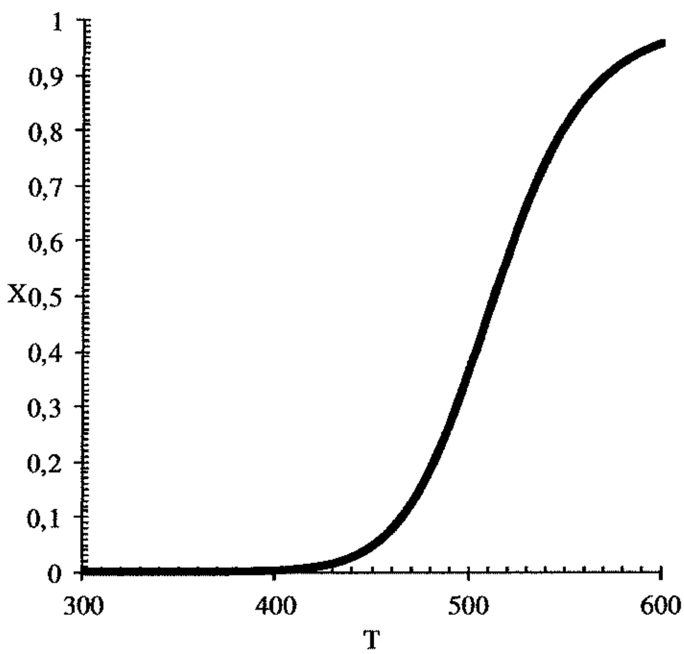
Reactores Químicos I
Ano lectivo 2012/13

3º Teste

A reacção reversível $A \rightleftarrows B$ é conduzida, na fase líquida, num reactor tubular adiabático. O reagente A é alimentado numa concentração 2 M, à temperatura de 580 K, a um caudal volumétrico de 20 $dm^3/min.$, juntamente com um sovente C, na concentração de 50,7 M, o qual se comporta como um inerte. A figura representa a variação da conversão de equilíbrio com a temperatura.

The reversible reaction $A \rightleftarrows B$ is carried out in the liquid phase in an adiabatic PFR. The reactant A is fed to the reactor at 2 M concentration, 580 K and 20 dm^3/min volumetric flow rate, along with a solvent C (50,7 M). The figure shows the plot of equilibrium conversion as a function of temperature.



1) Escreva a equação da curva representada na figura, substituindo todas as constantes pelos respectivos valores numéricos. Write the equation of the curve plotted in the figure, replacing all constant symbols by the corresponding numeric values.
2) Explique, justificando a sua resposta, se a reacção é exotérmica ou endotérmica. Explain, justifying your answer, if the reaction is exothermic or endothermic.
3) Escreva a equação de balanço de energia, substituindo todos os símbolos das constantes por valores numéricos. Write the energy balance equation replacing all the constant symbols by the corresponding numeric values.
4) Determine a conversão de equilíbrio adiabática e a correspondente temperatura de equilíbrio adiabática. Determine the adiabatic equilibrium conversion and the adiabatic equilibrium temperature.
5) Determine o valor da temperatura à saída do reactor. Determine the temperature value at the reactor exit.
6) Determine o valor da constante cinética à saída do reactor. Determine the rate constant value at the reactor exit.
7) Determine o valor da constante de equilíbrio à saída do reactor. Determine the value of the equilibrium constant at the reactor exit.
8) Escreva a expressão da lei cinética, substituindo todos os símbolos de constantes pelos correspondentes valores numéricos. Write the expression of the rate law, replacing all the constant symbols by the corresponding numeric values.
9) Calcule o volume do reactor necessário a uma conversão de 99% da conversão de equilíbrio. Calculate the reactor volume required to a conversion corresponding to 99% of equilibrium conversion.
10) Qual deverá ser o valor da concentração de A na alimentação, para que seja possível uma conversão de equilíbrio de 90%? What should be the value of the concentration of A in the reactor feed, in order to make possible an equilibrium conversion of 90%.

Dados (data): $\Delta H_R(580\ K) = 22$ kcal/mol; Peso molecular de A (molecular weight of A): 44; Peso molecular de C (molecular weight of C): 18; densidade da alimentação (feed density): 1; $Cp_A = Cp_B = 20$ cal/mol K; $Cp_I = 18$ cal/mol K; Constante cinética da reacção directa (rate constant of the direct reaction): $k(580\ K) = 1{,}6\ min^{-1}$; $K_e(580\ K) = 12$; Energia de activação (activation energy): $E = 18$ kcal/mol; $R = 1{,}987\ cal\ mol^{-1}\ K^{-1}$.

