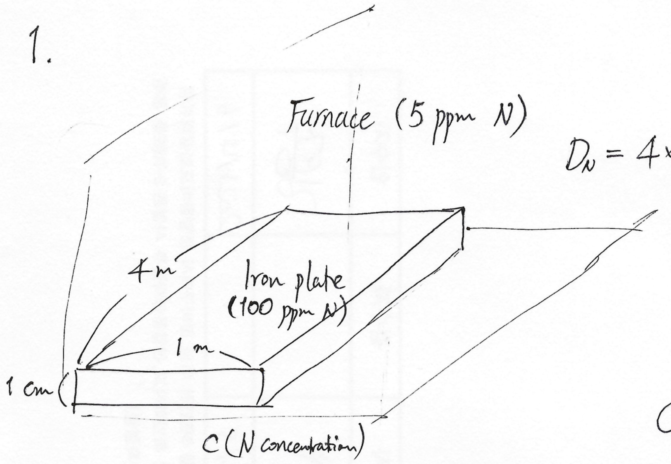
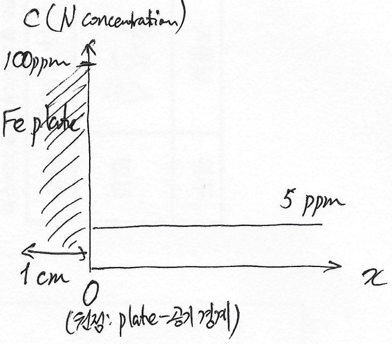
[AMSE 502] Phase Transformations Problemset #3 20202966 이정완.

1.



$D_N = 4 \times 10^{-7} cm^2 s^{-1}$



(a) According to Fick's 2nd law,

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

C: concentration of N / t: time.

D: diffusivity of N in Fe / x: distance from surface of Fe plate. (upper surface)

Initial and boundary condition:

$C(x<0,\ t=0) = 100$ ppm

$C(x>0,\ t=0) = 5$ ppm

$C(x=0,\ t) = 5$ ppm

(b)

Non-steady state solution of diffusion 의 thin film source 에서, $C(x,t) = \frac{A}{t^{\frac{1}{2}}} \exp\left(-\frac{x^2}{4Dt}\right)$

시간이 지남에 따라 질소가 확산되는데 전체 질소의 양은 M으로 일정하다.

이 경우는 한 방향으로 퍼지는 layer deposition 이므로 $C(x,t) = \frac{M}{\sqrt{\pi D t}} \exp\left(-\frac{x^2}{4Dt}\right)$

$$\rho(x,t) = \frac{M}{\sqrt{\pi D t}} \exp\left(-\frac{x^2}{4Dt}\right)$$

전체 질소의 양 M을 설명하기 위해, 무한 개의 thin film source로 나누어 thin film case로 생각.

Thin film의 넓이를 Δa_i라 하고 i번째 thin film의 x 방향 위치를 a_i, 그 농도를 ρ_i라 하면

$$\rho_i(x,t) = \frac{\rho_0 \Delta a_i}{\sqrt{\pi D t}} \exp\left(-\frac{(x-a_i)^2}{4Dt}\right)$$

이때, initial ρ_i ρ_0는 $\begin{cases} a_i<0 \text{ 일 때 } 100 \text{ ppm} \\ a_i>0 \text{ 일 때 } 5 \text{ ppm.} \end{cases}$

total N 농도

$$\rho(x,t) = \sum_{i=1}^{\infty} \rho_i = \int_{-1}^{0} \frac{100\,(\text{ppm})}{\sqrt{\pi D t}} \exp\left(-\frac{(x-a_i)^2}{4Dt}\right) da + \int_{0}^{\infty} \frac{5\,(\text{ppm})}{\sqrt{\pi D t}} \exp\left(-\frac{(x-a_i)^2}{4Dt}\right) da$$

$\frac{x-a}{\sqrt{4Dt}} = \xi$ 라 하면 $da = -2\sqrt{Dt}\, d\xi$

$$\rho(x,t) = -\frac{200}{\sqrt{\pi}} \int_{\frac{x+1}{2\sqrt{Dt}}}^{\frac{x}{2\sqrt{Dt}}} e^{-\xi^2} d\xi - \frac{10}{\sqrt{\pi}} \int_{\frac{x}{2\sqrt{Dt}}}^{-\infty} e^{-\xi^2} d\xi$$

$$= \frac{200}{\sqrt{\pi}} \int_{\frac{x}{2\sqrt{Dt}}}^{\frac{x+1}{2\sqrt{Dt}}} e^{-\xi^2} d\xi + \frac{10}{\sqrt{\pi}} \left(\int_{-\infty}^{0} e^{-\xi^2} d\xi + \int_{0}^{\frac{x}{2\sqrt{Dt}}} e^{-\xi^2} d\xi \right)$$

