36.- In order to carry out the decomposition of acetaldehyde in gas phase, which is an irreversible reaction and second order with respect to this compound, a continuous stirred tank reactor (CSTR) is employed. The reaction is:

\[ CH_3CHO \rightarrow CH_4 + CO \]

In the laboratory, a 100 L reactor has been employed operating at 520ºC and 1 atm with a feed rate of 0.025 kg/h. Under these conditions, a conversion degree of 80% was obtained. If we are going to work with a mass flow of 0.1 kg/s at industrial scale under the same conditions of pressure and temperature, and 75% conversion degree is required, which size of reactor will be needed?

37.- In a jacketed continuous stirred tank reactor, the first-order exothermic reaction \( A \rightarrow B \) is carried out in liquid phase. The feed rate consists of 90 kg/min of pure A. The aim is to generate 72 kg B/min. The reactor volume is 0.2 m\(^3\) and the coolant temperature is constant and equal to 273 K. The density of the mixture can be considered constant and equal to 0.9 kg/L. The average specific heat of the mixture is 2 J/(g·°C). The heat of the reaction can be considered independent of temperature and equal to -250 J/g of A. The global heat transfer coefficient is 300 W/(m\(^2\)·K) and the heat transfer area is 9 m\(^2\). The molecular weight of A and B is the same and equal to 90 g/mol. At 40ºC the rate constant is 1.127 min\(^{-1}\) and it is 1.421 min\(^{-1}\) at 50ºC. At which temperature the feeding should be introduced?

38.- In a CSTR, the endothermic and irreversible elementary reaction \( A + B \rightarrow C \) is performed in liquid phase. The reactor is heated by a steam jacket, and this steam is at its condensation temperature and pressure. The feeding, which is a mixture of A and B with both components at the same concentration equal to 2 kmol/m\(^3\), is introduced at 300 K with a flow rate of 30 L/min. The total volume of the reactor is 1.2 m\(^3\) and a conversion degree of 60% is required.

a) Find the steady-state temperature at which the reactor should operate to achieve the desired conversion.
b) Which will the condensation temperature of the heating steam be?
c) Which is the mass flow of the heating steam that condenses?

Data:

- \( k_{300 \, K} = 1.035 \, \text{m}^3/(\text{kmol} \cdot \text{h}) \), \( E = 10000 \, \text{kJ/kmol} \)
- Surface area of heat transfer: 6 m\(^2\)
- Global heat transfer coefficient: \( U = 15070 \, \text{kJ/(h} \cdot \text{m}^2 \cdot \text{K)} \)
- Latent heat of water vaporization: \( \lambda_a \, (\text{kcal/kg}) = 606.5 - 0.695 \, T \) (with T in ºC)
- \( \Delta H^{\circ}_{\text{f}, 300 \, K} = 41860 \, \text{kJ/kmol of A} \)
- \( C_{pA} = C_{pB} = 83.7 \, \text{kJ/(kmol} \cdot \text{K)} \), \( C_{pC} = 167.4 \, \text{kJ/(kmol} \cdot \text{K)} \) (assumed constants)
\[ R \text{ (gas constant)} = 2 \text{kcal/(kmol·K)} \]

39.- Acetic anhydride in an aqueous solution of 3 wt% is going to be hydrolyzed in order to obtain (after rectification) 50 kg/h of a solution of 98 wt% acetic acid. The hydrolysis should be conducted in a CSTR operating at 313 K, in order to reach a conversion degree of 85%. The reaction is:

\[ C_4H_6O_3 + H_2O \rightarrow 2 CH_3COOH \]

Calculate:

a) Volum of the reactor required
b) Heat exchange surface area needed
c) Cooling water flow rate

Data:
- Reaction is first order with respect to the molar concentration of acetic anhydride in solution, where \( k = 0.38 \text{ min}^{-1} \)
- Density of the solution fed: 1 g/cm\(^3\)
- Global heat transfer coefficient: \( U = 175 \text{ J/(s·m}^2\cdot\text{K)} \)
- Inlet temperature of cooling water: \( T_{\text{inl}} = 20^\circ\text{C} \)
- Outlet temperature of cooling water: \( T_{\text{out}} = 24^\circ\text{C} \)
- Heat of reaction (constant and independent of T): -29300 kJ/kmol of acetic acid
- The feeding is introduced at the reaction temperature
- Consider that the average molar specific heat of all the chemical species present in the system is 73.1 J/(mol·K)

