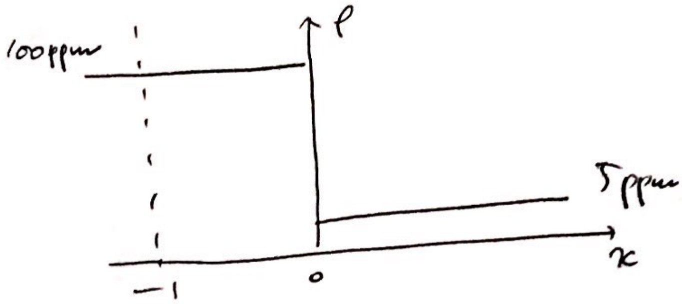
(a) Bottom 및 edge에서의 nitrogen loss는 고려하지 않으므로, 두께 방향으로의 diffusion만 고려한다. (x축 방향)

20192347 권현석

$$\Rightarrow \frac{\partial \rho}{\partial t} = -\nabla\cdot J = -\nabla(-D\nabla\rho) = D\nabla^2\rho = D\frac{\partial^2 \rho}{\partial x^2}$$



Initial & boundary condition.

$$\begin{cases} \rho(-1<x<0,\ t=0) = 100\ \text{ppm} \\ \rho(x>0,\ t=0) = 5\ \text{ppm} \\ \rho(x=0,\ t) = 5\ \text{ppm} \end{cases}$$

(b) Semi-finite sample에 대해,

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

Boundary condition: $\begin{cases} \rho_0(-1<x<0,t) = 100\text{ppm} \\ \rho_0(x>0,t) = 5\text{ppm} \end{cases}$

$$\Rightarrow \rho(x,t) = \int_{-1}^{0} \frac{100}{\sqrt{4\pi D t}} e^{-\left(\frac{x-\alpha}{\sqrt{4Dt}}\right)^2} d\alpha + \int_{0}^{\infty} \frac{5}{\sqrt{4\pi D t}} e^{-\left(\frac{x-\alpha}{\sqrt{4Dt}}\right)^2} d\alpha$$

$$= \sum_{i=1}^{\infty} \rho_i(x,t)$$

$\frac{x-\alpha}{\sqrt{4Dt}} = \eta$ 로 치환. $\Rightarrow -\frac{d\alpha}{\sqrt{4Dt}} = d\eta$. $d\alpha = -\sqrt{4Dt}\, d\eta$

$$\rho(x,t) = \frac{100}{\sqrt{\pi}} \int_{\frac{x}{2\sqrt{Dt}}}^{\frac{x+1}{2\sqrt{Dt}}} e^{-\eta^2} d\eta + \frac{5}{\sqrt{\pi}} \int_{-\infty}^{\frac{x}{\sqrt{4Dt}}} e^{-\eta^2} d\eta$$

$$= \frac{100}{\sqrt{\pi}}\left\{\int_0^{\frac{x+1}{\sqrt{4Dt}}} e^{-\eta^2}d\eta - \int_0^{\frac{x}{\sqrt{4Dt}}} e^{-\eta^2}d\eta\right\} + \frac{5}{\sqrt{\pi}}\left\{\int_{-\infty}^{0} e^{-\eta^2}d\eta + \int_0^{\frac{x}{\sqrt{4Dt}}} e^{-\eta^2}d\eta\right\}$$

$$= 50\left\{\operatorname{erf}\left(\frac{x+1}{\sqrt{4Dt}}\right) - \operatorname{erf}\left(\frac{x}{\sqrt{4Dt}}\right)\right\} + \frac{5}{2}\left\{\operatorname{erf}\left(\frac{x}{\sqrt{4Dt}}\right)+1\right\}$$

$$= 50\operatorname{erf}\left(\frac{x+1}{\sqrt{4Dt}}\right) - \frac{95}{2}\operatorname{erf}\left(\frac{x}{\sqrt{4Dt}}\right) + \frac{5}{2}$$

