

\[
c_i(z) = \begin{cases} 
\frac{\dot{m}_i}{280 \times 1.00003} \exp \left[ \frac{0.83}{2(10)} \left( 1 + 1.00003 \right) z \right] & \text{z} < 0 \\
\frac{\dot{m}_i}{280 \times 1.00003} \exp \left[ \frac{0.83}{2(10)} \left( 1 - 1.00003 \right) z \right] & \text{z} > 0
\end{cases}
\]

\[
c_i(z) = \begin{cases} 
0.00357 \dot{m}_i \exp(0.083z) & \text{z} < 0 \\
0.00357 \dot{m}_i \exp(-1.21 \times 10^{-6}z) & \text{z} > 0
\end{cases}
\]

\( \dot{m}_i \) is the mass flow rate of iodine into the stream. We will leave the units in \( \frac{\text{Bq} \cdot \text{m}^3}{\text{cm}^3 \cdot \text{s}} \) in order to reduce conversions.

\[
\dot{m}_i = 1.94 \text{ kg/s} \times \frac{1000 \text{ kg}}{\text{m}^3} \times 300000 \frac{\text{Bq}}{\text{cm}^3} = 582 \frac{\text{Bq} \cdot \text{m}^3}{\text{cm}^3 \cdot \text{s}}
\]
For downstream ($z > 0$), iodine travels 3,265 km.

For upstream ($z < 0$), iodine travels 0.048 km.

c. 

\[
c(z = 0) \frac{Bq}{cm^3} = 0.00357 \left( \frac{s}{m^3} \right) 582 \left( \frac{Bq \cdot m^3}{cm^3 \cdot s} \right) = 2.08 \frac{Bq}{cm^3}
\]

d. Dispersion/eddies/turbulence (not convection)

e.
\[ c_I(z) = \frac{\dot{m}_I}{Au\psi} \exp \left[ \frac{u}{2E} (1-\psi) z \right] \quad z > 0 \]

\[ \psi = \sqrt{1 + \frac{4Ek^n}{u^2}} \]

\[ n_z(0) = -E \frac{\partial c}{\partial z} + c(0)u \]

\[ E = 10^2 \text{m}^2/\text{s} \times \frac{100^2 \text{cm}^2}{1 \text{m}^2} = 10^4 \text{cm}^2/\text{s} \]

\[ u = 83.3 \text{cm/s} \]

\[ \frac{\partial c}{\partial z}_{z=0,z>0} = \left( \frac{\dot{m}_I}{Au\psi} \right) \times \left( \frac{u}{2E} (1-\psi) \right) \exp \left[ \frac{u}{2E} (1-\psi) 0 \right] \]

\[ = \left( \frac{\dot{m}_I}{Au\psi} \right) \times \left( \frac{u}{2E} (1-\psi) \right) \]

\[ = c(0) \left[ \frac{Bq}{\text{cm}^3} \right] \times -1.21 \times 10^{-6} \left[ \frac{1}{m} \right] \times \frac{1m}{100cm} \] (using earlier calculation)

\[ = 2.08 \left[ \frac{Bq}{\text{cm}^3} \right] \times -1.21 \times 10^{-8} \frac{1}{cm} \]

\[ = -2.51 \times 10^{-8} \frac{Bq}{\text{cm}^4} \]

\[ n_{I,\text{Dep}}(0^+) = -10^5 \text{cm}^2/\text{s} \times -2.51 \times 10^{-8} \frac{Bq}{\text{cm}^3} = 2.51 \times 10^{-3} \frac{Bq}{\text{cm}^2 \cdot s} \]

\[ n_{I,\text{Conv}}(0^+) = 83.3 \text{cm/m/s} \times 2.08 \left[ \frac{Bq}{\text{cm}^3} \right] = 173.3 \frac{Bq}{\text{cm}^2 \cdot s} \]

f.

It will be a lot less since this is a 1D transport model versus 2D/3D. Plus, there is fish/plants to eat some of the radiation changing the concentration.
Problem 4

Known:

Toluene properties in air and the grape. Dimensions of grape. Air properties including speed.

Find:

Convective mass transfer coefficient, time to reach a particular concentration at the core, surface concentration and the surface flux assuming error function solution.

