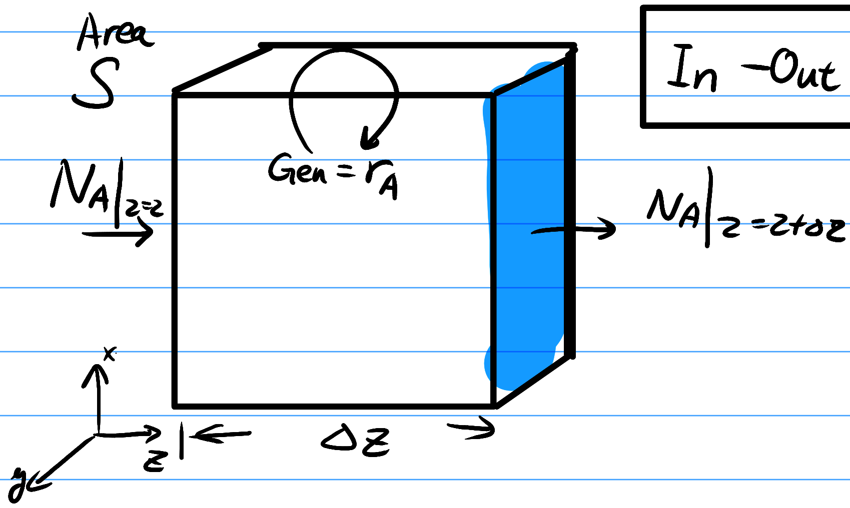
CHE 318 Lecture 09
Jan-21-2026

U.S.S mass transport



$$\boxed{\text{In} - \text{Out} + \text{Gen} = \text{Acc}}$$

Derivation of govern eqn

$$N_A|_{z=z} - N_A|_{z=z+\Delta z} = -\left(\frac{N_A|_{z+\Delta z} - N_A|_{z}}{\Delta z}\right)\cdot \Delta z$$

$\Downarrow$ Def. of derivative

$$= -\frac{\partial N_A}{\partial z}\cdot \Delta z$$

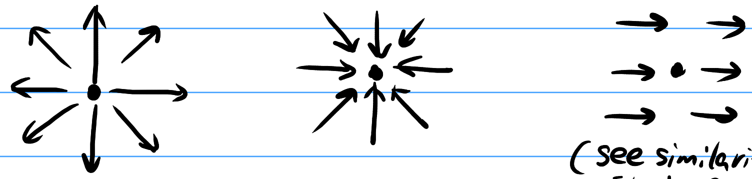
$$\Rightarrow \quad \frac{\partial c_A}{\partial t} = -\nabla \cdot N_A + r_A$$

1D $\quad \dfrac{\partial c_A}{\partial t} = -\dfrac{\partial N_A}{\partial z} + r_A$

Divergence operator $\nabla \cdot$ vector $\Rightarrow$ scalar

$$\nabla \cdot \vec{N}_A = \frac{\partial \vec{N}_A}{\partial x} + \frac{\partial \vec{N}_A}{\partial y} + \frac{\partial \vec{N}_A}{\partial z}$$

$\nabla \cdot \vec{N}_A > 0$ $\nabla \cdot \vec{N}_A < 0$ $\nabla \cdot \vec{N}_A = 0$



(see similarity with 1D S.S)

Gradient ∇ scalar $\rightarrow$ gradient

$$\nabla C \rightarrow \left(\frac{\partial c}{\partial x}, \frac{\partial c}{\partial y}, \frac{\partial c}{\partial z}\right)$$

Laplace operator ∇^2 scalar $\rightarrow$ scalar

$$\nabla^2 c \rightarrow \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2}$$

Special cases for U.S.S

$$\boxed{\frac{\partial c}{\partial t} = r_A - \nabla \cdot (-D_{AB} \nabla C_A + C_A v_m)}$$

Only 1 governing eq, different simplification

① Fick's second law

$$\begin{cases} v_m = 0 \Rightarrow \text{EMCD flux} \\ D_{AB} \text{ constant} \\ r_A = 0 \end{cases}$$

$$\frac{\partial c}{\partial t} = 0 - \nabla \cdot (-D_{AB} \nabla C_A + 0)$$

no negative sign $\rightarrow$ $= D_{AB} \nabla^2 C_A \Longrightarrow$ Fick's 2nd law