(c) $\int_{-1}^{0} \rho(x,t)\,dx = 50$ ppm일때의 t.

$$\Rightarrow \int_{-1}^{0}\left[50\operatorname{erf}\left(\frac{x+1}{\sqrt{4Dt}}\right) - \frac{95}{2}\operatorname{erf}\left(\frac{x}{\sqrt{4Dt}}\right) + \frac{5}{2}\right]dx$$

$$= 50\cdot\left[(x+1)\operatorname{erf}\left(\frac{x+1}{\sqrt{4Dt}}\right) + \sqrt{\frac{4Dt}{\pi}}\,e^{-\frac{(x+1)^2}{4Dt}}\right]_{-1}^{0}$$

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

$$= 50\operatorname{erf}\left(\frac{1}{\sqrt{4Dt}}\right) + 50\sqrt{\frac{4Dt}{\pi}}\,e^{-\frac{1}{4Dt}} - 50\sqrt{\frac{4Dt}{\pi}}$$

$$-\frac{95}{2}\sqrt{\frac{4Dt}{\pi}} - \frac{95}{2}\operatorname{erf}\left(\frac{-1}{\sqrt{4Dt}}\right) + \frac{95}{2}\sqrt{\frac{4Dt}{\pi}}\,e^{-\frac{1}{4Dt}} + \frac{5}{2}$$

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

$$\therefore\ t \simeq 621107\ \text{s}$$

(d) 같은 ρ에 대하여, Dt가 같으므로, $D \propto \frac{1}{t}$ $\Rightarrow$ shorter t required.

CamScanner로 스캔하기

2. (a) At 1173K, diffusion coefficient $= 1.1855 \times 10^{-9}\ m^2/s$.

length of simulation = 500

Initial composition = 0.01, boundary composition = 0.05

Reaction time = 10 hr = 36000 sec.

number of grid = 100.

Composition of B가 0.03인 지점

hour	distance
0	0
1	~20.20
2	~27.8
3	~35.35
4	~40.40
5	~45.45
6	~48
7	~51
⋮	

$\Rightarrow$ time $\propto$ (distance)^2

distance $\propto \sqrt{\text{time}}$

(b) For different diffusion coefficients for different temperatures,

($3.82824 \times 10^{-8}\ m^2/s$ for 1273K, $1.08583 \times 10^{-8}\ m^2/s$ for 1373K,

$2.61446 \times 10^{-8}\ m^2/s$ for 1473 K)

Composition of B가 0.03인 지점

temperature	distance after 1hr of injection
1173	~20.20
1273	~35.35
1373	~60.61
1473	~80.81

$\Rightarrow$ temperature $\propto \sqrt{\text{distance}}$

distance $\propto$ (temperature)^2

(c) distance $\propto \sqrt{\text{diffusion coefficient} \times \text{time}}$ 이므로,

$$\underset{d}{\text{distance}} \propto \sqrt{\underset{D}{\text{diffusion coefficient}} \times \underset{t}{\text{time}}}$$

$d^2 = kDt$ (for constant k).

1 hr of injection time에 대해,

$$1173K : \ 20.20^2 = k \cdot D_0 \exp\left(-\frac{Q}{R \cdot 1173}\right) \cdot 3600$$

$$1273K : \ 35.35^2 = k \cdot D_0 \exp\left(-\frac{Q}{R \cdot 1273}\right) \cdot 3600$$

$$\begin{cases} \ln(20.20)^2 = \ln k + \ln D_0 - \dfrac{Q}{1173R} + \ln 3600 \\ \ln(35.35)^2 = \ln k + \ln D_0 - \dfrac{Q}{1273R} + \ln 3600 \end{cases}$$

$$\Rightarrow 7.130587 - 6.011365 = \frac{Q}{R}\left(\frac{1}{1173} - \frac{1}{1273}\right)$$

$$1.119222 = \frac{Q}{R} \cdot 6.7 \times 10^{-5}$$

$$\therefore Q \simeq 138857.7 \ \text{J/mol}$$