ERQ I – Teste 1 Resolução

Felipe B. Pinto 61387 – MIEQB

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Conteúdo

Questão 1

The reversible reaction A $\rightleftharpoons$ B is carried out in a battery of two CSTR reactors arranged in series, it being known that the second reactor is double the volume of the first reactor. Reagent A is fed to the reactor battery in a concentration of $0.5\,\mathrm{mol\,dm^{-3}}$ at a volumetric flow rate of $20\,\mathrm{L/min}$. The direct and reverse reactions are elementary and the values of the direct reaction kinetic constant and the equilibrium constant are $0.15\,\mathrm{min^{-1}}$ and 28, respectively.

Q1 a.

Derive the expression of the rate law.

Resposta

$$-r_A = k\left([\mathrm{A}] - [\mathrm{B}]/k_e\right) = k\left([\mathrm{A}]_0(1-X) - [\mathrm{A}]_0 X/k_e\right) =$$
$$= k\,[\mathrm{A}]_0\left(1 - X\,(1+1/k_e)\right)$$

Q1 b.

For each of the reactors, derive the expressions that relate the volume of the reactor to the conversion.

Resposta

1 Reator:

$\tau_1 = V_1/v;$

$$0 = F_{A0} - F_A + r_{A1}V_1 = F_{A0} - F_{A0}(1-X_1) + r_{A1}V_1 =$$
$$= F_{A0}X_1 + r_{A1}V_1 \implies$$
$$\implies 0 = F_{A0}X_1/v + r_{A1}V/v = C_{A0}X_1 + r_{A1}\tau_1 \implies$$
$$\implies \tau_1 = \frac{C_{A0}X_1}{-r_{A1}} = \frac{C_{A0}X_1}{k\,C_{A0}\left(1 - X_1(1+1/k_e)\right)} =$$
$$= \frac{1}{k\,(1/X_1 - 1 - 1/k_e)}$$

2 Reator:

$\tau_2 = V_2/v;$

$$0 = F_{A1} - F_{A2} + r_{A2}V_2 =$$
$$= F_{A0}(1-X_1) - F_{A0}(1-X_2) + r_{A2}V_2 =$$
$$= F_{A0}(X_1 - X_2) + r_{A2}V_2 \implies$$
$$\implies 0 = F_{A0}(X_1-X_2)/v + r_{A2}V_2/v =$$
$$= C_{A0}(X_1-X_2) + r_{A2}\tau_2 \implies$$
$$\implies \tau_2 = \frac{C_{A0}(X_1-X_2)}{-r_{A2}} = \frac{C_{A0}(X_1-X_2)}{k\,C_{A0}\left(1 - X_2(1+1/k_e)\right)} =$$
$$= \frac{X_1 - X_2}{k\,\left(1 - X_2(1+1/k_e)\right)}$$

Q1 c.

Determine the value of the equilibrium conversion.

Resposta

$$X_e = \frac{[\mathrm{B}]_e}{[\mathrm{A}]_0} = 1 - \frac{[\mathrm{A}]_e}{[\mathrm{A}]_0};$$

$$\frac{[\mathrm{B}]_e}{[\mathrm{A}]_e} = \frac{[\mathrm{A}]_0 X_e}{[\mathrm{A}]_0(1-X_e)} = \frac{1}{1/X_e - 1} = k_e \implies$$
$$\implies X_e = \frac{1}{1/k_e + 1} = \frac{1}{1/28 + 1} \cong 0.966$$

Q1 d.

Knowing that the conversion at the exit of the 2nd reactor corresponds to 99% of the equilibrium conversion, determine the conversion at the exit of the 1st reactor.

Resposta

$$\frac{1}{k\,(1/X_1 - 1 - 1/k_e)} = \tau_1 =$$
$$= \tau_2/2 = \frac{X_1 - X_2}{2k\,\left(1 - X_2(1+1/k_e)\right)} \implies$$
$$\implies 0 = \begin{pmatrix} X_1^2\,(1+1/k_e) & + \\ -X_1\,(1 + X_2(1+5/k_e+4)) & + \\ +X_2 & \end{pmatrix} =$$
$$= \begin{pmatrix} X_1^2\,(1+1/k_e) & + \\ -X_1\,(1 + X_e\,0.99\,(1+5/k_e+4)) & + \\ +X_e\,0.99 & \end{pmatrix} \cong$$
$$\cong \begin{pmatrix} X_1^2\,(1+1/28) & + \\ -X_1\,(1 + 0.966 * 0.99\,(1+5/28+4)) & + \\ +0.966 * 0.99 & \end{pmatrix} \cong$$
$$\cong \begin{pmatrix} X_1^2\,1.036 & + \\ -X_1\,2.010 & + \\ +0.956 & \end{pmatrix} \begin{cases} 1.106 \\ 0.834 \end{cases} \quad \therefore X_1 \cong 0.834$$

Q1 e.

Determine the volumes of the reactors.