1)

$$Ke = \frac{C_{Be}}{C_{Ae}} = \frac{C_{A0}\,X_e}{C_{A0}\,(1-X_e)} = \frac{X_e}{1-X_e}$$

$$X_e = \frac{Ke}{1+Ke} = \frac{Ke(T_R)\,e^{-\frac{\Delta H_R}{R}\left(\frac{1}{T}-\frac{1}{T_R}\right)}}{1+Ke(T_R)\,e^{-\frac{\Delta H_R}{R}\left(\frac{1}{T}-\frac{1}{T_R}\right)}}$$

$$X_e = \frac{12\,e^{-\frac{22000}{1,987}\left(\frac{1}{T}-\frac{1}{580}\right)}}{1+12\,e^{-\frac{22000}{1,987}\left(\frac{1}{T}-\frac{1}{580}\right)}}$$

2)

A reacção é endotérmica, pois o calor de reacção é positivo.

This is an endothermic reaction because the heat of reaction has a positive value.

3)

$$X = \frac{\left(C_{pA}+\theta_C\,C_{pC}\right)(T-T_0)}{-\Delta H_R}$$

$$X = \frac{\left(20+\frac{50,7}{2}\times 18\right)\,(T-580)}{-22000}$$

4)

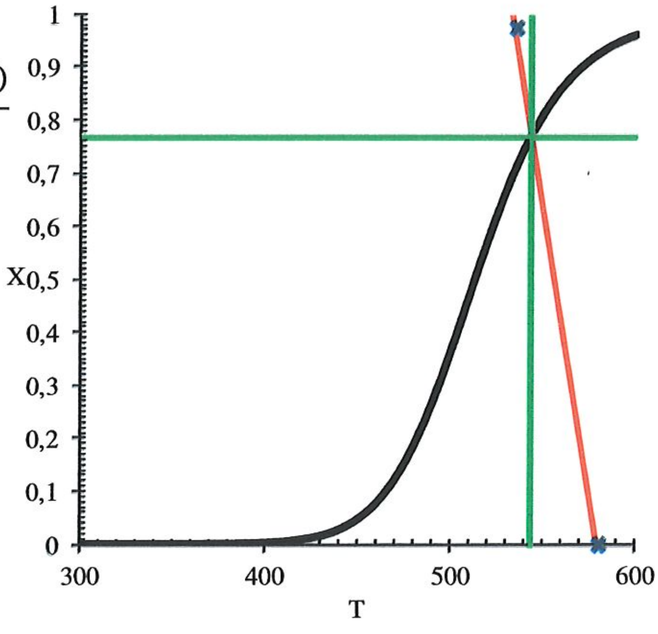
$$X = \frac{\left(20+\frac{50,7}{2}\times 18\right)\,(T-580)}{-22000}$$

X=0 T=580 K

X=0,974 T=535 K

Xe = 0,77

Te = 544 K



5)

$$X = \frac{\left(20 + \frac{50,7}{2} \times 18\right)\ (T - 580)}{-22000} = 0,99\ Xe = 0,99 \times 0,77$$

$$-22000\ X = \left(20 + \frac{50,7}{2} \times 18\right)\ (T - 580)$$

$$T = \frac{580\ \left(20 + \frac{50,7}{2} \times 18\right) - 22000\ X}{\left(20 + \frac{50,7}{2} \times 18\right)}$$

$$T = 580 - \frac{22000 \times 0,99 \times 0,77}{\left(20 + \frac{50,7}{2} \times 18\right)} = 544,8\ K$$

6)

$$k(T) = \ k(T_R)\ e^{-\frac{E}{R}\left(\frac{1}{T} - \frac{1}{T_R}\right)}$$

$$k(T) = \ 1,6 \times e^{-\frac{18000}{1,987}\left(\frac{1}{T} - \frac{1}{580}\right)}$$

$$k(544,8) = \ 1,6 \times e^{-\frac{18000}{1,987}\left(\frac{1}{544,8} - \frac{1}{580}\right)} = 0,69\ min^{-1}$$

7)

$$Ke(T) = \ Ke(T_R)\ e^{-\frac{\Delta H_R}{R}\left(\frac{1}{T} - \frac{1}{T_R}\right)}$$

$$Ke(T) = \ 12 \times e^{-\frac{22000}{1,987}\left(\frac{1}{T} - \frac{1}{580}\right)}$$

$$Ke(544,8) = \ 12 \times e^{-\frac{22000}{1,987}\left(\frac{1}{544,8} - \frac{1}{580}\right)} = 3,49$$

8)

$$-r_A = k\ \left(C_A - \frac{C_B}{Ke}\right)$$

$$-r_A = k\left(C_{A0}\,(1-X) \;-\; \frac{C_{A0}\,X}{Ke}\right)$$

$$-r_A = k\,C_{A0}\left(\,(1-X) - \frac{X}{Ke}\right)$$

$$-r_A = 2 \times 1{,}6\,e^{-\frac{18000}{1{,}987}\left(\frac{1}{T}-\frac{1}{580}\right)}\left(\,(1-X) - \frac{X}{12\,e^{-\frac{22000}{1{,}987}\left(\frac{1}{T}-\frac{1}{580}\right)}}\right)$$

$$T = 580 - \frac{22000\,X}{\left(20 + \frac{50{,}7}{2} \times 18\right)}$$

$$-r_A = 1{,}6\,e^{-\frac{18000}{1{,}987}\left(\frac{1}{T}-\frac{1}{580}\right)}\,C_{A0}\left(\,(1-X) - \frac{X}{12\,e^{-\frac{22000}{1{,}987}\left(\frac{1}{T}-\frac{1}{580}\right)}}\right)$$

