

MEsc 5025

Diffusion Homework Solutions

■

Problem 1

```
conc = 2 alpha/Sqrt[4 Pi Dif t] Exp[- x x/(4 Dif t)];
alpha=1.82 10^-4; Dif=3.42 10^-12; t=3(3600);
```

Solve for x:

```
Solve[conc == 0.01, x]//N
{{x -> 0.000766666}, {x -> -0.000766666}}
```

$x = 7.66 \cdot 10^{-4}$ cm or 7.66 microns

■ Problem 2

```
Clear[conc,x,Dif,t];
conc = A + B Erf[x/Sqrt[4 Dif t]];
```

From the boundary conditions:

```
0.1 = A + B Erf[infinity] ----> 0.1 = A + B
1 = A + B Erf[0] ----> A = 1,
B = -0.9
```

```
conc = 1 - 0.9 Erf[x / Sqrt[4 D t] ]
A = 1; B = -0.9; Dif = 1.4 10^-7;
x = 0.05;
FindRoot[A + B Erf[x/Sqrt[4 Dif t]] == 0.45, {t,100}]
{t -> 12026.4}
```

part a: time required to carburize $c=0.45$ at $x=0.05$ cm
is 12000 sec, or 3.33 hours.

```
x = 0.10;
FindRoot[A + B Erf[x/Sqrt[4 Dif t]] == 0.45, {t,100}]
{t -> 48105.7}
```

part b: time required to carburize $c=0.45$ to a depth of $x=0.10$ cm
is 48100 sec, or 13.36 hours.

```

Dif = 0.25 Exp[-34500/(1.987 (T+273))];
FindRoot[A + B Erf[x/Sqrt[4 Dif 12000]] == 0.45, {T,900}]
{T -> 1061.9}

```

part c: the temperature required to carburize $c=0.45$ to a depth of $x=0.10$ cm in 12000 sec is 1062 degrees C.

■ Problem 3

```
Clear[c, conc, x, Dif, t, A, L];
```

Assume the initial concentration profile in the slab is constant and the gas is r from both sides of the slab. The appropriate Fourier series solution is:

```
c = (A Sin[n Pi x/L] Exp[-(n Pi/L)^2 Dif t]);
```

The "A" coefficients are given by $2/L$ times the Integral from 0 to L of $\text{Sin}[n \text{ Pi} x/L] \text{Cos}[n \text{ Pi} x/L]$ evaluated at 0 and L, so the "A" coefficients are given by $2 \text{ Co} / (n \text{ Pi}) \text{Cos}[n \text{ Pi}]$. The first seven coefficients are

```
A = Table[2 Co/L Integrate[Sin[n Pi x/L], {x, 0, L}], {n, 7}]
```

```
{ 4 Co / Pi, 0, 4 Co / 3 Pi, 0, 4 Co / 5 Pi, 0, 4 Co / 7 Pi }
```

or $A = (4 \text{ Co} / n \text{ Pi})$ for all odd values of n
and $A = 0$ for all even values of n

The amount of gas remaining in the slab can be found by determining the average gas concentration, Cbar . This is found by integrating the concentration from one side of the slab to the other and dividing by the slab thickness:

```
Cbar=1/L Integrate[(4Co/(n Pi)Sin[n Pi x/L]Exp[-(n Pi/L)^2 Dif t]),
{x, 0, L}];
```

The fraction of gas remaining is the average concentration divided by the initial concentration, or $\text{FracRemain} = \text{Cbar}/\text{Co}$

```
FracRemain = 1/L Integrate[(4/(n Pi)Sin[n Pi x/L]
Exp[-(n Pi/L)^2 Dif t]),
{x, 0, L}];
```

```
term = Simplify[%]
```

$$\frac{8 \text{ Sin}\left[\frac{n \text{ Pi}}{2}\right]^2}{\text{E}^{(Dif n^2 \text{ Pi}^2 t)/L^2} n^2 \text{ Pi}^2}$$

This is the general term in the series solution for the amount of gas remaining (n =odd integers from 1 to infinity). However, since most of the gas is removed, the diffusion time is relatively long and the higher order terms ($n=3$ and higher) can safely be neglected. Substituting the size of the slab, the diffusivity, and

```

Dif = 10^-4; L = 7 (2.54);
summation = Sum[term, {n, 1, 1, 2}]

$$\frac{8}{E^{3.16327 \cdot 10^{-7} \cdot \text{Pi}^2 \cdot t \cdot \text{Pi}^2}}$$

N[FindRoot[summation==0.1, {t, 10000}], 10]
{t -> 670259.7059}

