

CHE318 L15

Feb -04 2026

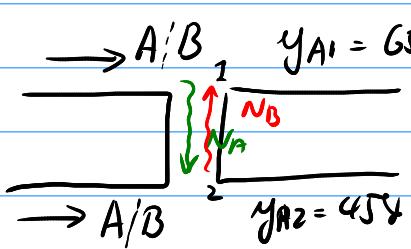
Recap: Boundary condition

$$\downarrow \quad k = \frac{C_{\text{interface 1}}}{C_{\text{interface 2}}}$$

$$k'_c: \text{M.T. coefficient} \quad N_A = k'_c(C_{Li} - C_i)$$

Various  $k_c$  forms:  $k_c \quad k'_c \quad k_x \quad k'_x \quad k_y \quad k'_y$

Solution to Q1



1 → 2

$$\begin{aligned} N_A &= k'_y \cdot (y_{A1} - y_{A2}) \\ &= 1.5 \times 10^{-4} \times (0.65 - 0.45) \\ &= 3.0 \times 10^{-5} \text{ kg mol/(m}^2 \cdot \text{s)} \end{aligned}$$

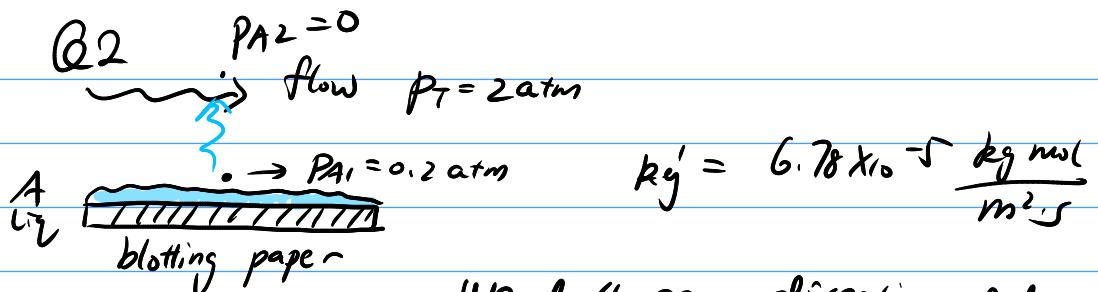
$$N_B = -N_A \quad 2 \rightarrow 1$$

We realize  $k'_y$  is dependent on total pressure!

$$k'_y \rightarrow k'_c \quad k'_y = k'_c \cdot C_T = k'_G \cdot P_T$$

$$k'_G = \frac{k'_y}{P_T} = \frac{1.5 \times 10^{-4}}{2000 \text{ kPa}} = 2.14 \times 10^{-7} \text{ kg mol/(m}^2 \cdot \text{s} \cdot \text{kPa})$$

$$k'_c = \frac{k'_y}{C_T} = \frac{k'_y}{P_T} \cdot R_T = k'_G \cdot R_T = \underbrace{6.65 \times 10^{-4} \text{ m/s}}_{\text{superficial vel}}$$



$$k_y' = 6.78 \times 10^{-5} \frac{\text{kg mol}}{\text{m}^2 \cdot \text{s}}$$

We don't care direction of  $N_A$  in fluid

All mass transfer coefficient  $\Rightarrow$  lumped

$$N_A = k_y' \cdot \frac{l}{y_{Bm}} \cdot (y_{A1} - y_{A2})$$

$\leftarrow$  Stagnant B

$$y_{Bm} \approx \frac{y_{B1} + y_{B2}}{2} = 0.95 \quad y_{A1} = 0.1 \quad y_{A2} = 0$$

$$N_A = 6.78 \times 10^{-5} \cdot \frac{1}{0.95} \cdot 0.1 = 7.14 \times 10^{-6} \text{ kg mol/(m}^2 \cdot \text{s)}$$

$$k_y = k_y' / y_{Bm} = 7.14 \times 10^{-5} \text{ kg mol/(m}^2 \cdot \text{s})$$

$$k_G = k_y / p_T = 3.57 \times 10^{-5} \text{ kg mol/(m}^2 \cdot \text{s, atm})$$

