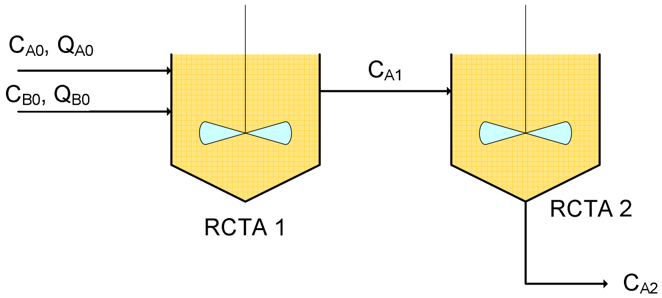
<u>CHEMICAL REACTORS</u> - <u>PROBLEMS OF REACTOR ASSOCIATION 47-60</u>

47.- *(exam jan'09)* The elementary chemical reaction in liquid phase $A + B \rightarrow C$ is carried out in two equal sized CSTR connected in series. The reagents are supplied separately to the first reactor (two streams). The reactors are initially filled with inert material. Each of the CSTR has a capacity of 200 L. The volumetric flow rates of entry into the first reactor are Q_{A0} = 10 L/min of A and Q_{B0} = 10 L/min of B, with $C_{A0} = C_{B0}$ = 2 mol/L. The kinetic rate constant k is 0.025 L/(mol·min).



a) Calculate the values of C_{A1} and C_{A2} in steady state. What is the global conversion of reactant A in steady state (from the first reactor inlet to the outlet of the second reactor)?
b) We will now study the system before reaching the steady state. For this, it is considered that t = 0 is the moment in which reagents begin to be delivered to the first reactor, although the volumetric flow had reached before the steady state with inert matter. Determine the time required to reach steady state in the first reactor (it can be assumed that this is virtually reached when C_{A1} exiting the first reactor is 99% of the value calculated for the steady state).
c) Represent on a graph the concentration of A leaving the first tank with time until steady state is reached.
d) Write (without solving) for the second reactor an equation similar to that mentioned in b). Espress it in terms of volumes and concentrations. Indicate in parentheses in the equation which variables change over time (for example, if the volume changes with time: V(t)). Indicate numerical subscripts for the variables that need them (for example, C_{A1} or C_{A2}).

48.- 1000 L/min of a solution having a concentration of 0.2 mol/L of A enter into a vertical tubular reactor. The reaction, at constant temperature, is first order and the volume of reactor is such that a conversion of 50% is achieved. After 3 years of work, the drip of the pump becomes 10% of the volumeric inflow. If this leak is collected and fed back into the reactor, which one will be the new conversion?

49.- The homogeneous gas-phase reaction $A \rightarrow 3B$ follows a second order kinetics. For a feed rate of pure A of 4 m^3/h at 5 atm and 350°C, an isothermal pilot reactor consisting of a tube with an internal diameter of 2.5 cm and 2 m length gave a conversion of 60%. A commercial plant will treat 320 m^3/h of feeding consisting of 60% A and 40% inerts at 25 atm and 350°C, with the aim of reaching a conversion degree of 80%. If two identical isothermal PFR are going to be connected in parallel, circulating half of the flow for each of them, which volume will each reactor have to achieve the required conversion?

50.- *(exam jan'07)* We want to obtain the product B by the elementary reversible reaction in gas phase $A \leftrightarrow B$ using a CSTR or a PFR, both adiabatic and working at constant P. The reactor is fed with a stream that only contains component A, with a molar flow rate of 1000 mol/min and an initial concentration of 4 mol/L of A, measured at the feeding temperature (T_0). If a conversion degree (ξ_A) of 0.8 is required, determine:

a) The minimum volumen if a CSTR is employed, and the corresponding T_0.
b) The minimum volumen if a PFR is employed, and the corresponding T_0.

Note: For ξ_A = 0.8 the temperature of the reaction can not be above 74°C (equilibrium condition).

<u>*Data*</u>:

Component	C_p^*(cal/(mol·K))
A	250
B	250

* C_p independent of temperature

ΔH_{ref} (25ºC)= -75.3 kJ/mol

Kinetics direct reaction			Kinetics reverse reaction		
k_{0d}	3.39×10^7	min^{-1}	k_{0i}	1.81×10^{18}	min^{-1}
E_{ad}	48900	J/mol	E_{ai}	124200	J/mol

51.- The irreversible gas phase reaction $A + B \rightarrow C$ is performed at 227°C and 10 atm. The reaction rate (mol/(L·min)) in terms of the conversion degree is:

$$-r_A = 0.0167 - 0.023(\xi_A - 0.1) + 0.0234(\xi_A - 0.1)(\xi_A - 0.7)$$

A feeding of 1 L/s containing 41% A, 41% B and 18% inerts (in molar basis) is going to be processed.

a) What is the total conversion if two continuous stirred tank reactors of 400 L each are connected in series?
b) What is the conversion if the two previous reactors are connected in parallel, with a volumetric flow rate entering each one being half of the initial?
c) What is the volume of the plug flow reactor necessary to achieve a conversion of 0.6 if the total molar flow of feeding is 2 mol/min, being the composition of the feeding the same as in previous cases?

