PROBLEMS OF PLUG FLOW REACTOR 13-25

13.- Data from the following table were obtained for the gas phase decomposition of reactant A in a constant volume batch reactor at 100°C fed with pure A. The stoichiometry of the reaction is $2A \rightarrow R + S$. Calculate the size of the plug flow reactor, operating at 100°C and 1 atm, capable of treating 100 mol/h of a feeding that contains 20% inerts in order to obtain a 95% conversion of A.

t (s)	0	20	40	60	80	100	140	200	260	330	420
P_A (atm)	1.00	0.80	0.68	0.56	0.45	0.37	0.25	0.14	0.08	0.04	0.02

14.- The homogeneous gas phase reaction $A \rightarrow 2B$ is conducted under isothermal conditions of 100°C at a constant pressure of 1 atm in a batch reactor. When starting from pure A, experimental data obtained are those shown in the following table. Calculate the size of the plug flow reactor operating at 100°C and 10 atm (both values kept constant during the reaction) for a 90% conversion of A with a total feed rate of 10 mol/s containing 40% inerts.

t (min)	0	2	4	6	8	10	12	14
V/V_0	1.00	1.35	1.58	1.72	1.82	1.88	1.92	1.95

15.- A tubular reactor is going to be designed to treat 1000 m^3/h of a gaseous mixture consisting of 80% (molar basis) acetylene and 20% inerts, measured at 550°C and 20 atm. The tubular reactor will consist of a combination of tubes in series. Each tube has a length of 3.5 m and an inner diameter of 20 cm. The reaction temperature will be 550°C and under these conditions acetylene is polymerized as:

$$4C_2H_2 \rightarrow (C_2H_2)_4 \qquad -r_{acetylene} = k \cdot C_{acetylene}^2 \qquad (k = 0.6\ L/(mol \cdot s))$$

If pressure drop through the tubes is neglected, calculate the number of tubes required for a 60% conversion of acetylene to tetramer complex. The pressure at the inlet of the first tube is 20 atm.

16.- Gas phase reaction $4A + B \rightarrow R + S$ is performed in a plug flow reactor. Formation rate of R is empirically correlated by the equation:

$$r_R = \frac{1 + C_A C_B}{1 + 0.5 C_B / C_A} \qquad (r_R \text{ in mol/(L·h)}, C_A \text{ and } C_B \text{ in mol/L})$$

The plug flow reactor is fed with a flow rate of 200 kmol A/ h, and the feeding is 50% A and 50% B. The reaction takes place at 3 atm and 150°C.

a) Calculate the space time required to get 80% conversion of limiting reactant.

b) How much R (kmol/h) will be produced using a plug flow reactor of 50000 litres, for the feeding and conditions specified?

17.- In an adiabatic plug flow reactor the gas phase reaction $A + B \rightarrow R + S$ is carried out at an absolute pressure of 2 atm. The kinetics of the reaction is given by $-r_A = kp_Ap_B$, where $k_{(100°C)} = 0.05$ and $k_{(500°C)} = 50$ (both in mol/(L·h·atm^2)). The reaction enthalpy can be considered constant in the range of working temperatures with a value of $\Delta H = 41.8$ kJ/mol$_A$. The reactor is fed with 5 kg/h of an equimolar mixture of A and B at 250°C and a conversion of 35% is desired. Calculate the volume of the reactor needed.

Data:

$C_{p\ \text{reactant mixture}} = 1.5$ cal/(g·ºC) (assumed constant)
$MW_{\text{reactant mixture}} = 40$ g/mole

18.- One of the key steps in the design of the equipment for the production of acetic anhydride is the cracking of acetone according to the reaction:

$$CH_3COCH_3 \rightarrow CH_2CO + CH_4$$

This reaction takes place in gas phase and follows a first order kinetics with respect to acetone. The rate constant is given by the expression:

$\ln k = 34.34 - (34222/T)$ (T in K, k in s^{-1})

8000 kg/h of acetone are going to be fed into a plug flow reactor. Considering that the reactor works adiabatically, the feeding is pure acetone, inlet temperature is 1035 K and pressure is 1.6 atm (the latter is constant along the reactor), what volume of reactor will be required to achieve a conversion of 20%?

Data:

$C_{p\ \text{acetone}} = 164$ J/(mol·K), $C_{p\ \text{ketene}} = 96$ J/(mol·K), $C_{p\ \text{methane}} = 60$ J/(mol·K)
$\Delta H_{(298K)} = 80.8$ kJ/mol$_{\text{acetone}}$

19.- In an adiabatic plug flow reactor of 1.5 m^3 volume, the elementary reaction $A + B \rightarrow C$ is performed in gas phase at constant pressure of 2 atm. The rate constant is given by the expression k = 9750exp(-4000/T) (T in K, k in L/(mol·s)). The reaction enthalpy at 298 K is 50 kJ/mol$_B$. The feeding introduced into the reactor consists of 16 mol/s of A, 16 mol/s of B and 8 mol/s of inerts. The inlet temperature is 700ºC. The heat capacity values are: $C_{pA} = C_{pB} = 75$ J/(mol·K), $C_{pC} = 150$ J/(mol·K) and $C_{p\ \text{inerts}} = 10$ J/(mol·K). Calculate the conversion obtained working under the conditions indicated above.