40.- Propylene glycol is obtained by hydrolysis of propylene oxide, a reaction that takes place at room temperature in liquid phase when using sulfuric acid as catalyst:

\[ \text{CH}_2-\text{CH}-\text{CH}_3 + \text{H}_2\text{O} \xrightarrow{\text{H}_2\text{SO}_4} \text{CH}_3-\text{CH} = \text{CH}_2 \]

Consider you are the engineer in charge of the adiabatic CSTR being used to produce propylene glycol by this method. Lately, the presence of leaks are being detected (repeatedly you have indicated to your boss that the steel used when the reactor was built is not of sufficient quality to withstand corrosion by sulfuric acid), so its replacement is being considered. There is a stored CSTR of 1.136 m\(^3\) available, with vitrified coating, which could be used.

Two streams are fed to the reactor, one with 1134 kg/h of propylene oxide and 32.6 kmol/h of methanol (the latter is inert), and another with 364.14 kmol/h of an aqueous solution of sulfuric acid 0.1 wt%. Although the mixture of water-methanol-propylene oxide undergoes a slight contraction in volume (3%) due to the mixing effect, this effect can be neglected in the calculations. The temperature of the two feeding streams is 14.4°C before mixing, but increases to 24°C due to the heat of mixing, so this will be the temperature to be taken for the feeding that enters the system.
Furusawa et al. (J. Chem. Eng Jpn. 2, 95 (1969)), working in similar conditions, found that the reaction was first order with respect to propylene oxide and apparent zero order with respect to water when this is in excess, where the rate constant is:
\[ k = 16.96 \cdot 10^{12} \cdot \exp(-9064/T) \text{ (in h}^{-1}).\]

The process has an important restriction, which is that propylene oxide has a low boiling point (34.3°C at 1 atm). This requires that the mixture used does not exceed an operating temperature of 51.7 °C, otherwise much of propylene oxide vapor would be lost in the purge system. In these conditions, would it be appropriate to use the stored CSTR available to replace the one with leaks when working under adiabatic conditions? If so, which would the conversion degree of oxide to glycol be?

**Data:**

<table>
<thead>
<tr>
<th></th>
<th>MW (g/mol)</th>
<th>( \rho ) (g/cm(^3))</th>
<th>( C_p ) (kcal/(kmol·°C))</th>
</tr>
</thead>
<tbody>
<tr>
<td>propylene oxide</td>
<td>58.08</td>
<td>0.8590</td>
<td>35</td>
</tr>
<tr>
<td>water</td>
<td>18.02</td>
<td>0.9941</td>
<td>18</td>
</tr>
<tr>
<td>propylene glycol</td>
<td>76.11</td>
<td>1.0360</td>
<td>46</td>
</tr>
<tr>
<td>methanol</td>
<td>32.04</td>
<td>0.7914</td>
<td>19.5</td>
</tr>
</tbody>
</table>

At 20°C the reaction enthalpy is -84663.7 J/mol of propylene oxide.

41.- Following the above problem, you suggest to your boss to use the replacing reactor after adding a coil to remove heat and cool down the temperature. The surface coil available in stock is 3.7 m\(^2\) and the cooling water flowing through it is at a constant temperature of 29.5°C. The global heat transfer coefficient indicated by the manufacturer for this type of coil is 567.7 W/(m\(^2\)·°C). Would this coil be appropriate? And if so, under which conditions would the reaction take place?

42.- A homogeneous reaction in liquid phase is going to take place in an adiabatic ideal CSTR. The reaction, represented by scheme \( A \rightarrow P \), is irreversible and first order. The concentration of A in the feeding is 3 kmol/m\(^3\), and this will be introduced with a volumetric flow rate of 6·10\(^{-5}\) m\(^3\)/s (free of products) in a reactor of 18·10\(^{-3}\) m\(^3\). The kinetic constant is \( k = 4.48 \cdot 10^6 \cdot \exp(-7500/T) \) (in s\(^{-1}\)). If the feeding is introduced at 298 K:

a) How many stationary states are possible with these conditions? Indicate whether they are stable or unstable and their coordinates (conversion degree and \( T \))

b) From which temperature should the feeding be introduced to obtain a single steady state with a high conversion degree?

