ERQ I – Teste 2023.2 Resolução

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09 de Dezembro de 2023

Conteúdo

Questão 1

- A $\rightleftharpoons$ B
- fase gásosa
- Reator tubular adiabático
- A (10%)
- $T_0 = 200\,°\mathrm{C} = 473.15\,\mathrm{K}$
- $v_0 = 10\,\mathrm{dm^3/s} = 600\,\mathrm{L/min}$
- gráfico $X \times T$
- $C_{p\,A} = C_{p\,B} = 5\,\mathrm{cal/mol\,K}$
- $C_{p\,I} = 12\,\mathrm{cal/mol\,K}$
- $k_{d\,(473\,\mathrm{K})} = 1.17\,\mathrm{min^{-1}}$
- $K_{e\,(473\,\mathrm{K})} = 40$
- $Ea = 20\,\mathrm{kcal/mol}$
- $R = 1.987\,\mathrm{cal\,mol^{-1}\,K^{-1}}$

Q1 a.

Endotermica/exotermica

Resposta

Exotérmica pois $X \propto T^{-1}$ ou seja diminui conforme a temperatura almenta.

Q1 b.

Calor de reação

Resposta

$$\Delta H_R : K_{e\,(T)} = K_{e\,(T_R)} \exp\left(-\frac{\Delta H_R}{R}(T^{-1} - T_R^{-1})\right) \implies$$

$$\implies \Delta H_R = \frac{-R}{(T^{-1} - T_R^{-1})} \ln \frac{K_{e\,(T)}}{K_{e\,(T_R)}};$$

$$K_{e\,(T)} : K_{e\,(T)} = \frac{p_{p\,B}}{p_{p\,A}} = \frac{C_{p\,B}\,R\,T}{C_{p\,A}\,R\,T} = \frac{C_{p\,A_0}\,X}{C_{p\,A_0}\,(1-X)} = \frac{1}{1/X - 1} \implies$$

$$\implies X = \frac{1}{1 + 1/K_e} \implies X = 0.5 \begin{cases} K_e = 1 \\ T \cong 619\,\mathrm{K} \end{cases}$$

$$\therefore \Delta H_R = \frac{-R}{(T^{-1} - T_R^{-1})} \ln \frac{K_{e\,(T)}}{K_{e\,(T_R)}} \cong \frac{-1.987}{(619^{-1} - 473^{-1})} \ln \frac{1}{40} \cong$$

$$\cong -14.701\,\mathrm{kcal/mol}$$

Q1 c.

$X_{eq} \wedge T_{eq}$

Resposta

$$X_{(520\,\mathrm{K})} = \frac{(C_{p\,A} + \theta_I\, C_{p\,I})(T - T_0)}{-\,\Delta H_R} = \frac{(C_{p\,A} + \frac{Y_{I\,0}}{Y_{A\,0}}\, C_{p\,I})(T - T_0)}{-\,\Delta H_R} \cong$$

$$\cong \frac{\left(5 + \frac{0.9}{0.1}\, 12\right)(520 - 473)}{14.701\,\mathrm{E}^3} \cong 0.360$$

$$\begin{cases} X_0 = 0; & T_0 = 473 \\ X_1 \cong 0.360; & T_1 = 520 \end{cases}$$

$$\boldsymbol{X_{eq} \cong 0.79} \quad \wedge \quad \boldsymbol{T_{eq} \cong 546}\,\mathrm{K}$$

Q1 d.

Volume do reator para $X_1 = 95\%\, X_e$

Resposta

$$V = \int_0^X \frac{F_{A\,0}\,\mathrm{d}X}{-r_A} = \int_0^X \frac{C_{A\,0}\,v_0\,\mathrm{d}X}{-r_A};$$

$$\begin{aligned}
-\,r_A &= k(C_A - C_B/K_e) = \\
&= k\left(\left(\frac{C_{A\,0}(1 - X)}{1 + \varepsilon\,X}\frac{T_0}{T}\right) - \left(\frac{C_{A\,0}\,X}{1 + \varepsilon\,X}\frac{T_0}{T}\right)/K_e\right) = \\
&= k\left(\frac{C_{A\,0}(1 - X(1 - 1/K_e))}{1 + \varepsilon\,X}\frac{T_0}{T}\right) = \\
&= k\left(\frac{C_{A\,0}(1 - X(1 - 1/K_e))}{1 + y_{A\,0}\,\delta\,X}\frac{T_0}{T}\right) = \\
&= k\left(\frac{C_{A\,0}(1 - X(1 - 1/K_e))}{1 + y_{A\,0}\,(1 - 1)\,X}\frac{T_0}{T}\right) = \\
&= k\,C_{A\,0}(1 - X(1 - K_e))\,\frac{T_0}{T} \implies
\end{aligned}$$

$$\implies V = \int_0^X \frac{C_{A0}\, v_0 \,\mathrm{d}X}{k\, C_{A0}(1 - X(1-K_e))\,\frac{T_0}{T}} =$$
$$= \int_0^X \frac{v_0 \;\mathrm{d}X}{k\,(1 - X(1-K_e))\,\frac{T_0}{T}} =$$
$$= \int_0^{.95*.79} \frac{600 \;\mathrm{d}X}{k\,(1 - X(1-K_e))\,\frac{473}{T}} =$$
$$\cong \int_0^{0.7505} \frac{1.268 \;\mathrm{d}X}{k\,(1 - X(1-K_e))/T}$$

