ERQ I – Teste 1 2020 Resolução

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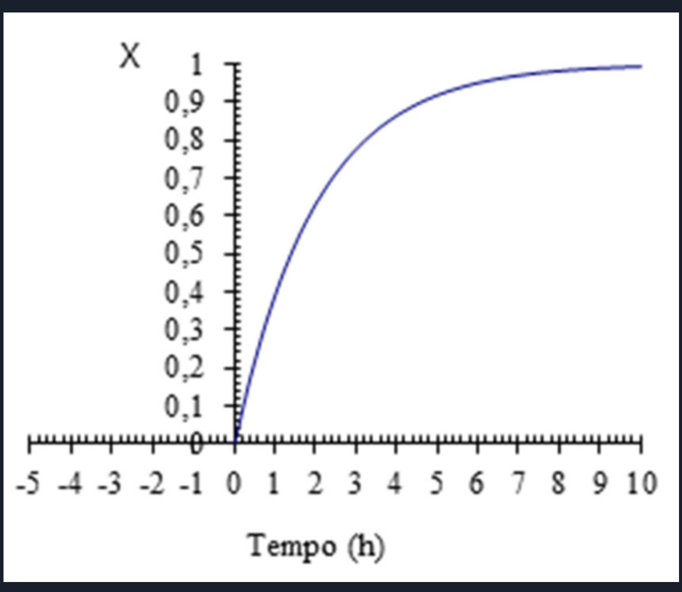
Conteúdo

Questão 1

The figure shows the kinetic curve obtained in a batch reactor, corresponding to the elemental liquid phase reaction $2\,A \longrightarrow B$. The reaction is carried out in batch reactors of $5\,m^3$, 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 $k = 0.074\,\mathrm{dm^3\,mol^{-1}\,h^{-1}}$.

Q1 a.

Write the expression of the rate law.

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

Q1 b.

Write the equation of the curve shown in the graphic.

Resposta

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

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

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

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

Q1 c.

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

Resposta

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

Q1 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:

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

Q1 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

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

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

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

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

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

Questão 2

A reacção de 1ª ordem $\mathrm{A} \longrightarrow 2\,\mathrm{B}$, em fase líquida, é conduzida num sistema de reactores contínuos, sendo uma solução de A com a concentração de $0.1\,\mathrm{mol/dm^3}$ alimentada a um caudal volumétrico de $10\,\mathrm{dm^3/min}$. Sabendo-se que a constante cinética à temperatura da reacção é $k = 0.02\,\mathrm{min^{-1}}$, e que se pretende obter uma conversão final de 70%, determine mostrando todos os cálculos:

Q2 a.

O volume de um único reactor CSTR.

Q2 b.

O número de reactores CSTR de $1\,\mathrm{m^3}$ de volume, associados em série.