**Data:**

Mixture density = 1000 kg/m\(^3\) (constant)
Specific heat of the mixture = 4.18 kJ/(kg·K) (independent of temperature)
\( \Delta H^* = -209000 \text{ kJ/kmol A} \)
43.- *(exam dec’06)* In a refrigerated CSTR working at constant pressure the following reversible and elementary reaction takes place:

\[ A + B \xrightleftharpoons[\gamma]{\kappa} 2C \]

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 of 20 mol A/s.

a) Obtain the conversion degree that will be achieved in this reactor

b) Determine the temperature at which heat generated by the reaction (J/mol) will be maximum. Calculate the new value of the heat exchange surface area necessary so that the CSTR could operate at the temperature that maximizes the heat generated

**Data:**

<table>
<thead>
<tr>
<th>Components</th>
<th>( C_{pj} ) (J/(mol·K))</th>
<th>( h_j^* ) (25°C) (J/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>25</td>
<td>-40000</td>
</tr>
<tr>
<td>B</td>
<td>15</td>
<td>-30000</td>
</tr>
<tr>
<td>C</td>
<td>20</td>
<td>-45000</td>
</tr>
</tbody>
</table>

*Note: \( C_{pj} \) independent of temperature*

<table>
<thead>
<tr>
<th>Kinetics direct reaction</th>
<th>Kinetics reverse reaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k_{0d} )</td>
<td>1.45\times10^7 m³/(mol·s)</td>
</tr>
<tr>
<td>( E_{ad} )</td>
<td>70000 J/mol</td>
</tr>
</tbody>
</table>

Volum | 1.6 m³
U | 10 J/(m²·s·K)
Area | 2 m²
\( T_{\text{coolant}} \) | 17 °C

44.- According to available data (AIChE Students Contest Problem, 1984), the potential market of dibutyl phthalate (DBP) was 10800 t/year. The product is obtained by liquid-phase reaction of n-butanol with monobutyl phthalate (MBP). The reaction is elementary and is catalyzed by sulfuric acid, taking place at 38°C:

\[ \text{HOOC} - C_6H_4 - \text{COO} - C_4H_9 + C_4H_9OH \xrightarrow{H_2SO_4} C_6H_4 - (\text{COO} - C_4H_9)_2 + H_2O \]

It is desired to meet a demand which is one third of this potential market, for which a CSTR will be used, mixing MBP and butanol with sulfuric acid just before entering the reactor so that the concentration of the first two when entering the reactor is 3.2 kmol/m³. The rate constant for the reaction temperature is 0.075 m³/(kmol·h). DBP has to be subsequently subjected to a separation process to be purified, reintroducing into the reactor unconverted MBP and butanol. If the sale price of DBP is 1.18 €/kg, the purchase price of MBP is 0.98 €/kg and that of butanol is 0.94 €/kg, under which conditions (\( \xi, V \)) will the process have to be performed to get the maximum benefit?

**Data and notes:**

Consider the operating cost of the reactor is 5 €/(h·m\(^3\)). The cost of separation of DBP is a function of conversion: 8/\(\xi\) €/h. Since the unprocessed reagents are reused, reagent consumption will be given by the production of DBP obtained after reaching the steady state.

45.- *(exam jul’09)* An effective way to remove nitrogen oxide (NO) that comes from a combustion process is through the reduction reaction with NH\(_3\). Unfortunately, at the same time that the reduction reaction takes place another undesirable reaction that consumes NH\(_3\) occurs. The reactions involved are:

\[
4 \text{NO}(g) + 4 \text{NH}_3(g) + \text{O}_2(g) \rightarrow 4 \text{N}_2(g) + 6 \text{H}_2\text{O}(g)
\]
\[
4 \text{NH}_3(g) + 3 \text{O}_2(g) \rightarrow 2 \text{N}_2(g) + 6 \text{H}_2\text{O}(g)
\]

The following data are known:

\[
\eta = \frac{k_1 C_{\text{NO}} a C_{\text{NH}_3}}{1 + a C_{\text{NH}_3}} \quad \text{and} \quad r_2 = k_2 C_{\text{NH}_3},
\]

where \( k_j = k_{j0} \exp\left(-\frac{E_j}{RT}\right) \) and \( a = a_o \exp\left(-\frac{A}{RT}\right) \).

