Lec 11-supplement: Scaling analysis of irreversible homogeneous reaction in a liquid

* problem:

$$D_A \frac{\partial^2 c_A}{\partial y^2} - k c_A = 0 \qquad c_A(y=L) = c_0$$

$$\frac{\partial c_A}{\partial y}(y=0) = 0$$

* solution:

$$c_A = c_0 \frac{\cosh(y/\lambda)}{\cosh(L/\lambda)} \qquad \lambda = \sqrt{\frac{D_A}{k}}$$

* OOM analysis:

$c_A \sim c_0$, $y \sim L$ ← $y \sim \lambda$ is also an ok length scale, but it zooms into the BL. Not good for plot.

* Dimensional analysis:

\# vars: c_A, y, D_A, k, L, c_0 = 6

(c_A ← dependent var; y ← independent var; D_A, k, L, c_0 ← params)

\# dimensions: length, time, moles = 3
(same fundamental unit as mass)

\# groups: 3

* Scaling analysis

let $\theta = \frac{c_A}{c_0}$, $\eta = y/L$

- problem (ODE): $D_A \cdot \dfrac{\partial^2 (C_o \theta)}{\partial (\eta L)^2} - k C_o \theta = 0$

$$D_A \cdot \frac{C_o}{L^2} \frac{\partial^2 \theta}{\partial \eta^2} - k C_o \theta = 0$$

$$\frac{\partial^2 \theta}{\partial \eta^2} - \frac{k L^2}{D_A} \theta = 0$$

$$Da = \frac{k L^2}{D_A} = \frac{k}{D_A / L^2} = \frac{\text{reaction rate}}{\text{diffusion rate}} = \frac{1/\text{time}}{1/\text{time}}$$

Damköhler number

(note: Da changes w/ order of reaction.)

$$\boxed{\frac{\partial^2 \theta}{\partial \eta^2} - Da\, \theta = 0}$$

- BC1 & BC2:

$$C_o \theta (\eta L = L) = C_o \Rightarrow \boxed{\theta(\eta = 1) = 1}$$

$$\frac{\partial (C_o \theta)}{\partial (\eta L)} (\eta L = 0) = 0 \Rightarrow \boxed{\frac{\partial \theta}{\partial \eta} (\eta = 0) = 0}$$

- Solution:

$$C_A = C_o \frac{\cosh(y/\lambda)}{\cosh(L/\lambda)} \qquad \lambda = \sqrt{\frac{D_A}{k}}$$

$$\theta \cancel{C_o} = \cancel{C_o} \frac{\cosh(L\eta/\lambda)}{\cosh(L/\lambda)} \qquad \frac{L}{\lambda} = \sqrt{\frac{k L^2}{D_A}} = \sqrt{Da}$$

$$\boxed{\theta = \frac{\cosh(\eta\, Da^{1/2})}{\cosh(Da^{1/2})}}$$

- limits :

  - Da<<1 → slow reaction, fast diffusion.

$$\cosh(x) \approx 1 + \frac{x^2}{2} + \ldots \qquad x \ll 1$$

$$\theta \approx \frac{1 + \eta^2 Da/2}{1 + Da/2} \approx \frac{2 + \eta^2 Da}{2 + Da}$$

$$\boxed{\theta \approx 1} \quad \text{as } Da \to 0$$

  - Da >> 1 → fast reaction, slow diffusion

$$\cosh(x) = \frac{e^x - e^{-x}}{2}$$

$$\lim_{x \to \infty} \cosh(x) = \frac{e^x}{2}$$

$$\theta \approx \frac{\frac{1}{2}\exp(\eta Da^{1/2})}{\frac{1}{2}\exp(Da^{1/2})} = \exp(\eta Da^{1/2} - Da^{1/2})$$

$$\boxed{\theta \approx \exp(Da^{1/2}(\eta - 1)) \quad \text{as } Da \to \infty}$$