9)

Balanço molar *Mole balance*:

$$F_A - \;(F_A +\; dF_A) +\; r_A\,dV = 0$$

$$dV = \frac{dF_A}{r_A}$$

$$V = \int_0^X F_{A0}\,\frac{dX}{-r_A}$$

Lei cinética *Kinetic law*:

$$-r_A = k\,C_{A0}\left(\,(1-X) - \frac{X}{Ke}\right)$$

Condensando o balance molar com a lei cinética:

$$V = \int_0^X F_{A0}\,\frac{dX}{k\,C_{A0}\left(\,(1-X) - \frac{X}{Ke}\right)}$$

$$V = \int_0^X v_0 \frac{dX}{k\left((1-X) - \frac{X}{Ke}\right)}$$

Arrhenius:

$$k(T) = 1{,}6\, e^{-\frac{18000}{1{,}987}\left(\frac{1}{T} - \frac{1}{580}\right)}$$

Van't Hoff:

$$Ke(T) = 12\, e^{-\frac{22000}{1{,}987}\left(\frac{1}{T} - \frac{1}{580}\right)}$$

Balanço de energia *Energy balance*:

$$T = 580 - \frac{22000\, X}{\left(20 + \frac{50{,}7}{2} \times 18\right)}$$

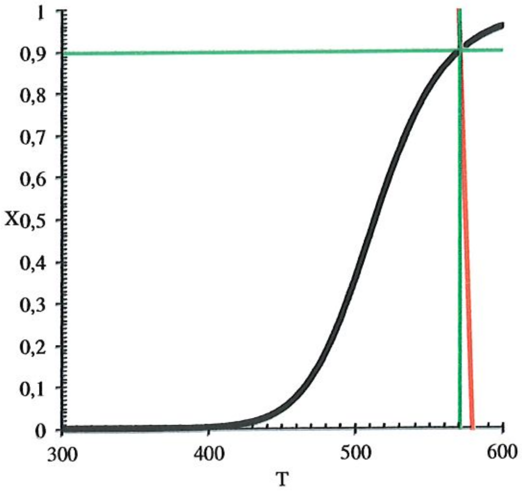
$$f(X) = \frac{v_0}{k\left((1-X) - \frac{X}{Ke}\right)}$$

$$V = \int_{X_1}^{X_3} f(X)\, dX = \frac{h}{3}\left(f(X_1) + 4\, f(X_2) + f(X_3)\right)$$

$$h = \frac{X_3 - X_1}{2}$$

X	$T = 580 - \frac{22000\, X}{\left(20 + \frac{50{,}7}{2} \times 18\right)}$	$k(T) = 1{,}6\, e^{-\frac{18000}{1{,}987}\left(\frac{1}{T} - \frac{1}{580}\right)}$	$Ke(T) = 12\, e^{-\frac{22000}{1{,}987}\left(\frac{1}{T} - \frac{1}{580}\right)}$	$f(X) = \frac{v_0}{k\left((1-X) - \frac{X}{Ke}\right)}$	$V = \int_0^X f(X)\, dX$	
0,000	580	1,6	12	12,5	12,5	
0,381	562,3838	1,064282	6,599156	33,49182	133,9673	
0,762	544,7676	0,689512	3,491405	1497,95	1497,95	
					209	dm^3

10)



Balanço de energia *Energy balance*:

$$X = \frac{(20 + 18\,\theta_C\,)\,(T - 580)}{-22000}$$

$$X = -\frac{(20 + 18\,\theta_C\,)}{22000}\,T + \frac{580\,(20 + 18\,\theta_C\,)}{22000}$$

$$-\frac{(20 + 18\,\theta_C\,)}{22000} = \frac{0{,}9 - 0}{572 - 580}$$

$$\theta_C = \frac{\frac{22000 \times 0{,}9}{580 - 572} - 20}{18} = 136{,}4$$

Base de cálculo *Calculation basis*: 1 dm^3

M = 1000 g

$$\begin{cases} 1000 = N_{A0}\,M_A + \,N_{C0}\,M_C \\ \theta_C = \dfrac{N_{C0}}{N_{A0}} \end{cases}$$

$$\begin{cases} 1000 = 44\,N_{A0} + 18\,N_{C0} \\ \dfrac{N_{C0}}{N_{A0}} = 136{,}4 \end{cases}$$

$$1000 = 44\,N_{A0} + 18 \times 136{,}4\,N_{A0}$$

$$N_{A0} = \frac{1000}{44 + 18 \times 136{,}4} = 0{,}4\ mol$$

$$\therefore\ C_{A0} = 0{,}4\ M$$