Problem 3

Equimolar Diffusion

Problem 3.1.a

Determine t when $x_{Xe} = 0.6$ in bulb 1

Starting with an integral mol balance,

$$\frac{d}{dt}\int c_{Xe}dV = -\int x_{Xe}cv_M \cdot adS - \int J_{Xe} \cdot adS + \int S_{Xe}dV \tag{1}$$

we know that $v_M = 0$ and there is no reaction so (1) goes to

$$\frac{d}{dt}\int c_{Xe}dV = -\int J_{Xe} \cdot adS$$

which can be evaluated to be

$$cV_0\frac{dx^0_{Xe}}{dt} = J^0_{Xe}A_c \tag{2}$$

Since $N = 0$ the following relationship holds

$$N_{Xe} = x_{Xe}N + J_{Xe} = J_{Xe} \tag{3}$$

so (2) becomes

$$cV_0\frac{dx^0_{Xe}}{dt} = N_{Xe}A_c \tag{4}$$

In is also true that

$$A_cJ^0_{Xe} = A_cJ^L_{Xe}$$

which implies that J_{Xe} and N_{Xe} are constant. </br></br> Using Fick's law to find N_{Xe}

$$J_{Xe} = N_{Xe} = -cD_{AB}\frac{dx_{Xe}}{dz}$$

rearranged is

$$N_{Xe}\int_0^L dz = -cD_{AB}\int_0^L dx_{Xe}$$

and evaluate to get

$$N_{Xe} = \frac{-cD_{AB}}{L}(x^L_{Xe} - x^0_{Xe}) \tag{5}$$

where L is the length of the tube

Now (5) can be substituted in for (4) to get

$$V_0 \frac{dx_{Xe}^0}{dt} = \frac{A_c D_{AB}}{L}(x_{Xe}^L - x_{Xe}^0) \tag{6}$$

x_{Xe}^L can be found by doing a total mol balance on both bulbs,

$$cx_{Xe}^0 V_0 + cx_{Xe}^L V_L = cx_{Xe}^\infty (V_0 + V_L)$$

which is rearranged to get

$$x_{Xe}^L = x_{Xe}^\infty (1 + \frac{V_0}{V_L}) - x_{Xe}^0 \frac{V_0}{V_L} \tag{7}$$

(7) can be inserted into (6) and evaluated to get

$$x_{Xe}^0 = x_{Xe}^\infty + (x_{Xe_0} - x_{Xe}^\infty) \exp(-\beta D_{AB} t) \tag{8}$$

where

$$\beta = \frac{A_c}{V_0 L}(1 + \frac{V_0}{V_L})$$

x_{Xe}^∞ can also be found by the overall mole balance because c cancels out and $V_0 = V_L$. </br> </br> $\therefore$

$$V(x_{Xe}^0 + x_{Xe}^L) = x_{Xe}^\infty (2V)$$

and rearranging gives

$$x_{Xe}^\infty = \frac{x_{Xe}^0 + x_{Xe}^L}{2}$$

At $t = 0$: $x_{Xe}^0 = 1$ and $x_{Xe}^L = 0$ which means $x_{Xe}^{\backslash\mathrm{infin}} = 0.5$ </br></br> (8) will be used in the following code to anser part a

In [ ]:

```
import numpy as np
import matplotlib.pyplot as plt
```

In [ ]:

```
d = .2                                          #tube diam cm
L = 10                                          #tube len cm
DAB = .180                                            #diffusiv cm2/sec
D = 15                                          #bulb diam cm
VL = 4/3*np.pi*(.5*D)**3                             #volume of bulb cm3
V0=4/3*np.pi*(.5*D)**3
xinf = .5                                           #x at t=inf
Ac = np.pi*(.5*d)**2                                #cross sectional area
xa00 = 1                                            #x at t=0 in bulb1

beta1 = Ac/V0/L*(1+V0/VL)
```

In [ ]:
```
def t(xa0):
    t = -np.log((xa0-xinf)/(xa00-xinf))/beta1/DAB
    return t/3600
print(t(.6))
```

```
698.5407606050782
```