Resposta

$V_i = v\,\tau_i;$

1 Reator

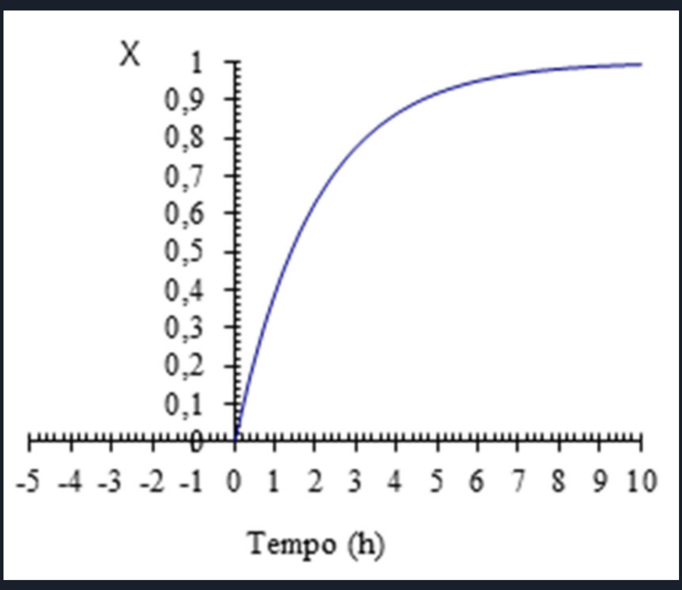
$$V_1 = v\,\tau_1 = v\left(\frac{1}{k\,(1/X_1 - 1 - 1/k_e)}\right) \cong$$
$$\cong \frac{20}{0.15\,(1/0.834 - 1 - 1/28)} \cong 817.409$$

2 Reator

$$V_2 = v\,\tau_2 = v\,2\,\tau_1 = 2\,V_1 \cong 2\,817.409 \cong 1634.819$$

Questão 2

The figure shows the kinetic curve obtained in a batch reactor, corresponding to the elemental liquid phase reaction $2\,\mathrm{A} \longrightarrow \mathrm{B}$. The reaction is carried out in batch reactors of $5\,\mathrm{m}^3$, which are loaded with pure A.



Data:

- $t_d = 120\,\mathrm{min}$.
- Molecular weight of A: $58\,\mathrm{g/mol}$.
- Molecular weight of B: $116\,\mathrm{g/mol}$.
- Density of A: $0.791\,\mathrm{g/L}$.
- If you were not able to solve b) use $k = 0.074\,\mathrm{dm^3\,mol^{-1}\,h^{-1}}$.

Q2 a.

Write the expression of the rate law.

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

Q2 b.

Write the equation of the curve shown in the graphic.

Resposta

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

$$\implies -\int_1^{1-X} \frac{\mathrm{d}(1-X)}{(1-X)^2} =$$
$$= -(-1)\,\Delta(X^{-1})\big|_1^{1-X} = 1/(1-X) - 1 = \frac{1}{1/X - 1} =$$

$$= \int_0^t k\,C_{A0}\,\mathrm{d}t = k\,C_{A0}\int_0^t \mathrm{d}t = k\,C_{A0}\,t \implies$$

$$\implies X = (1 + 1/k\,C_{A0}\,t)^{-1}$$

Q2 c.

Evaluate the value of the kinetic constant. Use the graphic.

Resposta

$$k : X = (1 + 1/k\,C_{A0}\,t)^{-1} \implies$$
$$\implies k = ((1/X - 1)\,C_{A0}\,t)^{-1} =$$
$$= ((1/X - 1)\,(N_{A0}/V)\,t)^{-1} =$$
$$= ((1/X - 1)\,(m_{A0}/M_A\,V)\,t)^{-1} =$$
$$= ((1/X - 1)\,(\rho_A\,V/M_A\,V)\,t)^{-1} =$$
$$= ((1/X - 1)\,(\rho_A/M_A)\,t)^{-1} \cong$$
$$\cong ((1/0.6 - 1)\,(791/58)\,1.9)^{-1}\ \mathrm{L/mol\,h} \cong$$
$$\cong 57.888\,\mathrm{mL/mol\,h}$$

Q2 d.

Calculate the optimal conversion and the optimal reaction time.

Resposta

Traça uma reta entre $(0, -t_d)$ e o gráfico, o ponto tangente é o optimo:

$$\boldsymbol{X_{opt} \cong 0.68} \qquad \boldsymbol{t_{opt} \cong 2.3}\,\mathrm{h}$$

Q2 e.

If the plant works $24\,\mathrm{h}$ day and $330\,\mathrm{d/year}$, determine the number of reactors needed for an annual production of B of $1500\,\mathrm{t}$. Use the conversion calculated in d) but if you were not able to, use any value at your choice.

Resposta

$$\mathrm{A} \longrightarrow \tfrac{1}{2}\mathrm{B}$$

$$N_R = \lceil V_R/5\,\mathrm{m}^2 \rceil = \lceil 1.15\,V/5\,\mathrm{m}^2 \rceil = \left\lceil \frac{1.15\,(N_{A0}/C_{A0})}{5\,\mathrm{m}^2} \right\rceil ;$$

$$N_{A0}\,X/2 = N_B = \frac{1500 * 10^6}{M_B * N_{batch}} = \frac{1500 * 10^6}{116 * \frac{330*24}{t_{batch}}} =$$
$$= \frac{1500 * 10^6}{\frac{116*330*24}{t_{opt}+t_d}} = \frac{1500 * 10^6}{\frac{116*330*24}{2.3+2}} \cong 7.021\ \mathrm{E3\,mol} \implies$$

$$\implies N_{A0} \cong 2 * 7.021\ \mathrm{E3}/0.68 \cong 20.649 \implies$$

$$\implies N_R \cong \left\lceil \frac{1.15 * 20.649}{(\rho_A/M_A)} \right\rceil = \left\lceil \frac{1.15 * 20.649}{5 * (0.791 * 10^3/58)} \right\rceil \cong$$
$$\cong \lceil 0.348 \rceil = 1$$