Fick's 1st law $J_{Az}^* = -D_{AB} \frac{\partial C_A}{\partial z}$

↑ negative sign

② Constant D_{AB} (no other simplification)

$$\frac{\partial c_A}{\partial t} = D_{AB}\nabla^2 c_A - \nabla\cdot(c_A \vec{v}_m) + r_A$$

$$\nabla\cdot(\lambda\vec{u}) = \boxed{\nabla\lambda}\cdot\boxed{\vec{u}} + \boxed{\lambda}\,\boxed{\nabla\cdot\vec{u}}$$

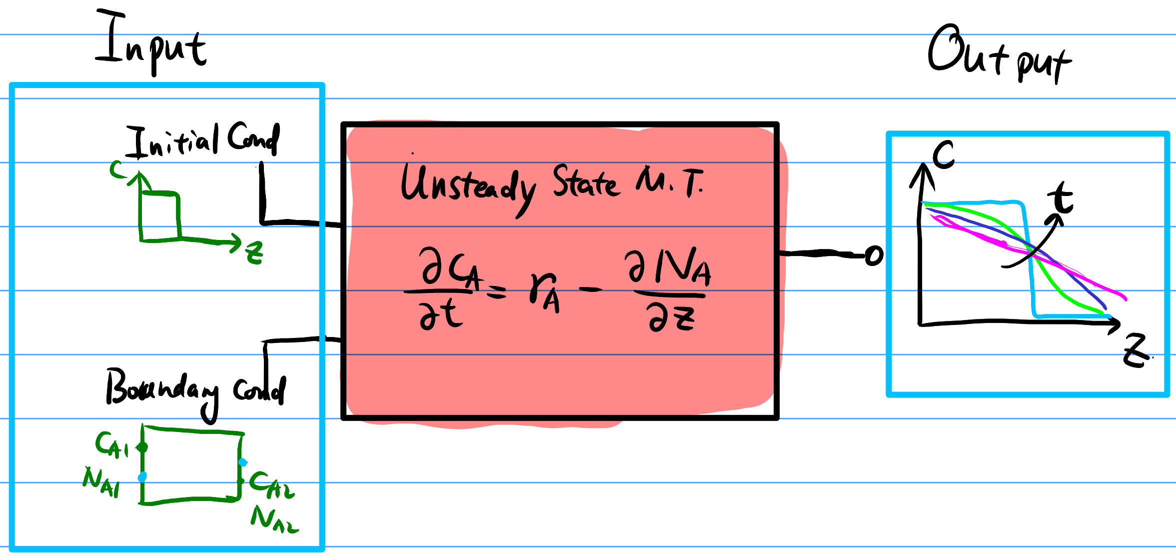
vector

scalar

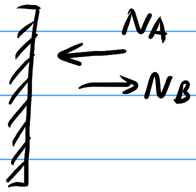
$$= D_{AB}\nabla^2 c_A - c_A\nabla\cdot\vec{v}_m - \nabla c_A\cdot\vec{v}_m + r_A$$

③ case ② But incompressible $(\nabla\cdot\vec{v}_m = 0)$

$$\frac{\partial c_A}{\partial t} = D_{AB}\nabla^2 c_A - \nabla c_A\cdot\vec{v}_m + r_A$$



B.C for reaction



$$xA \longrightarrow yB + wD$$

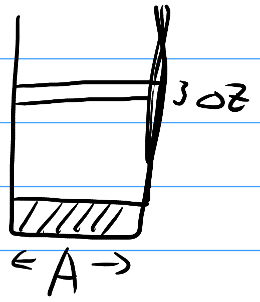
solid

$$\frac{N_A}{x} = -\frac{N_B}{y}$$

$$\underset{A}{CH_4(g)} \longrightarrow \underset{\text{coke}}{C(s)} + \underset{B}{4H(g)}$$ (assumption, not real reaction)

$$N_A = r_A$$
$$N_B = -4\,r_A$$
$$\Rightarrow \frac{N_A}{1} = -\frac{N_B}{4}$$

Solving U.S.S for stagnant B



Governing Eq (M.B)

$$\frac{\partial C_A}{\partial t} = -\frac{\partial N_A}{\partial z}$$

$$N_A = -C_T D_{AB}\frac{\partial x_A}{\partial z} + x_A(N_A+N_B)$$

Cannot directly say $N_B = 0$!