It will take about 699. hours for $x_{Xe} = 0.6$ in bulb 1

Problem 3.1.b

A similar approach was taken as part a to derive

$$x^L_{Xe} = x^\infty_{Xe} + (x^L_{Xe_0} - x^\infty_{Xe})exp(-\beta D_{AB}t) \tag{9}$$

where

$$\beta = \frac{A_c}{V_L L}(1 + \frac{V_L}{V_0})$$

In [ ]:
```
xa0L = 0                                                        #x in bulb2 at t=
beta2 = Ac/VL/L*(1+VL/V0)
def t(xaL):
    t = np.log((xaL-xinf)/(xa0L-xinf))/-beta2/DAB
    return t/3600
print(t(.3))
```

```
397.69563015371307
```

It will take about 398. hours for $x_{Xe} = 0.3$ in bulb 2

Problem 3.2

To determine the molar flux at $t = 90$ for both Xe and Ar, (8), (9), and (5) can be used. I will first use (8) and (9) to solve for the molar fractions in both bulbs and then plug those values into (5). $N_{Xe} = -N_{Ar}$. c will be found by using the ideal gas law.

$$\frac{n}{V} = c = \frac{P}{RT} \tag{10}$$

In [ ]:
```
P = 1                                                                  #pres
T = 105+273.15                                                             #
R = 82.057                                                   #gas constant
c = P/R/T                                                          #starting
def xa0(t):
    xa0 = xinf + (xa00-xinf)*np.exp(-beta1*DAB*t)
    return xa0

def xaL(t):
    xaL = xinf + (xa0L-xinf)*np.exp(-beta2*DAB*t)
    return xaL

def NA(xa0,xaL):
    NA = -c*DAB/L*(xaL-xa0)
```

```
    return NA

NA = NA(xa0(90*3600),xaL(90*3600))
print(NA)
```

4.7145197722612887e-07

$N_{Xe} = 4.71e-7\frac{mol}{cm^2 sec}$ </br></br> $N_{Ar} = -4.71e-7\frac{mol}{cm^2 sec}$

Problem 3.3

To find the velocities, I first derive an expression for $x_{Xe}(z)$. As established before:

$$J_{Xe} = N_{Xe} = -cD_{AB}\frac{dx_{Xe}}{dz}$$

which can be rewritten as

$$N_{Xe}\int_0^z dz = -cD_{AB}\int_{x_{Xe}^0}^{x_{Xe}^z} dx_{Xe}$$

and evaluated to be

$$x_{Xe}^z - x_{Xe}^0 = -\frac{N_{Xe}}{cD_{AB}}z$$

Now (5) can substitue into N_{Xe} to give

$$x_{Xe} = x_{Xe}^0 + (x_{Xe}^L - x_{Xe}^0)\frac{z}{L} \tag{11}$$

and

$$x_{Ar} = 1 - x_{Xe} \tag{12}$$

Velocity of each species can be written as

$$v_i = \frac{N_i}{cx_i} \tag{13}$$

N_i and c were calculated previously.

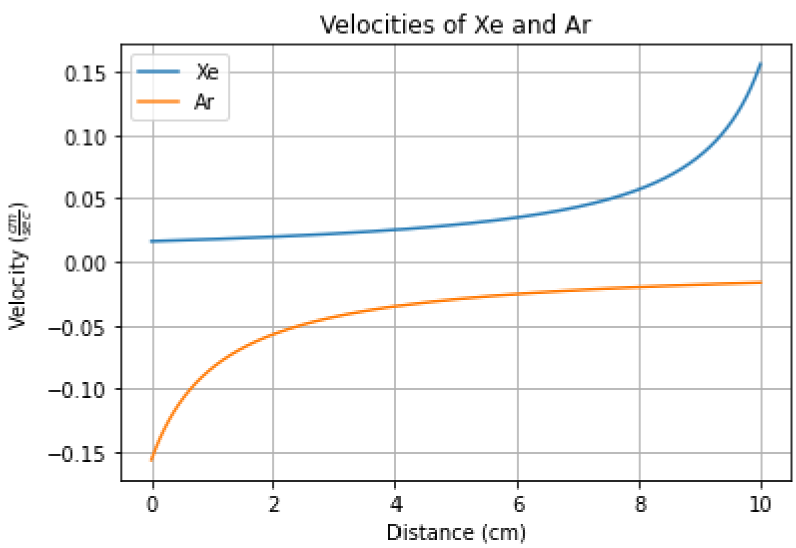
In [ ]:

```
def xA(z,xa0,xaL):
    xA = xa0 + (xaL-xa0)*z/L
    return xA

def v(x,spec):
    if spec == 1:
        return NA/c/x
    elif spec == 2:
        return -NA/c/x

z = np.linspace(0,10,999)
```

