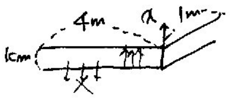
상 변태   HW 3   20202585   권재석

1.

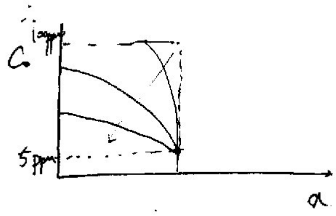
a) We neglect the N diffusion through other side.



Also, the total amount of N is restricted (100 ppm)

Concentration of N will gradually decrease during diffusion

Nitrogen at the surface will escape & immediately reach the surface (not rate determining step)



∴ Boundary condition become
$$\begin{cases} C(0<x<l,\ t=0) = 100\,ppm \\ C(x=L,\ t) = 5\,ppm \\ \dfrac{\partial C(x=0,t)}{\partial x} = 0 \end{cases}$$

The differential equation form is written by Fick's second law

$$\boxed{\frac{\partial C(x,t)}{\partial t} = D\frac{\partial^2 C}{\partial x^2}}$$

$d = 1cm$, $T = 1000K$ $D = 4\times10^{-7}\ cm/sec$

b) $l = 1cm < 4\sqrt{Dt}$: trigonal solution & 1st term approximation

$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$ using separation of variable $C(x,t) = X(x)T(t)$

$T(t) = \exp(-\lambda^2 Dt)$ $X(x) = A\cos\lambda x + B\sin\lambda x$

$\therefore C(x,t) = \sum_n (A\cdot\cos\lambda_m x + B\sin\lambda_m x)\cdot\exp(-\lambda^2 Dt)$

with first term approximation $C(x,t) = (A\cdot\cos\lambda_m x + B\sin\lambda_m x)\cdot\exp(-\lambda^2\cdot Dt)$

using boundary condition $\cancel{C(0<x<l)=0}$ $C(0=x)\neq0$ $C(x=L,t) = 5ppm$ B term vanishes.

$$\therefore \underline{C(x,t) = A\cos\lambda_m x\cdot\exp(-\lambda_n^2 Dt) + 5\,ppm} \quad \left(\lambda_m = \frac{m\pi}{l}\right)$$

using orthogonality thm,

$$\boxed{C(x,t) = \frac{4C_0}{\pi}\cos\frac{\pi x}{2l}\cdot\exp\left(-\frac{\pi^2}{4l^2}Dt\right)+5}$$

c) Too see the time for $C = \frac{C_0}{2}$, I solved the equation

$\frac{C_0}{2} = \frac{4C_0}{\pi}\int_0^1 \cos\frac{\pi}{2}x\ \exp(-\pi^2 Dt)dx + 5$,   since t is independent to x.

$\frac{\pi}{8} - 5 = \int_0^1 \cos\frac{\pi}{2}x\,\exp(-\pi^2 Dt)\,dx = \frac{2}{\pi}\exp(-\pi^2 Dt)$,   solution t for this is $\underline{540000\ sec}$

d) The time reaching half concentration will increase if D is dependent to concentration.

As time goes by, the concentration decrease and so does for D. therefore the diffusion amount will decrease compare to independent D.

This is why I assume that t will increase for this case.

2.

c) Using $l \propto \sqrt{Dt}$. write the equation $\underline{l = a\sqrt{Dt}}$

for different time step the difference can be written as

$$\ln\left(\frac{l_1}{l_2}\right) = \frac{1}{2}\ln\left(\frac{D_1}{D_2}\right) + \ln\left(\frac{t_1}{t_2}\right)$$

Diffusion coefficient can be written as

$$D = D_0 \exp\left(-\frac{Q}{RT}\right)$$

→ activation barrier

Substituting D in the above equation gives. and comparing for same time

$$\underline{\ln\frac{l_1}{l_2} = -\frac{Q}{2R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)}$$

