Problema A

1ª Orden

$$-r_A = \frac{1}{X}\frac{dX}{dt}$$

Partícula Esférica

$V = 150\ mL \Rightarrow C_A = 0{,}1\ M$

$m_c = 0{,}1\ g$

$t = 1$ hora

Exper	d_p (mm)	X
1	0,22	0,932
2	1,85	0,298

a)

$$k'_{ap} = \eta\, k'$$ ← Intrínseca (Reação)

BM batch

$$r'_{A_{ap}} W = \frac{dN_A}{dt} \rightarrow N_{A_0}(1-X)$$

$$-r'_{A_{ap}} W = N_{A_0}\frac{dX}{dt}$$

$$r_X \quad -r'_{A\,ap} = k'_{ap}\, C_{A_0}(1-X)$$

1ª Ordem

Eq. Condensada

$$\int_0^t dt = \frac{V}{W.k'_{ap}} \int_0^X \frac{dX}{1-X}$$

$$t = \frac{V}{W.k'_{ap}} \ln\left(\frac{1}{1-X}\right) \Leftrightarrow$$

$$\Leftrightarrow k'_{ap} = \frac{V}{W.t} \ln\left(\frac{1}{1-X}\right)$$

$$k'_{ap,1} = \frac{0,15}{0,1 \times 60} \ln\left(\frac{1}{1-0,932}\right) = 0,067206$$

$$L/(min.g)$$

$$k'_{ap,2} = \frac{0,15}{0,1 \times 60} \ln\left(\frac{1}{1-0,298}\right) = 0,008846$$

b)

$$\phi = r\sqrt{\frac{k'.\rho_c}{De}}$$

$$\phi_2 = \frac{d_{p2}}{2}\sqrt{\frac{k'.\rho_c}{De}} \qquad \phi_1 = \frac{d_{p1}}{2}\sqrt{\frac{k'.\rho_c}{De}}$$

$$\frac{\phi_1}{\phi_2} = \frac{d_{p1}}{d_{p2}} \Leftrightarrow \phi_1 = \phi_2 \frac{d_{p1}}{d_{p2}}$$

$$\frac{\eta_1}{\eta_2} = \frac{\frac{k'_{ap1}}{k'}}{\frac{k'_{ap2}}{k'}} = \frac{k'_{ap,1}}{k'_{ap,2}}$$

$$\frac{3}{\phi_1^2}\left(\phi_1 \coth(\phi_1) - 1\right) = \eta_1$$

$$\frac{3}{\phi_2^2}\left(\phi_2 \coth(\phi_2) - 1\right) = \eta_2$$

$$\frac{k'_{ap,1}}{k'_{ap,2}} = \frac{\frac{3}{\phi_1^2}\left(\phi_1 \coth(\phi_1) - 1\right)}{\frac{3}{\phi_2^2}\left(\phi_2 \coth(\phi_2) - 1\right)}$$

$$= \frac{\frac{3}{\left(\phi_2 \frac{d_{p1}}{d_{p2}}\right)^2}\left(\phi_2 \frac{d_{p1}}{d_{p2}} \coth\left(\phi_2 \frac{d_{p1}}{d_{p2}}\right) - 1\right)}{\frac{3}{\phi_2^2}\left(\phi_2 \coth(\phi_2) - 1\right)}$$

$$f(\phi_2) = \frac{\phi_2 \frac{d_{p1}}{d_{p2}} \coth\left(\phi_2 \frac{d_{p1}}{d_{p2}}\right) - 1}{\left(\frac{d_{p1}}{d_{p2}}\right)^2 \left(\phi_2 \coth(\phi_2) - 1\right)} - \frac{k'_{ap1}}{k'_{ap2}} = 0$$

$$\phi_2 = 77{,}79$$

$$\phi_1 = \phi_2 \frac{dp_1}{dp_2} = 9{,}251$$

coth ≈ 1

$$\eta_2 = \frac{3}{77{,}79^2}\left(77{,}79 - 1\right) = 0{,}012855)$$

$$\eta_1 = \eta_2 \frac{k'_{ap1}}{k'_{ap2}} = 0{,}097665$$

c) k' e De

$$k' = \frac{k'_{ap1} - k'_{ap2}}{\eta_1 - \eta_2} = 0{,}6881 \ L/(min \cdot g)$$

$$\phi_1 - \phi_2 = \frac{dp_1}{2}\sqrt{\frac{k' \rho_c}{De}} - \frac{dp_2}{2}\sqrt{\frac{k' \cdot \rho_c}{De}} \Leftrightarrow$$

$$\Leftrightarrow \frac{De}{k' \cdot \rho_c} = \left(\frac{\frac{dp_1 - dp_2}{2}}{\phi_1 - \phi_2}\right)^2$$

$$D_e = 1,9459 \times 10^{-9} \ m^2/s$$

d)

$$\phi_3 = 0,001 \sqrt{\frac{0,6881 \times 1,2 \times 10^3}{1,9459 \times 10^{-9}}} = 84,098$$

$$\eta_3 = \frac{3}{84,098}\left(84,098 \cdot \underbrace{\coth(84,098)}_{\approx 1} - 1\right) =$$

$$= 0,03525$$

$$k'_{ap,3} = k' \eta_3 = 0,03525 \times 0,6881 =$$

$$= 0,02425 \ L/(g \cdot min)$$

e)