Q3



$$\overline{\text{Flux}} = \frac{[\text{weight}]}{[\text{molar mass}][\text{time}]}$$

$$N_A \cdot 4\pi r_0^2 = \frac{m_1 - m_2}{M_A \cdot \delta t} = k_L (C_{AS} - 0)$$

$$k_L = \frac{1}{4\pi r_0^2} \cdot \frac{m_1 - m_2}{C_{AS} \cdot M_A \cdot \delta t}$$

≈ ← Get from solubility

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## Theories of Mass Transfer Coefficient

Different theories of  $k_c'$

① Film theory



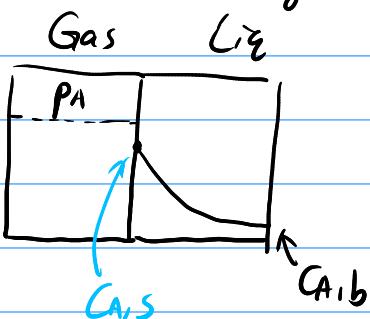
$$N_A = \bar{J}_A z^* \\ = \frac{D_{AB}}{\delta_f} (C_{A,s} - C_{A,b}) \\ k_c' = \frac{1}{\delta_f}$$

1) Physically intuitive ✓

2)  $k_c' \propto D_{AB}^{1/3}$  ✗ (Chilton - Colburn result)  
 $k_c' \propto D_{AB}^{-1/3}$

② Penetration theory

Dankwerts 1950



$$\text{Solve } D_{AB} \frac{\partial^2 C_A}{\partial z^2} : \frac{\partial C_A}{\partial t}$$

$$\text{B.C. } \begin{cases} C_A(z=0) = C_{A,s} \\ C_A(z=\infty) = C_{A,b} \end{cases}$$

Solution

$$\frac{C_A(z,t) - C_{A,b}}{C_{A,s} - C_{A,b}} = 1 - \operatorname{erf}\left(\frac{z}{\sqrt{4D_{AB}t}}\right)$$

$$N_A = -D_{AB} \frac{\partial C_A}{\partial z} \Big|_S$$

$$\operatorname{erf} = \frac{2}{\sqrt{\pi}} \int_0^z e^{-x^2} dx$$

$$= \sqrt{\frac{D_{AB}}{\pi t}} (C_{A,s} - C_{A,b})$$

$$\frac{\partial C_A}{\partial z} = -\frac{2}{\sqrt{\pi}} \cdot (C_{A,s} - C_{A,b}) \cdot \frac{1}{\sqrt{4D_{AB}t}} \cdot e^{-\left(\frac{z}{\sqrt{4D_{AB}t}}\right)^2}$$

depend on time

If contact time is short

$$\int t^{-\frac{1}{2}} = 2t^{\frac{1}{2}} + C_{\text{const}}$$

$$\Rightarrow N_A = \frac{\int_0^{t_0} N_A|_{z=0} dt}{t_L} = \frac{\sqrt{\frac{4D_{AB}}{\pi t_0}} (C_{A,S} - C_{A,b})}{k_c'}$$

$t_0$  = penetration time scale

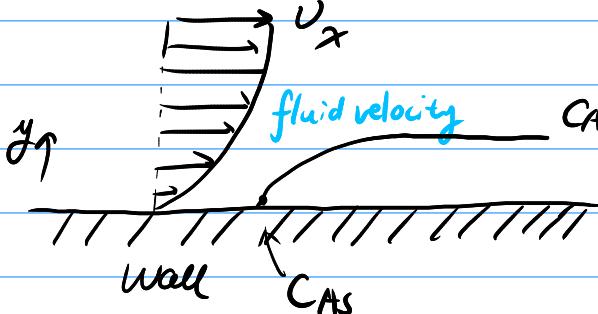
Penetration theory  $\Rightarrow k_c' \propto \sqrt{D_{AB}}$  (close to practical  
 $n = 0.8 \text{ to } 0.9$ )

