ERQ I – Teste 1 2023 Resolução

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Conteúdo

Questão 1

- Fase liq
- A + B $\longrightarrow$ C
- 3 reatores batch
- $V = 5\,\mathrm{m}^3$
- $C_{A0} = C_{B0} = 1\,\mathrm{M}$
- $t_d = 2\,\mathrm{h}$
- $M_A = 60\,\mathrm{g/mol}$
- $M_B = 130\,\mathrm{g/mol}$
- Caso n res a): $k = 2.8\,\mathrm{dm}^3\,\mathrm{mol}^{-1}\,\mathrm{h}^{-1}$

Q1 a.

Lei cin

Resposta

$$-r_A = k\,(C_A\,C_B) = k\,(C_{A0}(1-X)\,C_{A0}(1-X)) =$$
$$= k\,C_{A0}^2(1-X)^2$$

Q1 b.

eq da curva $X = f(t)$

Resposta

$X = f(t)$:

$$-r_A\,V = (k\,C_{A0}^2(1-X)^2)\,V = k\,C_{A0}^2(1-X)^2\,V =$$
$$= \frac{\mathrm{d}N_A}{\mathrm{d}t} = \frac{\mathrm{d}(N_{A0}(1-X))}{\mathrm{d}t} = N_{A0}\frac{\mathrm{d}(1-X)}{\mathrm{d}t} \implies$$

$$\implies \int_0^t k\,C_{A0}^2(1-X)^2\,V\;\mathrm{d}t = k\,C_{A0}^2\,V\int_0^t \mathrm{d}t = k\,C_{A0}^2\,V\,t =$$

$$= \int_1^{1-X} N_{A0}\frac{\mathrm{d}(1-X)}{(1-X)^2} =$$
$$= N_{A0}\int_1^{1-X}\frac{\mathrm{d}(1-X)}{(1-X)^2} = -N_{A0}\,\Delta(1-X)^{-1}\Big|_1^{1-X} =$$
$$= N_{A0}\left(\frac{1}{1-X} - 1\right) = \frac{N_{A0}}{1/X - 1} \implies$$

$$\implies X = \left(1 + \frac{N_{A0}}{k\,C_{A0}^2\,V\,t}\right)^{-1} = \left(1 + \frac{C_{A0}\,V}{k\,C_{A0}^2\,V\,t}\right)^{-1} =$$
$$= (1 + 1/k\,C_{A0}\,t)^{-1}$$

Q1 c.

const cine

Resposta

$$k : X = (1 + 1/k\,C_{A0}\,t)^{-1} \implies$$
$$\implies k = \left(C_{A0}\,t\,(X^{-1} - 1)\right)^{-1} \cong \left(1 * 1.5 * (0.8^{-1} - 1)\right)^{-1} \cong$$
$$\cong 2.667\,\mathrm{M}^{-1}\,\mathrm{h}^{-1}$$

Q1 d.

$t_{opt} \wedge X_{opt}$ (usando graf)

Resposta

traçando do ponto $(0, -t_d)$ até tangenciar o gráfico temos:

$$\boldsymbol{X_{opt} \cong 0.7} \qquad \boldsymbol{t_{opt} \cong 1}\,\mathrm{h}$$

Q1 e.

Prod anual de C

- 24 h/d
- 330 d/year

Resposta

$$m_C = N_C\,M_C\,N_{batches} = N_C * 130 * (3 * 24 * 330/t_{batch}) =$$
$$= N_C\,3088800/(t_{opt} + t_d) = N_C\,3088800/(1+2) = N_C\,1029600;$$

$$N_C = N_{A0}\,X = C_{A0}\,V * 3\,X \cong$$
$$\cong 1 * 5 * 0.7 \cong 3.5 \implies$$

$$\implies m_C \cong 3.604\,\mathrm{t}$$

Q1 f.

expl proc p det analit $X_{opt} \wedge t_{opt}$

Questão 2

- $\mathrm{A} \longrightarrow 3\,\mathrm{B}$
- $T_0 = 500\,^\circ\mathrm{C} = 773.15\,\mathrm{K}$
- $k = 0.03\,\mathrm{min}^{-1}$

$$\int \frac{1 + a\,X}{1 - X}\,\mathrm{d}X = -a\,X + (1 + a)\,\ln\frac{1}{1 - X}$$

