PRACTICAL SESSIN

⑥

GAS/LIQUID REACTORS

2 FILM THEORY

$$r'''' = \frac{P_A}{\frac{1}{K_G a} + \frac{H_A}{K_L a E} + \frac{H_A}{K_e' f_L}}$$

volumetric overall rate of change (kmol/m^3 s)

P_A = partial pressure of A

K_G, K_L = mass transfer coefficients

a = interfacial gas/liquid area per unit of volume

H_A = Henry's constant

K_e' = pseudo first order kinetic constant

f_L = fraction of liquid volume

EXERCISE 1

$$A_{(g\to l)} + 2B_{(l)} \rightarrow C_{(l)} \qquad \tau = K_c C_A C_B^2$$

third order reaction!

! Problem

The analysis carried out in the classroom was done assuming a second order reaction $\tau = K_c C_A C_B$
On the basis of this kinetics, a pseudo-1st order kinetic constant was defined: $K_c' \overset{def}{=} K_c C_B$

Now we have a 3rd order reaction, so in principle the results obtained in the classroom cannot be applied

Idea 💡 (simplification):

We define the reaction rate as $\tau = \underbrace{K_c C_B}_{K_c^*} \cdot C_A C_B$

$$\tau = K_c^* C_A C_B$$

If we proceed in this way,
by introducing this K_c^* pseudo
kinetic constant, we have a pseudo 2nd order reaction
rate and we can continue according with the usual procedure

$$\tau = K_c^* C_A C_B \longrightarrow \tau = K_c' C_A$$

where $K_c' = K_c^* C_B = K_c C_B^2$

$$\Downarrow$$

$$\tau''' = \frac{P_A}{\frac{1}{K_G a} + \frac{H_A}{K_L a E} + \frac{H_A}{K_c' f_L}}$$

of course this
is a trick introduci
errors!!

The overall rate can be determined if we know p_A and C_B (which is hidden in the k_l' constant). This is fine because p_A and C_B will be available from the mass balance equations at the reactor level

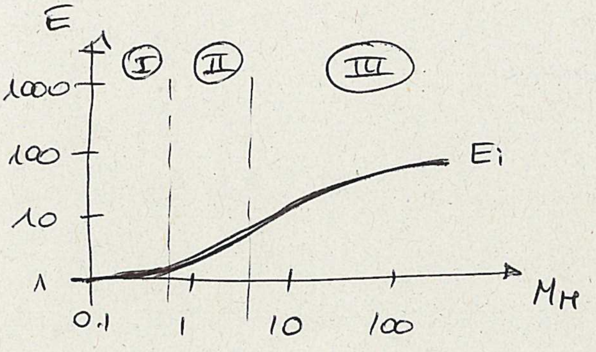
However we have to calculate E, the enhancing factor

$$E = E(M_H, E_i) \qquad \begin{cases} M_H = \text{HATTA modulus} \\ E_i = E \text{ @ infinitely fast chemistry} \end{cases}$$

$$M_H \overset{\text{def}}{=} \frac{\sqrt{k_l^* C_B \mathcal{D}_A}}{k_L} \qquad E_i = 1 + \frac{\mathcal{D}_B}{\mathcal{D}_A} \frac{C_B H_A}{b \, \boxed{p_{AI}}}$$

stoichiom. coefficient

partial pressure at the interface



analytical expressions

$$E = \begin{cases} \text{if } M_H < 1 & \begin{cases} \text{if } M_H < 0.3 & E = 1 \\ \text{if } M_H > 0.3 & E = 1 + \dfrac{M_H^2}{3} \end{cases} \\ \text{if } M_H > 1 & \begin{cases} \text{if } M_H < 5E_i & E = M_H \\ \text{if } M_H > 5E_i & E = E_i \end{cases} \end{cases}$$

<u>Problem</u>: $E_i = 1 + \dfrac{\mathcal{D}_B}{\mathcal{D}_A} \dfrac{C_B H_A}{b \, \boxed{p_{AI}}} \longrightarrow$ we do not this value

To determine p_{AI} we can exploit the fact that the overall rate of change r'''' is also equal to the rate of change associated to the mass transfer in the gaseous phase

$$\underset{\substack{\uparrow\\ \text{overall}\\ \text{rate of}\\ \text{change}}}{r''''} = r''''_{\substack{gas\\layer}} = K_G a \left(p_A - p_{AI} \right)$$

$$p_{AI} = p_A - \frac{r''''}{K_G a}$$

but r'''' is a function of p_{AI} itself, so we need an iterative procedure

Iterative procedure

1) First guess of p_{AI} $(p_{AI} < p_A)$

2) Calculation of E_i

3) Calculation of E

4) Calculation of r''''

5) Estimation of a new value of p_{AI}

$$p_{AI} = p_A - \frac{r''''}{K_G a}$$

NO 6) Convergence ?