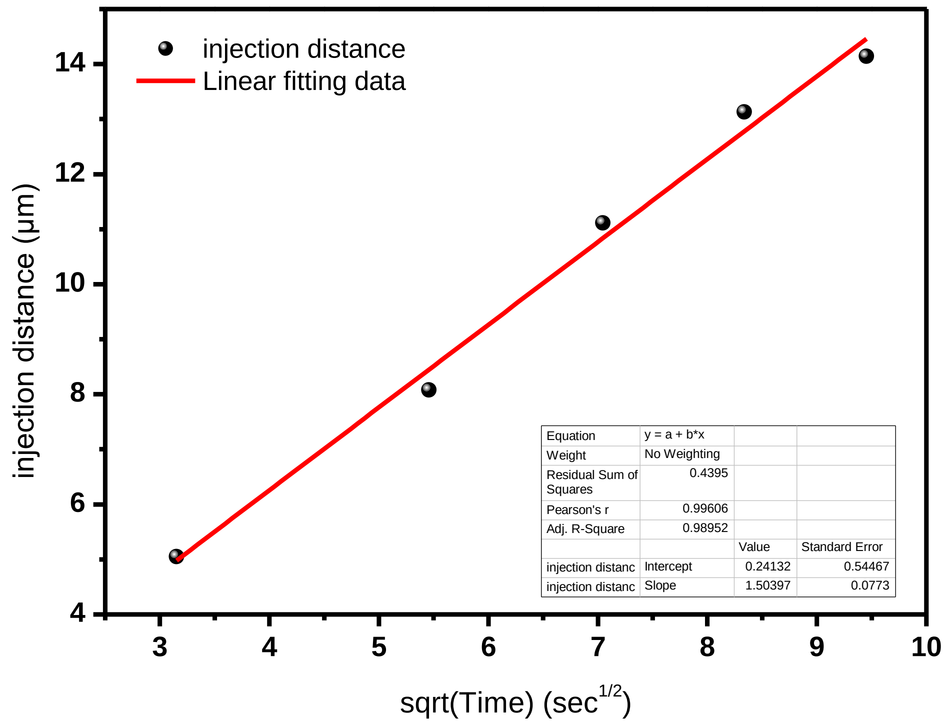
using data for $\underline{t = 90\text{sec}}$

$l_1 = 3\mu m$ $l_2 = 14\mu m$ $T_1 = 1173K$ $T_2 = 1473K$

$\therefore$ $\underline{\Delta Q = 147723 J.}$

2-a)

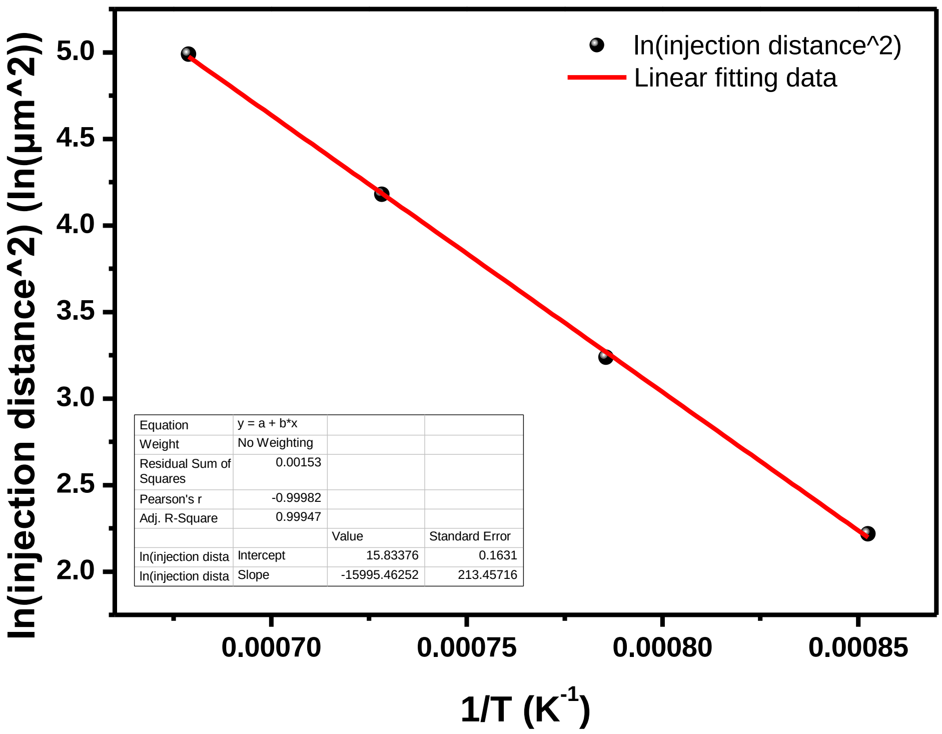
T=1473 data



$l \propto \sqrt{Dt}$에 비례하는 수식을 고려하여 fitting 하였습니다.

2-b)

t~60



$\ln(l^2) \propto {}^{1}/_{T}$ 의 관계가 성립하는 것을 확인할 수 있습니다.