Constraints between N_A & N_B

$$\frac{\partial C_T}{\partial t} = -\frac{\partial N_T}{\partial z} = -\frac{\partial N_A}{\partial z} - \frac{\partial N_B}{\partial z} = 0$$

$$\frac{\partial N_A}{\partial z} = -\frac{\partial N_B}{\partial z} \qquad N_T \text{ is constant}$$

B.C.s

$x_A(z=0,t) = x_{A0}$ $\qquad x_A(L,t) = 0$

$N_B(z=0,t) = 0$ $\longrightarrow$ $N_A(0,t) = -\frac{C_T D_{AB}}{1-x_{A0}}\frac{\partial x_A}{\partial z}\Big|_{z=0}$

$z=0$ $\qquad$ No flux BC

$$\frac{\partial C_A}{\partial t} = C_T\frac{\partial x_A}{\partial t} = -\frac{\partial\left(-C_T D_{AB}\frac{\partial x_A}{\partial z}\right)}{\partial z} - \frac{\partial\left[x_A\cdot(N_A+N_B)\right]}{\partial z}$$

2 parts

$$= -C_T D_{AB}\frac{\partial^2 x_A}{\partial z^2} - \frac{\partial x_A}{\partial z}\cdot(N_A+N_B) - x_A\cancel{\frac{\partial(N_A+N_B)}{\partial z}}$$

What is $N_T = N_A + N_B$?

$$N_T(z\neq 0,t) = N_T(z=0,t) = N_A(0,t) + \cancel{N_B(0,t)}$$

$$= -\frac{C_T D_{AB}}{1-x_{A0}}\frac{\partial x_A}{\partial z}\Big|_{z=0}$$

Not a constant over t !

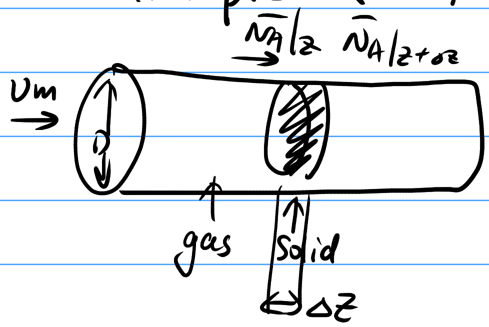
Final expression for Govern. Equ.

$$\frac{\partial x_A}{\partial t} = +D_{AB}\frac{\partial^2 x_A}{\partial z^2} + \left[\frac{D_{AB}}{1-x_{A0}} \underbrace{\left.\frac{\partial x_A}{\partial z}\right|_{z=0}}_{\text{inital gradient !}}\right]\frac{\partial x_A}{\partial z}$$

And initial conditions

$x_A(z\neq 0, 0) = 0$ Analytical solution exhists

Example 2 Reaction through catalyst wall



Reaction & M.T.

In the catalyst region Rate of reaction
$r = k(C_{As} - C_A)$

$$In - Out + \boxed{Gen}^{\neq 0} = Acc$$

$$\frac{\pi D^2}{4}\left(N_A|_z - N_A|_{z+\Delta z}\right) + \pi D \cdot \Delta z \cdot k(C_{As} - C_A)$$

$$= \frac{\pi D^2}{4} \cdot \frac{\partial C_A}{\partial t}$$

$$\hookrightarrow \quad -\frac{\partial N_A}{\partial z} + \left(\frac{4k}{D}\right)(C_{As} - C_A) = \frac{\partial C_A}{\partial t}$$

Use flux eq with v_m (easier!)

$$N_A = -D_{AB}\frac{\partial C_A}{\partial z} + C_A \cdot v_m$$

Constant v_m case

$$\frac{\partial N_A}{\partial z} = -D_{AB}\frac{\partial^2 C_A}{\partial z^2} + \frac{\partial C_A}{\partial z} v_m$$

$$\Downarrow$$

$$\frac{\partial C_A}{\partial t} = -\left(-D_{AB}\frac{\partial^2 C_A}{\partial z^2} + \frac{\partial C_A}{\partial z} v_m\right) + \frac{4k}{D}(C_{As} - C_A)$$

1) Need initial & BC
2) Numerical integration