52.- Certain substance is polymerized in solution at high temperature. If the temperature is above 105°C a product of inadequate properties is obtained, leading to operating at a temperature of 102°C. At this temperature the polymerization proceeds via a reaction that is represented by a kinetic equation of order 2 with respect to the monomer. The monomer is being treated in two equally sized CSTR connected in series, yielding a final product in which the monomer content is approximately 20%. The production is planned to be increased by incorporating a third reactor equal to the above two. To what percentage can the feeding flow rate increase in order to keep obtaining a product containing not more than 20% of the monomer, if the third reactor is connected in series to receive what comes from the second one?

53.- A CSTR and a PFR of 1 m^3 each one are used, connected in series, to perform the liquid-phase irreversible reaction $A \rightarrow P$ at constant T, with k = 0.5 L/(mol·min). If Q_v = 1000 L/min and C_{A0} = 1 mol/L, which is the most appropriate layout in order to obtain maximum conversion? Repeat the problem for the cases where the reaction order is 0 and 1 (with the same value of k and the corresponding units), and justify the results in each case.

54.- The elementary reaction $A + B \rightarrow R + S$ in liquid-phase is being carried out at constant T in a PFR using equimolar amounts of A and B. The conversion is 96% for a volumetric flow of 100 m^3/h. Calculate how much the inlet flow rate can be increased keeping the same final conversion if a CSTR ten times bigger than the PFR is coupled in series to the output of the PFR. If the CSTR was coupled before the PFR, should the flow rate increase more or less than in the previous case? Will the initial concentration influence? And the reaction order?

55.- The irreversible elementary reaction in liquid phase $A + B \rightarrow C$ is carried out adiabatically in a continuous reactor. An equimolar feeding of A and B at 27°C enters into the reactor, and the volumetric flow rate is 2 L/s (C_{A0} = 1 mol/L). Calculate:

a) Volume of PFR and CSTR needed to achieve in each case a 85% conversion. Indicate what volume of each reactor represents in the graph (1/r) versus ξ_A.
b) Maximum inlet temperature of the feeding that could be taken without exceeding the boiling point of liquid (550 K) at complete conversion (100%).
c) Conversion that can be achieved in an adiabatic CSTR of 500 L compared with two adiabatic CSTR of 250 L in series, being the conditions for the feeding of the first reactor in the last case those previously indicated.

Data:

$h_A^*{}_{(273\ K)}$ = -20 kcal/mol ; $h_B^*{}_{(273\ K)}$ = -15 kcal/mol; $h_C^*{}_{(273\ K)}$ = -41 kcal/mol
$C_{pA} = C_{pB}$ = 15 cal/(mol·K) ; C_{pC} = 30 cal/(mol·K)
$k_{(300\ K)}$ = 0.01 L/(mol·s) , E = 10000 cal/mol

56.- The liquid phase reaction $A \rightarrow P$ is carried out in a system of three CSTR of equal volume in series. 0.416 mol/s of A are fed into the first reactor. The molecular weight of A is 100 kg/kmol and the initial concentration of A is 1 kmol/m^3. The reaction is first order and the value of k is given by the expression $k = 4\cdot10^6\cdot\exp(-7900/T)$ (in s^{-1}). The reaction is exothermic and the enthalpy of reaction can be considered independent of temperature and equal to $-1.67 \cdot 10^6$ J/kg of A. The value (ρC_p) of the mixture is constant and equal to $4.2 \cdot 10^6$ J/(m^3·°C). If a final conversion of 0.9 is desired:

a) What is the volume of each reactor if they work isothermally ($T = T_0$) at 95°C?
b) What is the temperature at which the feeding must enter the first tank to work adiabatically at 95°C?
c) Consider that the first tank still works adiabatically at 95°C, and second and third tanks work isothermally, using heat exchangers for that. By using a coolant at 20°C and given a global coefficient of heat transfer of 1180 W/(m^2·°C), what is the heat transfer area required in each of tanks 2 and 3?

Note:

Consider that in sections b) and c) the volume and conversions for each reactor are those obtained in section a).

57.- *(exam dec'07)* The liquid phase reaction $A + 2B \rightarrow C$, whose kinetic equation corresponds to the expression $-r_A = kC_AC_B$ (in mole/(L·min)), is carried out in two CSTR in series. The volumetric flow rate is 80 L/min, with C_{A0} = 1 mol/L and C_{B0} = 2 mol/L. Considering that the volume of each reactor is 300 L, they work adiabatically and the final conversion at the output of the second reactor has to be 92.244%, at what temperature the feeding must be introduced in the first reactor?