Specific data for these reactions are:

\[
k_{1,0} = 1\times10^6 \text{ s}^{-1}; \quad E_1 = 60 \text{kJ/mol}
\]
\[
k_{2,0} = 6.8\times10^7 \text{ s}^{-1}; \quad E_2 = 85 \text{kJ/mol}
\]
\[
a_o = 2.68\times10^{-17} \text{ m}^3/\text{mol}; \quad A = -213 \text{kJ/mol}
\]

Other data of interest are:

<table>
<thead>
<tr>
<th>(\Delta H_r) (kJ/mol) (25°C)</th>
<th>(C_p) (\text{NH}_3) (J/mol K)</th>
<th>(C_p) (\text{N}_2) (J/mol °C)</th>
<th>(C_p) (\text{H}_2\text{O}) (J/mol K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-1627.7</td>
<td>35.15</td>
<td>29.1</td>
<td>37.6</td>
</tr>
<tr>
<td>-1266.22</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(C_p) (\text{O}_2) (J/mol °C)</td>
<td>29.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(C_p) (\text{NO}) (J/mol K)</td>
<td>29.9</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Assume that these reactions can be carried out in a steady state CSTR of 200 L volume (actually, they are heterogeneous reactions performed in a fluidized bed of catalyst). Knowing that the reactor is fed with a flow rate of 0.15 m\(^3\)/s (assuming the same output value) with a concentration of 0.022 mol/m\(^3\) \(\text{NH}_3\), 0.016 mol/m\(^3\) NO and 0.947 mol/m\(^3\) \(\text{O}_2\):

- a) Calculate the maximum degree of progress of each reaction if they occur independently.
- b) Write the mass balances for \(\text{NH}_3\) and NO in this reactor in terms of the degree of progress of each reaction considering the simultaneous reactions.
- c) Calculate the degree of progress of each reaction if the reactor operates at 500 K (reactions are simultaneous).
- d) Knowing that the reactor operates adiabatically (simultaneous reactions), at which temperature does the feeding have to be provided for the reactor operating at 500 K?
46.-(exam jul’10) The following process is being carried out where two liquid streams are mixed in a continuous stirred tank reactor at steady state with the aim of obtaining the product R by means of reaction 1. Unfortunately, the by-product S is also produced by reaction 2.

![Diagram of a reactor with two streams](image)

The stream $Q_0$ only contains component A (with a concentration of 20 mol/L) and water (36 mol/L). In the stream $Q_0'$ only component B (with a concentration of 40 mol/L) and water (25 mol/L) are present. The water acts as an inert in this process. Both streams enter at 30°C.

Other data:
$Q_0 = Q_0' = 50$ L/min
$r_1 \text{ (mol/(L·min))} = k_1 c_A^{1.5} c_B^{0.3}$ (C_A and C_B in mol/L)
$r_2 \text{ (mol/(L·min))} = k_2 c_A^{0.5} c_B^{1.8}$ (C_A and C_B in mol/L)
$k_{10} = 3.7 \times 10^7$ (corresponding units where the volume is in L, the amount of matter in mole and the time in minutes).
$k_{20} = 1.0 \times 10^7$ (corresponding units where the volume is in L, the amount of matter in mole and the time in minutes).
$E_1 = 49000 \text{ J/mol}, E_2 = 50000 \text{ J/mol}$
$V_{\text{reactor}} = 385$ L
$T_{\text{air}} = 18 \text{ °C}$
$C_{p,A} = 15 \text{ cal/(mol}_A\text{·K)}, C_{p,B} = 11 \text{ cal/(mol}_B\text{·K)}, C_{p,R} = 12 \text{ cal/(mol}_R\text{·°C)}, C_{p,S} = 14 \text{ cal/(mol}_S\text{·°C)}, C_{p,\text{water}} = 1 \text{ cal/(g}_\text{water}\text{·°C)}$
Global heat transfer coefficient between the reactor and air = 1200 W/(m²·°C)
$\Delta H_1^* = -3765 \text{ J/mol}_A$, $\Delta H_2^* = -3855 \text{ J/mol}_A$
(Note: reference temperature $T^*$ is 25°C)

a) Indicate the units of $k_{10}$ and $k_{20}$.
b) If it is intended that 85% of A reacts, which concentration will A and B have in the output stream? Which percentage of B has reacted?
c) Which is the working temperature of the reactor?
d) Which are the concentrations of R and S when exiting the reactor?
e) Which are the degrees of progress of each reaction?
f) Which heat flow does the reactor gain or lose? (indicate whether it gains or loses)
g) Which is the heat transfer area?