1-(b) 계속.

$$\rho(x,t) = 5\left(1+\frac{2}{\sqrt{\pi}}\int_0^{\frac{x}{2\sqrt{Dt}}} e^{-\xi^2}d\xi\right) + 100\left(\frac{2}{\sqrt{\pi}}\int_0^{\frac{x+1}{2\sqrt{Dt}}} e^{-\xi^2}d\xi - \frac{2}{\sqrt{\pi}}\int_0^{\frac{x}{2\sqrt{Dt}}} e^{-\xi^2}d\xi\right)$$

$$= 5\left(1+\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)\right) + 100\left\{\mathrm{erf}\left(\frac{x+1}{2\sqrt{Dt}}\right) - \mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)\right\}$$

(c) How long time takes for ρ in the plate drops to 50% of initial value.

(b) 문제의 결과에서,

$$\int_{-1}^{0}\rho(x,t)\,dx = \int_{-1}^{0}\left\{5\left(1+\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)\right) + 100\left\{\mathrm{erf}\left(\frac{x+1}{2\sqrt{Dt}}\right) - \mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)\right\}\right\}dx$$

이때, $\int \mathrm{erf}(x)\,dx = x\,\mathrm{erf}(x) + \frac{e^{-x^2}}{\sqrt{\pi}} + C$

$$\int \mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)dx = \left(\frac{x}{2\sqrt{Dt}}\,\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right) + \frac{e^{-\frac{x^2}{4Dt}}}{\sqrt{\pi}}\right)\cdot 2\sqrt{Dt} + C$$

$$= x\,\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right) + \frac{2\sqrt{Dt}}{\sqrt{\pi}}e^{-\frac{x^2}{4Dt}} + C$$

$$\int \mathrm{erf}\left(\frac{x+1}{2\sqrt{Dt}}\right)dx = (x+1)\,\mathrm{erf}\left(\frac{x+1}{2\sqrt{Dt}}\right) + \frac{2\sqrt{Dt}}{\sqrt{\pi}}e^{-\frac{(x+1)^2}{4Dt}} + C$$

$$\therefore \int_{-1}^{0}\rho(x,t)\,dx = \int_{-1}^{0}\left\{5 - 95\,\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right) + 100\,\mathrm{erf}\left(\frac{x+1}{2\sqrt{Dt}}\right)\right\}dx$$

$$= 5 - 95\left[x\,\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right) + \frac{2\sqrt{Dt}}{\sqrt{\pi}}e^{-\frac{x^2}{4Dt}}\right]_{-1}^{0} + 100\left[(x+1)\,\mathrm{erf}\left(\frac{x+1}{2\sqrt{Dt}}\right) + \frac{2\sqrt{Dt}}{\sqrt{\pi}}e^{-\frac{(x+1)^2}{4Dt}}\right]_{-1}^{0}$$

$$= 5 - 195\left(\frac{2\sqrt{Dt}}{\sqrt{\pi}} - \frac{2\sqrt{Dt}}{\sqrt{\pi}}e^{-\frac{1}{4Dt}}\right) + 195\,\mathrm{erf}\left(\frac{1}{2\sqrt{Dt}}\right)$$

$$= 5 - 195\left(\frac{2\sqrt{Dt}}{\sqrt{\pi}} - \mathrm{erf}\left(\frac{1}{2\sqrt{Dt}}\right) - \frac{2\sqrt{Dt}}{\sqrt{\pi}}e^{-\frac{1}{4Dt}}\right)$$

When $t=0$, $\int_{-1}^{0}\rho(x,t)\,dx = 100$ ppm. $\int_{-1}^{0}\rho(x,t)\,dx = 50$ ppm일 때 $t = 621{,}107$ sec.

(d) (b)의 결과에서 D가 증가하면 $\rho(x,t)$가 감소.

따라서, 농도가 50ppm이 되는 시간이 감소.

2번 문제는 #4 H.W 와 함께 제출하겠습니다.