Simpson:

$$f(X) = \frac{1.268 \;\mathrm{d}X}{k\,(1 - X(1-K_e))/T};$$

$$T : X = \frac{(C_{p\,A} + \theta_I\, C_{p\,I})(T - T_0)}{-\,\Delta H_R} \implies$$
$$\implies T = T_0 - \frac{X \;\Delta H_R}{C_{p\,A} + \theta_I\, C_{p\,I}} \cong 473 - \frac{-X\, 14.701\,\mathrm{E}^3}{5 + \frac{.9}{.1}\,12} \cong$$
$$\cong 473 + X\; 130.094;$$

$$k_{(T)} = k_{(T_R)}\; \exp\left(-\frac{Ea}{R}(T^{-1} - T_R^{-1})\right) =$$
$$\cong 1.17\; \exp\left(-\frac{20\,\mathrm{E}^3}{1.987}(T^{-1} - 473^{-1})\right) \cong$$
$$\cong 1.17\; \exp\left(-10.064\,\mathrm{E}^3(T^{-1} - 473^{-1})\right);$$

$$K_{e\,(T)} = K_{e\,(T_R)}\; \exp\left(-\frac{\Delta H}{R}\,(T^{-1} - T_R^{-1})\right) \cong$$
$$\cong 40\; \exp\left(\frac{14.701\,\mathrm{E}^3}{1.987}\,(T^{-1} - 473^{-1})\right) \cong$$
$$\cong 40\; \exp\left(7.398\,\mathrm{E}^3\,(T^{-1} - 473^{-1})\right)$$

$$h = \frac{0.7505}{2} = 0.37525 \begin{cases} X_0 = 0 \\ X_1 = 0.37525 \\ X_2 = 0.7505 \end{cases}$$

$$\therefore V = \frac{h}{3} \left(f_{(X_0)} + 4\, f_{(X_1)} + f_{(X_2)} \right)$$

Encontramos com os 3 pontos de X os valores para T, $k_{(T)}$, $K_{e\,(T)}$ que podem ser usados para encontrar $f(X)$ que finalmente são usados para encontrar V

Q1 e.

$Y_{A\,0}$ para $X_{eq} = 90\%$

Resposta

$$Y_{A\,0} : -X_{(T)}\ \Delta H_R = (C_{p\,A} + \theta_I\, C_{p\,I})\,(T - T_0) =$$
$$= \left(C_{p\,A} + \frac{Y_{I\,0}}{Y_{A\,0}}\, C_{p\,I} \right) (T - T_0) =$$
$$= \left(C_{p\,A} + \frac{1 - Y_{A\,0}}{Y_{A\,0}}\, C_{p\,I} \right) (T - T_0);$$
$$T_{eq} \cong 473 + 0.9 * 130.094 \cong 590.085 \implies$$
$$\implies Y_{A\,0} = \left(1 + \frac{\frac{-X_{(T)}\ \Delta H_R}{T - T_0} - C_{p\,A}}{C_{p\,I}} \right)^{-1} =$$
$$= \left(1 + \frac{\frac{0.9 * 14.701\,\mathrm{E}^3}{590.085 - 473} - 8}{12} \right)^{-1} \cong 0.103$$

Questão 2

- A $\longrightarrow$ B
- CSTR não adiabático
- $V = 6\,\mathrm{m}^3$
- Em estado estacionário
- $v_0 = 6\,\mathrm{L/min} = 360\,\mathrm{L/h}$
- $Y_{A\,0} = 0.1$
- $\Delta H_R = -100.7\,\mathrm{kJ/mol}$
- $C_{p\,A} = C_{p\,B} = 34.6\,\mathrm{J/mol\,K}$
- $C_{p\,I} = 75.4\,\mathrm{J/mol\,K}$
- $R = 8.314\,\mathrm{J\,mol^{-1}\,K^{-1}}$
- $C_{A\,0} = 1\,\mathrm{M}$
- $T_0 = 298\,\mathrm{K}$
- $k_{(298\,\mathrm{K})} = 0.0227\,\mathrm{h^{-1}}$
- com parede envolvida até 85% com agua a $100\,°\mathrm{C} = 373\,\mathrm{K}$

Q2 a.

Equações das curvas

Resposta

$$G_{(T)} = -\,\Delta H_R\, X$$

$$X : r_{(T)} = G_{(T)} = \frac{Ua}{F_{A0}}\,(T - T_0) + \sum \theta_i\, Cp\, i(T - T_0) =$$
$$= \frac{\left(\frac{Q^{\cdot}}{T_0 - T}\right)}{F_{A0}}\,(T - T_0) + \frac{1 - Y_{A0}}{Y_{A0}}\, C_{p\,B}(T - T_0) =$$
$$= \frac{-Q^{\cdot}}{C_{A0}\, v_0} + (1/Y_{A0} - 1)\, C_{p\,A}\, X(T - T_0) \implies$$
$$\implies X = \frac{G_{(T)} + \frac{Q^{\cdot}}{C_{A0}\, v_0}}{(1/Y_{A0} - 1)\, C_{p\,A}(T - T_0)} \implies$$

$$\implies G_{(T)} =$$
$$= -\,\Delta H_R \left(\frac{Q^{\cdot}}{C_{A0}\, v_0}\right) \left((1/Y_{A0} - 1)\, C_{p\,A}(T - T_0) + \Delta H_R\right)^{-1} =$$
$$= -100.7\,\mathrm{E}^3 \left(\frac{Q^{\cdot}}{1 * 360}\right) \left((1/0.1 - 1)\, 1(T - 298) - 100.7\,\mathrm{E}^3\right)^{-1} \cong$$
$$\cong \frac{-31.080\, Q^{\cdot}}{T - 11.487\,\mathrm{E}^3}$$

Por não conseguir calcular $Q^{\cdot}$ deixei como variável, se mostra necessário uma vez que a equação final deve ser uma reta, $Q^{\cdot} \propto T^2$ o que nao verificou

Q2 d.

Ea usando gráfico