↓ YES

STOP

can be also written as

$$\underbrace{\frac{p_A}{R_{GAS} + R_{LIQ} + R_{KIN}}}_{r''''} - \underbrace{K_G a \left(p_A - p_{AI} \right)}_{r''''_{gas}} = 0$$

OPERATING LINE

$$\begin{cases} \dfrac{dF_A}{dV} = -r'''' \\[2ex] \dfrac{dF_B}{dV} = -b r'''' \end{cases} \longrightarrow \frac{dF_B}{dV} = +b \frac{dF_A}{dV}$$

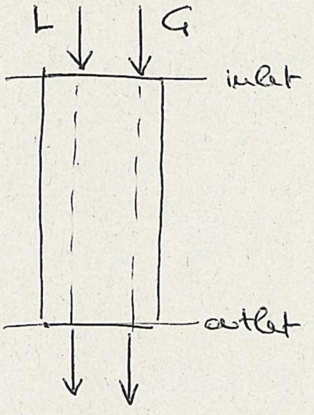
$$\frac{F^L_{TOT}}{C_{TOT}} \frac{dC_B}{dV} = +b \frac{F^G_{TOT}}{p_{TOT}} \frac{dp_A}{dV}$$

$$dC_B = +b \frac{F^G_{TOT}}{F^L_{TOT}} \frac{C_{TOT}}{p_{TOT}} dp_A$$

$$C_B = C_B^{in} + b \frac{F^G_{TOT}}{F^L_{TOT}} \frac{C_{TOT}}{p_{TOT}} \left(p_A - p_A^{in} \right)$$

EXERCISE 2

CO-CURRENT
BUBBLE TOWER



$$\begin{cases} p_A^{in} = 5000 \text{ Pa} \\ C_B^{in} = 100 \text{ mol/m}^3 \end{cases}$$

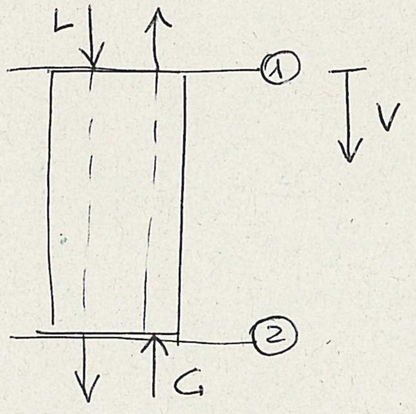
GOVERNING EQUATIONS

$$\begin{cases} \frac{dF_A^G}{dV} = -r'''' \\ \frac{dF_B^L}{dV} = -b r'''' \\ \frac{dF_C^L}{dV} = +r'''' \end{cases} \oplus \text{ ICs}$$

in case of diluted conditions

$$\begin{cases} \frac{dp_A}{dV} = -\frac{p_{TOT}}{F_{TOT}^G} r'''' \\ \frac{dC_B}{dV} = -\frac{C_{TOT}}{F_{TOT}^L} b r'''' \\ \frac{dC_C}{dV} = \frac{C_{TOT}}{F_{TOT}^L} r'''' \end{cases} + IC \begin{cases} p_A(V=0) = p_A^{in} \\ C_B(V=0) = C_B^{in} \\ C_C(V=0) = 0 \end{cases}$$

EXERCISE 3



COUNTER-CURRENT

$$\begin{cases} C_B^{in} = 100 \text{ mol/m}^3 \\ p_A^{out} = ? \end{cases}$$

$$\begin{cases} C_B^{out} = ? \\ p_A^{in} = 5000 \text{ Pa} \end{cases}$$

GOVERNING EQUATIONS

$$\begin{cases} \dfrac{dp_A}{dV} = \dfrac{p_{TOT}}{F_{TOT}^{G}}\,\tau'''' \\ \dfrac{dC_B}{dV} = -\dfrac{C_{TOT}}{F_{TOT}^{L}}\,b\,\tau'''' \\ \dfrac{dC_C}{dV} = \dfrac{C_{TOT}}{F_{TOT}^{L}}\,\tau'''' \end{cases} + \begin{cases} p_A(V=V_{TOT}) = p_A^{in} \\ C_B(V=0) = C_B^{in} \\ C_C(V=0) = 0 \end{cases}$$

BVP BOUNDARY VALUE PROBLEM

SHOOTING METHOD

1) Guess value of p_A^{out}

2) Solve the system of equations as a regular ODE + IC problem

3) Check the error on the section 1

$$\varepsilon = p_A(V=V_{TOT}) - p_A^{in}$$

4) If $\varepsilon <$ threshold? $\xrightarrow{\text{YES}}$ STOP

↓ NO

Guess a new value: $p_{A\,new}^{out} = p_{A\,old}^{out} - \alpha\varepsilon$