Q2 a.

det P de conv

- batch
- vol const
- fase gas
- $X = 0.99$
- Carreg A puro
- $P_0 = 2\,\mathrm{atm}$

Resposta

$$P = P_0\,\frac{V_0}{V}\,\frac{T}{T_0}\,(1 + \varepsilon\,X) = 2\,(1 + (-1 + 3)\,0.99)\,\mathrm{atm} \cong 5.960\,\mathrm{atm}$$

Q2 b.

nas cond de a), qual o t para $X = 99$

Resposta

$$t = C_{A0}\int_0^X \frac{\mathrm{d}X}{-r_A} = C_{A0}\int_0^X \frac{\mathrm{d}X}{k\,C_A} = C_{A0}\int_0^X \frac{\mathrm{d}X}{k\,(F_A/v)} =$$
$$= C_{A0}\int_0^X \frac{(v_0(1 + \varepsilon\,X))}{k\,(F_{A0}(1 - X))}\,\mathrm{d}X =$$
$$= \frac{C_{A0}}{k\,(F_{A0}/v_0)}\int_0^X \frac{1 + \varepsilon\,X}{1 - X}\,\mathrm{d}X =$$
$$= \frac{C_{A0}}{k\,(C_{A0})}\,\Delta\left(-\varepsilon\,X + (1 + \varepsilon)\,\ln\frac{1}{1 - X}\right)\Big|_0^X =$$
$$= k^{-1}\left(-\varepsilon\,X + (1 + \varepsilon)\,\ln\frac{1}{1 - X}\right) =$$
$$= (0.03 * 60)^{-1}\left(-2 * 0.99 + (1 + 2)\,\ln\frac{1}{1 - 0.99}\right) \cong 6.575\,\mathrm{h}$$

Q2 c.

Det o vol

- PFR
- $v_A = 100\,\mathrm{L/s}$
- $P = 2\,\mathrm{atm}$

Resposta

$$V : \mathrm{d}V = F_{A0}\,\frac{\mathrm{d}X}{-r_A} = C_{A0}\,v_0\,\frac{\mathrm{d}X}{k\,(F_A/v)} =$$
$$= C_{A0}\,v_0\,\frac{\mathrm{d}X}{\frac{k\,(C_{A0}(1 - X))}{(1 + \varepsilon\,X)\,(T/T_0)\,(P_0/P)}} = \frac{v_0}{k}\,\frac{\mathrm{d}X}{\frac{1 - X}{1 + \varepsilon\,X}} = \frac{v_0}{k}\,\frac{1 + \varepsilon\,X}{1 - X}\,\mathrm{d}X \implies$$

$$\implies V = \frac{v_0}{k}\int \frac{1 + \varepsilon\,X}{1 - X}\,\mathrm{d}X =$$
$$= \frac{v_0}{k}\,\Delta\left(-\varepsilon\,X + (1 + \varepsilon)\,\ln\frac{1}{1 - X}\right)\Bigg|_0^X =$$
$$= \frac{v_0}{k}\left(-\varepsilon\,X + (1 + \varepsilon)\,\ln\frac{1}{1 - X}\right) =$$
$$= \frac{100}{(0.03/60)}\left(-2 * 0.99 + (1 + 2)\,\ln\frac{1}{1 - 0.99}\right) \cong 2.367\,\mathrm{E6\,L}$$

Questão 3

Det numero de reatores

- A $\longrightarrow$ B
- bateria de R CSTR
- $V_r = 1\,\mathrm{m}^3$
- $k = 0.5\,\mathrm{h}^{-1}$
- $C_{A0} = 5\,\mathrm{M}$
- $v_0 = 1759\,\mathrm{dm}^3/\mathrm{h}$
- $X \geq 89\%$

Resposta

$N_R = \lceil V_R/V_r \rceil = \lceil 1.15 * V/1 \rceil = \lceil 1.15 * (N_{A0}/C_{A0}) \rceil =$
$= \lceil 1.15 * (N_A/(1-X))/C_{A0} \rceil;$

$-r_A = k\,C_A = k\,C_{A0}\,(1-X)$