Data:

$k = \exp(18.90 - 8000/T)$ (T in K, k in L/(mol·min))
C_{pA} = 20 J/(mol·K), C_{pB} = 40 J/(mol·K), C_{pC} = 100 J/(mol·K)
ΔH_{298K}^{*} = -20000 J/mol_A

58.- *(exam sep'07)* 1000 kg/h of a solution containing acetic acid (HAc) at 40% w/w are going to be produced by hydrolysis of acetic anhydride (AAc) in a cylindrical CSTR with L/D ratio equal to 1, using a feeding of acetic anhydride in water at 20°C. The final conversion has to be 85%, with acetic anhydride being the limiting reactant. The reaction takes place in liquid phase, being this:

$$AAc + H_2O \rightarrow 2HAc$$

Design the reactor considering the different possibilities below. Moreover, calculate in each case the total investment cost of the reactor, taking into account the following:

-Cost/ reactor volume = 0.70 €/L
-Cost/ cooling jacket area = 50 €/m^2
-Coste/ insulator area = 25 €/m^2

The design options are the following:

a) Operate the reactor isothermally, at the temperature of the feeding. In this case, a water-cooled jacket is employed to keep the temperature. The temperature inside the jacket is constant and equal to 15°C and the global coefficient of heat transfer is 940.5 kJ/(m^2·h·°C).

b) Operate the reactor at 50°C. A cooling jacket is also employed, with the same values of coolant temperature and global coefficient U as above.
c) Operate the reactor adiabatically.
d) Replace the CSTR with a PFR (L/D = 5) operating under adiabatic conditions.
e) Combine a PFR and a CSTR, both adiabatic, in the layout that provides a minimum total volume (suggestion for the choice: use the graph $1/(-r_A)$ vs ξ_A).

<u>Additional data</u>:

$k = 2.1338 \cdot 10^9 \exp(-5745.2/T)$ k in h^{-1}, T in K

-The partial order of reaction for water is 0.

-Density of solution = 1.027 kg/L, constant.

-Average specific heat of the solution = 3.5948 kJ/(L·ºC), constant.

-Enthalpy of the reaction constant.

-For the purposes of calculating the insulator surface area, assume that it covers only the lateral surface of the reactor

-In all cases, the feeding temperature is 20ºC.

	MW (kg/kmol)	h_f^* (298 K) (kJ/mol)
AAc	102	-647,90
H_2O	18	-285,49
HAc	60	-485,72

59.- *(exam jan'10)* In a continuous stirred tank reactor the reversible elementary gas phase reaction $2A \underset{2}{\overset{1}{\rightleftarrows}} 3R$ at constant pressure is carried out. 20% conversion of A is required.

a) Which working temperature allows to operate with the minimum volume of reactor? Which is this minimum volume?
b) What will be the heat removed/ added to the reactor?
c) What is the area of heat exchanger required to keep the temperature at the value calculated in section a)?
d) If an adiabatic plug flow reactor operating at the same pressure is connected in series at the output of this CSTR, what volume this PFR must have to achieve a value of 25% for total conversion of the system (CSTR + PFR)? At which temperature will the mixture exit the second reactor?

<u>Data:</u>

Input molar flow to the first reactor = 1000 mol A/min

Concentration of A entering the first reactor = 1 mol/L

Concentration of R entering the first reactor = 0 mol/L

$r_A = -k_1 C_A^2 + k_2 C_R^3$

k_{10} (L/(mol·min)) = 3.2×10^7

k_{20} (L^2/(mol^2·min))= 2.2×10^{18}

E_1 = 49000 J/mol

E_2 = 124200 J/mol

Inlet fluid temperature to the first reactor = 25ºC
Fluid temperature inside the heat exchanger = 225ºC
C_{pA} = 150 cal/(mol_A·K)
C_{pR} = 100 cal/(mol_R·K)
U = 1200 W/(m^2·ºC)
ΔH* (J/mol_A) = -37650 (reference temperature: 25ºC)

60.- *(exam jul'11)* The elementary reaction in liquid phase $2A \underset{2}{\overset{1}{\rightleftarrows}} B + C$ is carried out in two adiabatic CSTR connected in series. The feeding stream to the first reactor, with a volumetric flow rate of 2.8 m³/h and a temperature of 38ºC, contains only component A with a concentration of 24 kmol/m³. If a final conversion of 80% is required, determine:

a) The volume of both reactors, if they have to be of equal size
b) The volume that would be needed if only one CSTR is available

Data:

$k_{0,d}$= 39363 m³/(kmol·h) , $k_{0,rev}$= 0.204 m³/(kmol·h) (referred to reaction r_i)
Ea_d= 32281 kJ/kmol , Ea_{rev}= 8850 kJ/kmol
ΔH_i= -8000 kJ/kmol (at the temperature of the feeding stream, referred to unitary kmol of reaction)
Consider an average heat capacity of the mixture constant and equal to 251 kJ/(kmol·K).