BM Leito fixo

$$dW = \frac{dF_A}{r'_{ap}} = F_{A0} \frac{dX}{-r'_{ap}}$$

eq. condensada $\quad dW = C_{A0} \nu_0 \dfrac{dX}{k'_{ap} C_{A0} (1-X)} =$

$$= \frac{\nu_0}{k'_{ap}} \frac{dX}{1-X}$$

$$W = \frac{\nu_0}{k'_{ap}} \int_0^X \frac{dX}{1-X} = \frac{\nu_0}{k'_{ap}} \ln\left(\frac{1}{1-X}\right)$$

$$X = 1 - e^{-\frac{k'_{ap}}{\nu_0} W}$$

$$V_R = V_{cat} + V_{vazios} = \frac{W}{\rho_c} + \varepsilon_b V_R$$

$$\varepsilon_b = 0{,}48$$

$$\left.\begin{array}{l} \phi_4 \\ \eta_4 \end{array}\right\} k'_{ap,4} = 0{,}009772 \ L/(\min \cdot g)$$

$$W = \rho_c (1-\varepsilon_b) \frac{\pi d^2}{4} L =$$

$$= 1{,}2 \times 10^6 (1 - 0{,}48) \frac{\pi \times 0{,}2^2}{4} \times 2 =$$

$$= 39\,207 \ g$$

$$X \approx 1$$

Problema B

Leito fixo

Partícula Esférica

$N_{tubos} = 50$

$d_p = 6\ mm$

$L = 1\ m$

$D = 2,5\ cm$

$\nu_0 = 100\ L/min$

$T = 673\ K$

$P = 1\ atm$

$X = 0,35$

a) $V_R = V_{cat} + V_{vazios} = \dfrac{W}{\rho_c} + \varepsilon_b V_R$

$V_R = N_{tubos} V_{Tubos} = N_{Tubos} \dfrac{\pi D^2}{4} \times L =$

$= 0,024544\ m^3$

$W = \underset{1,3\ g/cm^3}{\rho_c} (1 - \underset{0,46}{\varepsilon_b}) V_R = 17,23\ Kg$

b)

B. M.

$$dW = F_{A_0} \frac{dX}{-r_{A,obs}} \qquad \Bigg| \quad -r'_{A,obs} = k'_{obs} C_{A_0} (1-X)$$

Eq. Condensada

$$dW = F_{A_0} \frac{dX}{k'_{obs} C_{A_0} (1-X)}$$

$$W = \frac{\nu_0}{k'_{obs}} \int_0^X \frac{dX}{1-X}$$

$$k'_{obs} = \frac{\nu_0}{W} \ln\left(\frac{1}{1-X}\right)$$

$$k'_{obs} = 0{,}0025 \; L/(min.g)$$

c)

$$k'_{ap} = \eta k'$$

$$\phi = 0{,}03 \sqrt{\frac{0{,}018 \times 1{,}3 \times 10^6}{1000 \times 60 \times 1{,}3 \times 10^{-8}}} = 16{,}4$$

$$\eta = \frac{3}{16{,}4} \Big(16{,}4 \cdot \underbrace{\coth(16{,}4)}_{\simeq 1} - 1 \Big) = 0{,}171$$

$$k'_{ap} = 0{,}171 \times 0{,}018 = 0{,}00309 \ L/(g \cdot min)$$

d)

$$k'_c (C_{AB} - C_{AS}) = -r'_A = k'_{ap} \cdot C_{AS}$$

$$C_{AS} = C_{AB} \frac{k'_c}{k'_{ap} + k'_c}$$

$$k'_c = \frac{k'_{obs} \, k'_{ap}}{k'_{ap} - k'_{obs}} = 0{,}013166 \ L/(min \cdot g)$$

Converter para m/s para usar no nº Adimensional Sherwood

$$k_c = k'_c \times a = k'_c \times \frac{d_p \times \rho_c}{6} =$$

$$= 0{,}013166 \ \frac{L}{min \cdot g} \times 13 \ \frac{g}{dm^2}$$

$$v = \frac{V_{tubo}}{A_c} = \frac{V_0 / N_{tubos}}{\varepsilon_b \, A_{tubo}} = \frac{100}{50 \times 0{,}46 \times \frac{\pi \, 0{,}25^2}{4}} =$$

$$= 0{,}14762 \ m/s$$

$$Re = 410 = \frac{u \cdot d_p}{V(1-\varepsilon_b)}$$

$$Sh = Re^{1/2} \cdot Sc^{1/3}$$

$$\frac{k_c \, d_p}{D_A} \cdot \frac{\varepsilon_b}{1-\varepsilon_b} = Re^{1/2} \cdot \frac{V^{1/3}}{D_A^{1/3}}$$

$$D_A^{2/3} = \frac{k_c \cdot d_p}{Re^{1/2} \, V^{1/3}} \, \frac{\varepsilon_b}{1-\varepsilon_b}$$

$$D_A = 9{,}66 \times 10^{-9} \ m^2/s$$

e)

$$\left.\begin{array}{l} \phi >> 3 \\ \eta << 1 \end{array}\right\}$$ Fortes limitações difusionais intraparticulares.

A cinética não é o passo limitante

Ao contrário → Cinética

$k'_c > k_{ap}$ ← Não há limitações difusionais externas.

Ao contrário ($k'_c < k_{ap}$) → Há limitações externas

Reator em regime difusional interno