In [ ]:
```
xa0_90 = xa0(90*3600)
xaL_90 = xaL(90*3600)
xa_z = xA(z,xa0_90,xaL_90)
va = v(xa_z,1)

xb0_90 = 1-xa0_90
xbL_90 = 1-xaL_90
xb_z = 1-xa_z
vb = v(xb_z,2)
```

In [ ]:
```
plt.plot(z,va,label='Xe')
plt.plot(z,vb,label='Ar')
plt.legend()
plt.grid()
plt.title('Velocities of Xe and Ar')
plt.xlabel('Distance (cm)')
plt.ylabel(''.join(['Velocity ',r'($\frac{cm}{sec}$)']))
;
print(va[-1],'\n',vb[-1])
```

```
0.1562327457619987
 -0.016140418446698973
```



At $z = L$, </br></br> $v_{Xe} = 0.156\frac{cm}{sec}$ </br></br> $v_{Ar} = -1.61e-2\frac{cm}{sec}$

Problem 3.4

At $z = L$, $v_M = 0$ as shown by

$$v_M = \frac{N}{c} = \frac{0}{c}$$

Problem 3.5

The mass averaged velocity can be determined using

$$v_m = \frac{\Sigma m_i v_i}{m_{tot}}$$

m_i can be determined by using the ideal gas law and the molar masses of each species

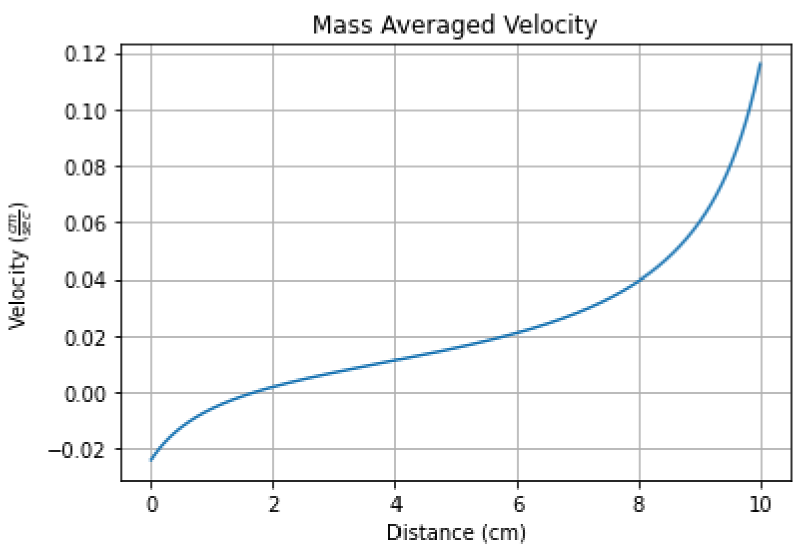
$$m = nM$$

where M is molar mass

In [ ]:

```
Mx = 131.29                                     #molar mass of xe g/mol
Ma = 39.948                                     #molar mass of ar g/mol
n = P*V0/R*T                                    #number of moles of each species
mx = n*Mx                                       #mass xe g
ma = n*Ma                                       #mass ar g

vm = (mx*va+ma*vb)/(ma+mx)
plt.plot(z,vm)
plt.grid()
plt.title('Mass Averaged Velocity')
plt.xlabel('Distance (cm)')
plt.ylabel(''.join(['Velocity ',r'($\frac{cm}{sec}$)']));
print(vm[-1])
```

```
0.11601992405297935
```



At $z = L$, </br></br> $v_m = 0.116\frac{cm}{sec}$