Dankwes  $\Rightarrow$  (modified factor for turbulent m.t.  
 | surface renewal)

$$k_c' = \sqrt{D_{AB} \cdot s}$$

↑ renewal factor

### ③ Boundary layer theory



① Developed for laminar flow

② Intuition =

- 1) NA has  $x, y$  component
- 2)  $\rightarrow x$  convection only  
 $\uparrow y$  diffusion / conv.

3) velocity ( $v_x, v_y$ ) known

Mass balance

$$\text{In}_x + \text{In}_y - \text{Out}_x - \text{Out}_y = \text{Acc}$$

$$v_x \frac{\partial C_A}{\partial x} + v_y \frac{\partial C_A}{\partial y} = D_{AB} \frac{\partial^2 C_A}{\partial y^2}$$

$\underbrace{v_x \frac{\partial C_A}{\partial x} + v_y \frac{\partial C_A}{\partial y}}$

$\downarrow$  Diffusive div

$\underbrace{v_x \frac{\partial C_A}{\partial x}}$

Convection div

Boundary Condition

$$\begin{cases} \frac{\partial u_x}{\partial y} \Big|_{y=0} = 0 \\ \frac{C_A - C_{As}}{C_{A,\infty} - C_{As}} \Big|_{y=0} = 0 \end{cases}$$

$$\begin{cases} \frac{\partial u_x}{\partial y} \Big|_{y=\infty} = 1 \\ \frac{C_A - C_{As}}{C_{A,\infty} - C_{As}} \Big|_{y=\infty} = 1 \end{cases}$$

Laminar flow,  $u_x$  profile is

$$N_{Re,I} = \frac{\rho \cdot U_{\infty} \cdot \rho}{\mu}$$

$$N_{Sc} = 1 \quad \left( \frac{\partial u_x}{\partial y} \Big|_{y=0} = 0.332 \frac{U_{\infty}}{L} \sqrt{N_{Re,I}} \right) \quad \text{Reynolds Number}$$

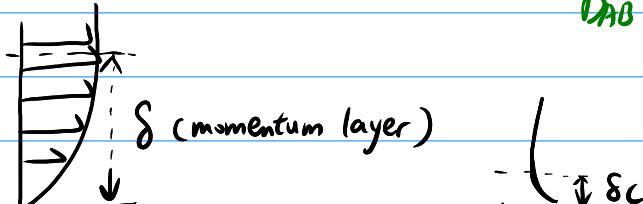
Same boundary  $\left( \frac{\partial C_A}{\partial y} \Big|_{y=0} = \frac{0.332}{L} \sqrt{N_{Re,I}} \cdot (C_{A,\infty} - C_{As}) \right)$

$$N_A = -D_{AB} \left( \frac{\partial C_A}{\partial y} \Big|_{y=0} \right) \Rightarrow k'_c = \frac{0.332 D_{AB} \sqrt{N_{Re,I}}}{L}$$

Steady State

this is when  $N_{Sc} = 1$

$$N_{Sc} = \frac{L \cdot k'_c}{D_{AB}} \quad \text{Schmidt number}$$



We have in general Boundary thickness relation

$$\frac{\delta}{\delta_c} = N_{Sc}^{-\frac{1}{3}}$$

General eqn for boundary layer theory

$$\frac{k'_c \cdot L}{D_{AB}} = 0.332 N_{Re,I}^{1/2} N_{Sc}^{1/3}$$

$$N_{Sc} \propto \frac{1}{D_{AB}} \Rightarrow k'_c \propto D_{AB}^{-\frac{2}{3}} \quad (\text{very close to practical results})$$