Schematic and given data:

\[ R = 0.0125 \text{m} \]
\[ K^* = 3.39 \times 10^{-3} \]
\[ D_{\text{tol-grape}} = 1.15 \times 10^{-7} \text{ m}^2/\text{s} \]
\[ D_{\text{tol-air}} = 8.11 \times 10^{-6} \text{ m}^2/\text{s} \]
\[ u = 0.254 \text{ m/s} \]
\[ c_{\infty} = 2.18 \times 10^{-3} \text{ g/ m}^3 \]
\[ \rho = 1.24 \text{ kg/ m}^3 \]
\[ \mu = 1.98 \times 10^{-5} \text{ kg/ m} \cdot \text{s} \]

Strategy:

Calculation of \( h_m \) is straightforward using formulas in the text, in this case, for flow over a sphere. We then calculate Biot number to see if a lumped parameter solution is valid. If not, then we use Heisler chart to obtain time for the given concentration. It is important to note that the surface concentration in the grape is not the same as surface concentration in the air, but related by \( K^* \)

Assumptions:

Short time and long distance for part d), therefore using the flux from the error function.

Solution:

a.
Re = \frac{(2 \times 0.0125[m])\left(1.24 \left[\frac{kg}{m^3}\right]\right)\left(0.254\left[\frac{m}{s}\right]\right)}{1.98 \times 10^{-5}\left[\frac{kg}{m \cdot s}\right]} = 397.68

Sc = \frac{1.98 \times 10^{-5}\left[\frac{kg}{m \cdot s}\right]}{\left(1.24\left[\frac{kg}{m^3}\right]\right)\left(8.11 \times 10^{-6}\left[\frac{m^2}{s}\right]\right)} = 1.97

Sh = \frac{h_m(2R)}{D_{Tol-Air}} = 2 + Sc^{0.4} \left(0.4 \text{Re}_{D}^{\frac{1}{2}} + 0.06 \text{Re}_{D}^{\frac{2}{3}}\right) = 16.7

h_m = 5.42 \times 10^{-3}\left[\frac{m}{s}\right]

b. This is an unsteady state mass transfer problem. We will first check the Biot number.

Bi = \frac{h \cdot K \cdot (R)}{D_{Tol-grape}} = \frac{(5.42 \times 10^{-3}\left[m/s\right])\left(3.39 \times 10^{-3}\right)(0.0125[m])}{1.15 \times 10^{-7}\left[m^2/s\right]} = 2 > 0.1

Biot number being greater than 0.1, we cannot use a lumped parameter solution. We will then use the Heisler chart to calculate \( t \) for the given concentration at the center by finding \( Fo \).

\[ m = \frac{1}{Bi} = 0.5 \]

\[ n = 0 \]

\[ \frac{0.8c_{\infty} - c_{\infty}}{0 - c_{\infty}} = -0.2c_{\infty} = 0.2 \]

From figure B.3 on page 329, we get:

\[ Fo = \frac{D_{Tol-grape} t}{R^2} = 0.5 \]

\[ t = \frac{(0.0125^2)0.5}{1.15 \times 10^{-7}\left[m^2/s\right]} = 679.3s = 11.3 \text{ min} \]

c. If \( h_m \) is infinite, \( c_{\infty}^{\text{fluid}} \) equals \( c_{\infty} \) since there is no resistance between the bulk and surface. Hence,

\[ c_s^{\text{grape}} = \frac{c_{\infty}^{\text{fluid}}}{K*} = \frac{c_{\infty}}{K*} = 0.643 \left[\frac{g}{m^3}\right] \]

d. \[ n_s = \frac{g}{m^2s} = \sqrt{\frac{D}{\pi t}(c_s - c_i)} \]

\[ n_s \propto \sqrt{D} \]
Problem 5

1. Yes, since diffusion is still there and mass transfer coefficient includes the effects of diffusion and flow.

2. Infinite since there is almost zero resistance

3. To reach the same concentration or temperature, for a size $L_c$,

$$\frac{Dt}{L_c^2} = \text{Constant}$$

$$L_c^2 \propto t$$

$$\left(\frac{L_2}{L_1}\right)^2 = \frac{t_2}{t_1}$$

Therefore $t$ increases as the SQUARE of $L_c$

4. i. Eddies/turbulence in water
   ii. Variation in the length and diameter of capillaries
   iii. Variation in length and diameter of pores in the soil

5. The corresponding terms in heat and mass are analogous; $J$ for amount of energy while $kg$ for amount of mass......

$$\begin{align*}
[h] &= \frac{[q]}{[A][T_s - T_\infty]} = \frac{[J/s]}{[m^2][K]} = \frac{W}{m^2K} \\
[h_m] &= \frac{[n]}{[A][c_s - c_\infty]} = \frac{[kg/s]}{[m^2][\frac{kg}{m^3}]} = \frac{m}{s}
\end{align*}$$

F. Electric potential and resistors