HW4_2

February 23, 2022

1 HW 4

1.1 Problem 2.1

Estimate time for benzene to completely evaporate from beaker assuming N_A doesn't change with time.

Starting with a mole balance,

$$\frac{d}{dt}\int c_i dV = -\int N_i \cdot a dS + \int S_i dV \tag{1}$$

which simplifies to

$$\frac{d}{dt}\int c_A dV = -\int N_A \cdot a dS \tag{1.1}$$

$dV = A_c dh$ and $dh = -dz$ so (1.1) goes to

$$-A_c \frac{d}{dt}\int c_A dz = -\int N_A \cdot a dS \tag{1.2}$$

Assuming a negligible amount of air dissolved in the benzene, $c_A = \frac{\rho}{M}$ and is constant with respect to z so the left side of (1.2) becomes

$$-A_c \frac{\rho}{M}\frac{d}{dt}\int dz$$

For the right hand side of (1.2), N_A is constant with respect to S so the RHS becomes

$$-N_A A_c \tag{1.3}$$

now equating (1.2) and (1.3),

$$\frac{\rho}{M}\frac{d}{dt}\int dz = N_A$$

N_A can be expanded to

$$N_A = x_A N + J_A \tag{2}$$

assuming $N_B = 0$ and applying Fick's Law (2) is simplified to

$$N_A = x_A N_A - cD_{AB}\frac{dx_A}{dz}$$

and rearanged to get

$$N_A = -\frac{cD_{AB}}{1-x_A}\frac{dx_A}{dz}$$

which can then be seperated and integrated,

$$\int_{z_1}^{z_2} dz = -\frac{cD_{AB}}{N_A}\int_{x_{A_1}}^{x_{A_2}} \frac{dx_A}{1-x_A}$$

$$N_A = \frac{cD_{AB}}{z_2 - z_1}\ln(\frac{1-x_{A_2}}{1-x_{A_1}}) \tag{2.1}$$

∴

$$\frac{\rho}{M}\frac{d}{dt}\int dz = \frac{cD_{AB}}{\Delta z}\ln(\frac{1-x_{A_2}}{1-x_{A_1}})$$

separating gives

$$\int_0^t dt = \frac{\rho}{McD_{AB}\ln(\frac{1-x_{A_2}}{1-x_{A_1}})}\int_{z_1}^{z_2} zdz$$

where $z = \Delta z$ After integrating,

$$t = \frac{\rho}{McD_{AB}\ln(\frac{1-x_{A_2}}{1-x_{A_1}})}(\frac{z_2^2 - z_1^2}{2}) \tag{3}$$

The script below uses the following values to solve for t $M = 78.11\frac{g}{mol}$ $D_{AB} = 0.0905\frac{cm^2}{sec}$ $\rho = 0.876\frac{g}{cm^3}$ $z_1 = L$ $z_2 = H$ where L and H are taken from the book to be 0.5cm and 6cm respectively. x_{A_1} was calculated using Raoult's law: $x_A = \frac{p_A}{P} = \frac{0.12518}{1}$ T was assumed to be $298K$ and P to be $1atm$ c was calculated using the ideal gas law, $c = \frac{P}{RT}$

[ ]:
```
import numpy as np
M = 78.11                                  #g/mol
P = 1                                                   #atm
pA = .12518
DAB = .0905                                    #cm2/sec
ro = .876                                      #g/cm3
xa1 = pA/P
xa2 = 0
R = 8.2057*1000000                                       #cm3atm/mol/k
T = 273.15+25                                           #k
c = P/R/T                                               #mol/cm3
L = .5                                                  #cm
H = 6                                                           #cm
t = (ro/M/c/DAB/np.log((1-xa2)/(1-xa1))*(H**2-L**2)*.5)/60/60/24
print(round(t),'days')
```

```
469007 days
```

It would take about 469007 days to evaporate if N_A is constant in time

1.2 Problem 2.2

Account for changing N_A with liquid level

(2.1) still holds but the left side of the mole balance becomes

$$\frac{d}{dt}c_A h A_c = c_A A_c \frac{dh}{dt} \tag{4}$$

(3) can be rearanged to solve for z_2 as a function of time,

$$z_2 = \sqrt{\frac{2McD_{AB}\ln(\frac{1-x_{A_2}}{1-x_{A_1}})t}{\rho} + z_1^2} \tag{5}$$

Given that $h = H - z$,

$$h = H - \sqrt{\frac{2McD_{AB}\ln(\frac{1-x_{A_2}}{1-x_{A_1}})t}{\rho} + z_1^2}$$

∴

$$\frac{dh}{dt} = -\frac{\frac{2McD_{AB}\ln(\frac{1-x_{A_2}}{1-x_{A_1}})}{\rho}}{2\sqrt{\frac{2McD_{AB}\ln(\frac{1-x_{A_2}}{1-x_{A_1}})}{\rho}t + z_1^2}}$$

Putting it all back together gives

$$-\frac{\frac{2McD_{AB}\ln(\frac{1-x_{A_2}}{1-x_{A_1}})}{\rho}}{2\sqrt{\frac{2McD_{AB}\ln(\frac{1-x_{A_2}}{1-x_{A_1}})}{\rho}t + z_1^2}}\frac{\rho}{M} = \frac{cD_{AB}}{z_2 - z_1}\ln(\frac{1-x_{A_2}}{1-x_{A_1}})$$

which can be solved for t,

$$t = -\frac{\left(\frac{\frac{2McD_{AB}\ln(\frac{1-x_{A_2}}{1-x_{A_1}})}{\rho}}{2\frac{cD_{AB}}{z_2-z_1}\ln(\frac{1-x_{A_2}}{1-x_{A_1}})}\frac{\rho}{M}\right)^2 - z_1^2}{\frac{2McD_{AB}\ln(\frac{1-x_{A_2}}{1-x_{A_1}})}{\rho}}$$

[ ]:
```
a = 2*M*c*DAB*np.log((1-xa2)/(1-xa1))
b = c*DAB*np.log((1-xa2)/(1-xa1))/(H-L)
t = ((a*ro/M/2/b)**2 - L**2)/a
print(t/60/60/24)
```

```
343898.65074998315
```

Accounting for changing flux with liquid level, it would take about 343899 days to fully evaporate. This is less than if N_A is assumed to be constant in time. I think that it is more accurate to account for changing N_A because it does change with time and typically, the fewer assumptions that are made the more accurate the model.