PRACTICAL SESSION 7

EXERCISE 1

2 FILM THEORY

$$r = \frac{p_A}{\frac{1}{K_G a} + \frac{H_A}{K_L a E} + \frac{H_A}{K' C_B f_L}}$$

volumetric overall rate of change $[kmol/m^3 s]$

p_A = partial pressure of A

K_G = mass transfer coefficient (gas phase)

K_L = mass transfer coefficient (liquid phase)

a = gas/liquid interfacial area per unit of volume

H_A = Henry's constant

K' = kinetic constant (second order reaction)

f_L = liquid volume fraction

C_B = concentration of specie B

$$A_{(g \to l)} + 2B_{(l)} \longrightarrow C_{(l)}$$

$r = K C_A C_B^2$ third order reaction

$$r = \underbrace{K C_B}_{} \cdot C_A C_B = K' C_A C_B$$

pseudo 2nd order reaction

$K' = K \cdot C_B$

$$r = \frac{p_A}{\frac{1}{K_G a} + \frac{H_A}{K_L a}\frac{1}{E} + \frac{H_A}{k' C_B f_L}}$$

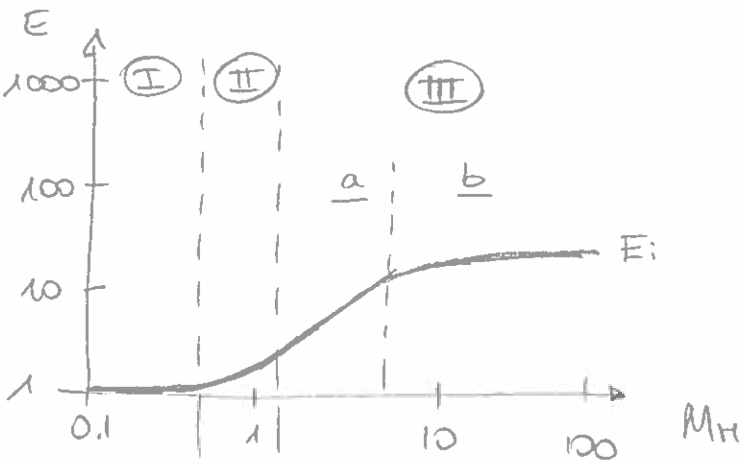
everything is known, but $\frac{1}{E}$ (ENHANCING FACTOR)

$E = E(M_H, E_i)$

- M_H = HATTA MODULUS
- E_i = E @ infinitely fast chemistry

$$M_H \overset{def}{=} \frac{\sqrt{k' \mathcal{D}_A C_B}}{K_L} \qquad E_i = 1 + \frac{\mathcal{D}_B}{\mathcal{D}_A}\frac{C_B H_A}{b\, p_{AI}}$$

b: stoichiometric coefficient; p_{AI}: partial pressure at interface



$E = ?$

- if $M_H < 1$
  - if $M_H < 0.3$ $\quad E = 1$
  - if $M_H > 0.3$ $\quad E = 1 + \frac{M_H^2}{3}$
- if $M_H > 1$
  - if $M_H < 5E_i$ $\quad E = M_H$
  - if $M_H > 5E_i$ $\quad E = E_i$

Problem: $E_i = 1 + \frac{\mathcal{D}_B}{\mathcal{D}_A}\frac{C_B}{b}\frac{H_A}{p_{AI}}$

we do not know this value

$\downarrow$

Solution: iterative procedure

Iterative procedure

1) First guess value of p_{AI} $\quad (p_{AI} \leq p_A)$

2) Calculation of E_i

3) Calculation of E

4) Calculation of r

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

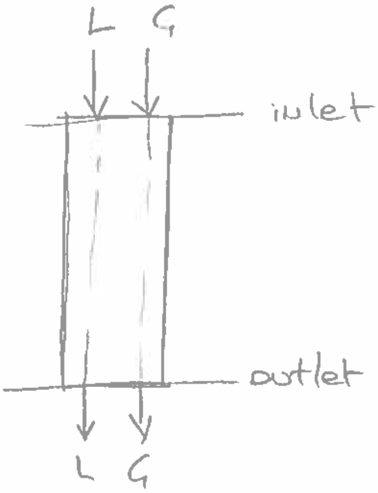
$$r = K_G a (p_A - p_{AI})$$

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

6) Repeat up to convergence

EXERCISE 2

CO-CURRENT BUBBLE TOWER



$$\left\{ \begin{array}{l} p_{A\,in} = 5000 \text{ Pa} \\ C_{B\,in} = 100 \text{ mol/m}^3 \end{array} \right.$$