```

The time required to remove 90% of the gas is 670259.7059 sec or 7.76 days.
 Note: including the next term results in the marginally more accurate solution
 {t -> 670259.7077720129 sec}

■ Problem 4

Assuming the initial oxygen concentration in the film is uniform we wish to find time required to reach the steady state profile. The appropriate solution to the equation is a Fourier series. Steady state is reached when the time component of Fourier series becomes insignificant (goes to zero). i.e. $\text{Exp}[-(n \text{ Pi}/L)^2 D t]$ is approximately zero. The first time dependent factor has $n=1$ ($n=0$ is the steady $\text{Exp}[-(\text{Pi}/L)^2 D t]$ can be neglected when $L^2 = D t$ (i.e. $\text{Exp}[-\text{Pi}^2] = \text{Exp}[-9.9]$)
 For $t = 48 \text{ hrs} = 172800 \text{ s}$, $D = 4 \text{ Exp}[-112000/(8.3 \cdot 10^{-8} \text{ m}^2/\text{sec})] = 4.31 \times 10^{-4}$
 Using $L = \text{Sqrt}[D t]$, $L = 8.6 \times 10^{-8} \text{ m}$ or $8.6 \times 10^{-6} \text{ cm}$

■ Problem 5

The only way the hydrogen gas can leave the tank is for it to diffuse through the During steady state, the concentration profile is not changing with time. Using 2nd law it can be demonstrated that the concentration profile from the inside wall tank to the outside wall must be linear during steady state. To determine the drop, one must determine the amount of hydrogen leaving the tank per sec. This is the flux of hydrogen through the walls times the area of the walls. Thus, the of finding the hydrogen flux. This is given by:

$$J = -D \frac{dc}{dx} \quad (\text{Fick's 1st Law})$$

First, we determine the concentration profile (so we can determine what dc/dx is)
 $c = \text{Const} \cdot \text{Sqrt}(P)$ and the solubility of H at 1 atm pressure is 3 ppm.

converting the hydrogen concentration to reasonable units:

$\{(3 \text{ g of H}) / (1,000,000 \text{ g of Ni})\} (8.91 \text{ g of Ni per cm}^3 / 1.01 \text{ g of H per mol}) = 2$
 mol of H per cubic cm of Ni at a pressure of 1 atmosphere. The pressure inside 132 psi or 9 atm; thus, the concentration of H at the inside wall, c_i , is

$$c_i = 2.65 \cdot 10^{-5} \text{ Sqrt}[9] \text{ mol/cm}^3$$

$$\frac{0.0000795 \text{ mol}}{\text{cm}^3}$$

and the concentration at the outside wall, $c_o = 0$.

The concentration profile for a wall of thickness, W , is thus:

$$c = [(c_o - c_i)/W] x + c_i$$

and the concentration gradient is simply:

$$(c_o - c_i)/W$$

The flux per unit area is:

$$J = -D \frac{dc}{dx} = - (c_o - c_i)/W$$

and the total number of moles of H lost per second is

$$J A \quad \text{where } A \text{ is the area of the square tank } (A = 6 \text{ L}^2)$$

$$\frac{dn}{dt} = J A = - 6 D (c_o - c_i) \text{ L}^2/W$$

Next we relate the loss of hydrogen moles to a decrease in pressure. Assuming the gas in the tank behaves ideally and the number of moles of hydrogen gas is $0.5n$ hydrogen atoms (i.e. hydrogen is a diatomic gas and we are using n to represent n moles of hydrogen atoms):

$$P = 0.5nRT/V = 0.5n (3.4 \cdot 10^{-6} \text{ liter} \cdot \text{atm}/(\text{K} \cdot \text{mol})) (673 \text{ K}) / (1 \text{ liter}) = (0.$$

$$\text{differentiating this expression for } P, \quad R = (0.8206 \text{ L} \cdot \text{atm}/(\text{K} \cdot \text{mol}))$$

$$\frac{dP}{dt} = (0.00115 \text{ atm/mol}) \frac{dn}{dt}$$

substituting the previous expression for dn/dt ,

$$\frac{dP}{dt} = - 0.00115 (6 D (c_o - c_i) \text{ L}^2/W)$$

employing the values stated in the problem, the rate of pressure drop becomes:

$$\text{PressureDrop} = -0.00115(6 \cdot 10^{-6})(0 - 0.0000795)10^2/0.1 \text{ atm/sec}$$

$$\frac{5.4855 \cdot 10^{-10} \text{ atm}}{\text{sec}}$$

or the pressure drops 1 atm every 52 years.