20.- *(exam dec'06)* In an adiabatic plug flow reactor working at constant pressure the following reversible and elementary reaction takes place:

$$A + B \underset{2}{\overset{1}{\rightleftarrows}} 2C$$

The stream fed into the reactor consists of a gas phase mixture at 77°C and 580.5 kPa of A and B in stoichiometric proportion and molar flow rate of 20 mol A/s.

a) Determine the conversion of equilibrium in adiabatic conditions for the PFR
b) Determine the volume of PFR needed to achieve a conversion equal to 85% of the previous value

Data:

Components	C_{pj} (J/(mol·K))	h_j^* (25ºC) (J/mol)
A	25	-40000
B	15	-30000
C	20	-45000

Note: C_{pj} independent of temperature

Kinetics direct reaction			Kinetics reverse reaction		
k_{0d}	1.45×10^7	m³/(mol·s)	k_{0i}	1.85×10^6	m³/(mol·s)
E_{ad}	70000	J/mol	E_{ai}	90000	J/mol

21.- The gas phase reaction $2A \rightarrow B$, with $r_B = \exp(14 - 7000/T)\cdot C_A^2$ (T in K, r_B in mol/(L·min)) is carried out in a PFR of 1000 L at a given pressure. The feeding, with volumetric flow rate of 100 L/min (measured at 25°C and at the same pressure), contains 90% A and 10% inerts (molar basis), and the concentration of A (measured under the same conditions as the volumetric flow) is C_{A0} = 20 mol/L. Other data are:

$\Delta H^*_{(293\ K)} = 3.5$ kcal/mol$_B$
$C_{pA} = 0.02$ kcal/(mol$_A$·K), $C_{pB} = 0.03$ kcal/(mol$_B$·K), $C_{p\ inerts} = 0.01$ kcal/(mol$_{inerts}$·K)

a) Find the temperature at which the reactor would work under isothermal conditions to obtain a final conversion of 90%
b) Find the temperature at which the reaction mixture should enter in order to achieve a final conversion of 90% working adiabatically

22.- The gas coming from the oxidation of ammonia is rapidly cooled to room temperature to remove most of the water vapor that contains. Once cool, the mixture contains 9% NO, 1% NO_2, 8% O_2 (in mole %), together with water vapor and N_2. The cooled gas is assumed to be saturated with water vapor. Before using this mixture as feeding to produce nitric acid in absorption towers the mixture has to be oxidized so that the ratio is 5:1 NO_2/NO. This oxidation is performed in an adiabatic PFR, introducing the feeding at 293 K. Which volume of reactor will be needed if a volumetric flow rate of 10700 m^3/h is introduced (measured at 293 K and 1 atm) and the working pressure is 1 bar?

Data:

The kinetic expression of reaction $NO + 0.5O_2 \rightarrow NO_2$ is:

$r = 119844\exp(-629.11/T)C_{NO}^2 C_{O_2}$ (r in kmol/(m^3·s) and C in kmol/m^3)

Vapor pressure of H_2O $_{(20ºC)}$ = 17.5 mm Hg

$\Delta H_{(20ºC)}$ = -56.6 kJ/mol NO_2

Average heat capacities for the working temperature range:

Compound	O_2	NO	NO_2	N_2	H_2O
C_p (J/(mol·K))	29.4	29.9	37.9	29.1	37.6

23.- *(exam jan'13)* n-butane (n-C_4H_{10}) is going to be isomerized to isobutane (i-C_4H_{10}) according to the following reversible reaction:

$$\text{n-}C_4H_{10} \leftrightarrow \text{i-}C_4H_{10}$$

The reaction is going to be carried out adiabatically in liquid phase and at high pressure. Find out the volume of the PFR necessary to process a feed flow rate of 163 kmol/h with an inlet temperature of 330 K so that the conversion reached is 65%. The feed stream has a molar fraction composition of 0.9 of n-butane and 0.1 of isopentane. The substance isopentane can be considered as an inert here.

Data:

ΔH^*_r = -6900 J/mol n-butane

C_{A0} = 9.3 mol/L

Reversible reactions are always elementary

$k_{o,forward} = 1.7\cdot 10^{11}$ h^{-1}

$k_{o,reverse} = 6.9\cdot 10^{11}$ h^{-1}

$E_{a,forward}$ = 65.7 kJ/mol

$E_{a,reverse}$ = 72.6 kJ/mol

	C_{pj} (J/(mol·K))
n-butane	141
i-butane	141
i-pentane	161

24.- A PFR is going to be employed to produce 1000 mol R/h from an aqueous solution of component A (C_{A0} = 1 mol/L). The reaction is $A \rightarrow R$, with $-r_A = 2\ C_A$ (mol/(L·h)), at constant T. The cost of the reactant stream is 0.4 €/mol$_A$ and the cost of the reactor is 0.2 €/(L·h). If the reactive A that is not used is discharged, find the optimal operating conditions (V, X_A, n_{A0}) to achieve a minimum cost of R. Which is the minimum cost of R under these conditions?

25.- *(exam jan'11)* The elementary gas-phase reaction $2A \rightarrow B + 2C$ is going to be carried out in an adiabatic plug flow reactor working at constant P. The kinetic equation is given by the following expression: $-r_A = 79980\cdot exp(-1683/T)C_A^2$ (k in L·mol^{-1}·h^{-1}). The operating cost of the reactor is 0.05 €/(L·h). The cost of the reactive A is 0.35 €/mol, and reactive A unconsumed is not reused. If we want to produce 100 mol/h of B, the feeding contains A (C_{A0}

= 0.4 mol/L) and inert (10% mol) and it is introduced into the reactor at a temperature of 25°C, working at constant pressure, obtain:

- Conversion of A in the PFR so that the total cost is minimum
- Volume of the corresponding PFR
- Total cost in the PFR

Other data:

C_{pA} = 18 cal/($mol_A \cdot K$), C_{pB} = 14 cal/($mol_B \cdot K$)
C_{pC} = 12 cal/($mol_C \cdot K$), C_{pI} = 10 cal/($mol_I \cdot K$)
$\Delta H^{*}_{(20°C)}$ = -60500 J/mol_A