Governing equations

$$\left\{ \begin{array}{l} \dfrac{dF_A^{(G)}}{dV} = -r \\[2ex] \dfrac{dF_B^{(L)}}{dV} = -b\,r \\[2ex] \dfrac{dF_C^{(L)}}{dV} = r \end{array} \right.$$

in case of diluted conditions

$$\left\{ \begin{array}{l} F_{tot}^{(G)} \dfrac{dy_A}{dV} = -r \\[2ex] F_{tot}^{(L)} \dfrac{dx_B}{dV} = -b\,r \\[2ex] F_{tot}^{(L)} \dfrac{dx_C}{dV} = r \end{array} \right.$$

$$y_A = p_A / P_{TOT}$$

$$x_B = C_B / C_{TOT}$$

$$x_C = C_C / C_{TOT}$$

$$\Longrightarrow \left\{ \begin{array}{l} \dfrac{dp_A}{dV} = -\dfrac{P_{TOT}}{F_{tot}^{(G)}}\, r \\[2ex] \dfrac{dC_B}{dV} = -\dfrac{C_{TOT}}{F_{tot}^{(L)}}\, b\,r \\[2ex] \dfrac{dC_C}{dV} = +\dfrac{C_{TOT}}{F_{tot}^{(L)}}\, r \end{array} \right.$$

system of ODEs with initial conditions

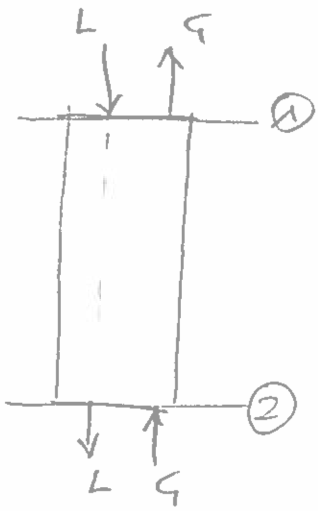
$$\begin{cases} \dfrac{dp_A}{dV} = -\dfrac{P_{TOT}}{F_{tot}^{(G)}} r \\[2ex] \dfrac{dC_B}{dV} = -\dfrac{C_{TOT}}{F_{tot}^{(L)}} b\, r \\[2ex] \dfrac{dC_C}{dV} = +\dfrac{C_{TOT}}{F_{tot}^{(L)}} r \end{cases}$$

$+$

$$\begin{cases} p_A(V=0) = p_A^{in} \\ C_B(V=0) = C_B^{in} \\ C_C(V=0) = 0 \end{cases}$$

EXERCISE 3

COUNTER-CURRENT CONFIGURATION



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

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

system of ODEs with boundary conditions

$$\begin{cases} \dfrac{dp_A}{dV} = +\dfrac{P_{TOT}}{F_{tot}^{(G)}} r \\[2ex] \dfrac{dC_B}{dV} = -\dfrac{C_{TOT}}{F_{tot}^{(L)}} b\, r \\[2ex] \dfrac{dC_C}{dV} = +\dfrac{C_{TOT}}{F_{tot}^{(L)}} r \end{cases}$$

$+$

$$\begin{cases} p_A(V=V_{TOT}) = p_A^{in} \quad A \\ C_B(V=0) = C_B^{in} \\ C_C(V=0) = 0 \end{cases}$$

SHOOTING METHOD ON p_A

1. Guess a value of p_A^{out}

2. Use the following initial condition for pressure of A (instead of Ⓐ)

$$p_A(V=0) = p_A^{out} \quad \text{(guessed)}$$

3. Solve the corresponding system of ODEs with ICs

4. Check the error in terms of the guess

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

5. If the error $\mathcal{E}$ is sufficiently small, solution OK!

6. Otherwise guess a new value

$$p_{A\,new}^{out} = p_{A\,old}^{out} - \alpha \cdot \mathcal{E}$$

under-relaxation factor (must be sufficiently small)

STOP