PROBLEMS OF NON IDEAL REACTORS 50-63

50.- According to several experiments carried out in a continuous stirred tank reactor we suspect that the behaviour of the reactor is non ideal. The response to a pulse tracer test is given by equation $C(t) = 5\exp(-2.5t)$ (with t in min and C in mg/L). It seems that the reactor can be modeled considering that the fluid elements of different ages do not mix with each other, behaving like if small batch reactors were operating inside the continuous reactor (complete segregation). Obtain:

a) The plots of E(t) and F(t)
b) The mean residence time t_m and the real volume of the reactor, if the tracer test has been carried out with a value of Q_v equal to 2 L/min
c) Which fraction of the effluent remains in the reactor after the first minute after injection of the tracer?
d) Which conversion could be achieved in this reactor with the model previously commented if a second-order reaction was carried out in liquid phase at constant T with $kC_{A0} = 23.75\ min^{-1}$? (k referred to-$r_A$)

51.- The second-order reaction of dimerisation $2A \rightarrow B$ (with $r_A = -kC_A^2$) takes place in liquid phase, with k = 0.01 dm^3/(mol·min) at the reaction temperature. The feeding is pure A with an input concentration of 8 mol/L. The theoretical volume of the reactor is 1000 L and the volumetric flow rate of the feed for the reaction is 25 L/min.

In order to understand the behaviour of the reactor better, which does not behave ideally, a pulse tracer test has been performed with a volumetric flow rate of 25 L/min, and the results are shown in the following table:

t (min)	0	5	10	15	20	30	40	50	70	100	125	150	175	200
C (mg/L)	112	95.8	82.2	70.6	60.9	45.6	34.5	26.3	15.7	7.67	5.11	2.55	1.73	0.90

a) We want to know the limits within which the conversion can vary depending on the degree of micromixing.
b) What is the real volume of the reactor?

52.- A pulse tracer test produces a signal with a parabolic shape that fits to the following equation (time in minutes, concentration in $kmol/m^3$):

$$C = (t-2)^2, \quad 0 \le t \le 2$$
$$C = 0, \quad \text{any other } t$$

Calculate:
a) The mean residence time.
b) The equations for E(t), E(θ) and F(t).

c) The conversion obtained under completely segregated flow conditions for an elementary liquid-phase reaction with a rate equation $r = kC_A$, with $k = 1\ min^{-1}$.
d) The parameters of the dispersion model that represent this curve, for closed-closed vessels.

53.- Consider the first-order reaction $A \rightarrow B$ carried out in a tubular reactor of 10 cm diameter and 6.36 m length in liquid phase. The kinetic constant is 0.25 min^{-1}. A pulse tracer test is performed in the reactor with the following results:

t (min)	0	1	2	3	4	5	6	7	8	9	10	12	14
C (g/m^3)	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0

Calculate the conversion in the system obtained using: a) the dispersion model for a closed-closed vessel, b) tanks-in-series model, c) ideal PFR model d) complete segregation model, e) ideal CSTR model.

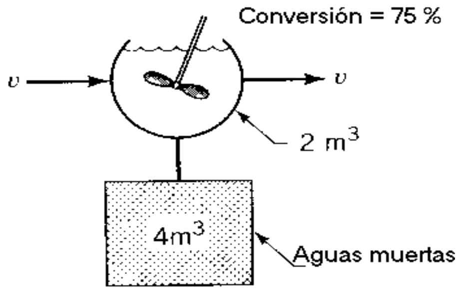
54.- In order to characterise the flow in a reactor a pulse tracer test was carried out, obtaining the following experimental values with a volumetric flow rate of 10 L/min:

t (min)	1	2	3	4	5	6	8	10	15	20	30	41	52
C (mg/L)	9	35	52	65	82	77	70	56	47	32	15	7	3

Based on these results, it is suspected that the flow in this reactor could be modeled by a dispersion model or a tanks-in-series model. In the reactor, the reaction $A + B \rightarrow P$ is carried out in liquid phase. Since there is a large excess of B, the reaction can be considered pseudo first order. If the reactor behaved as an ideal PFR, it would yield a 99% conversion. Determine the conversion to be obtained in each of the following cases:

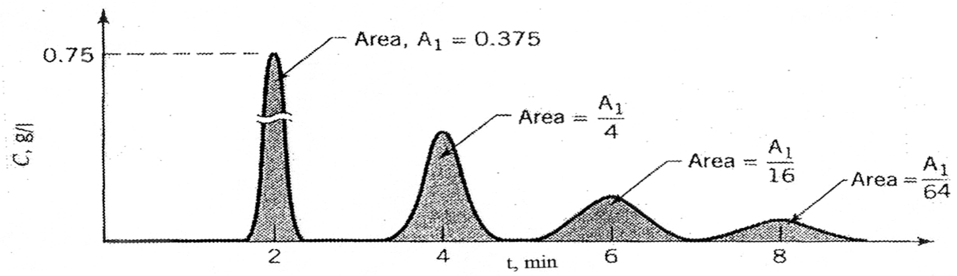
a) Assuming a dispersion model for a closed-closed vessel.
b) With the tanks-in-series model.
c) From the direct use of the experimental tracer curve.
d) With the model of an ideal CSTR.

55.- We have a tank reactor of 6 m^3 that gives a conversion of 75% for the first-order reaction in liquid phase $A \rightarrow R$. However, it is suspected that the mixture is incomplete and there is an undesirable flow pattern, since the reactor is stirred with a stir operating at low power. An experiment with pulse tracer input shows that it is like this and provides the flow model shown schematically in the figure. Calculate the conversion that can be obtained if the stirrer is replaced by a high-powered one to ensure a thorough mixing. What is the conversion in both cases if the fluid used is a macrofluid?



56.- A tank of 860 L is used as a liquid-gas reactor. The gas bubbles rise through the reactor and exit the top part. The liquid flows in the opposite direction to the gas, with a volumetric flow rate of 5 L/s. To get an idea of the pattern of fluid flow in this tank, a pulse tracer is injected (M = 150 g) at the entrance of the liquid and the concentration is measured at the exit as shown in the figure.

a) Is this experiment well done? Is all the injected tracer collected?
b) If so, calculate the fraction of reactor occupied by the liquid.
c) Determine the E curve as a function of the concentration curve measured.
d) Qualitatively, what do you think that is happening in the reactor?
e) If the liquid is a macrofluid (C_{A0} = 2 mol/L) with rate constant k = 0.5 L/(mol·min) (referring k to $-r_A$), what will be the final conversion?



57.- *(exam feb'08)* We want to perform in a tank reactor the liquid phase reaction $2A \rightarrow B$. It has been determined that the rate equation is:

$$r = \frac{0.5 \cdot C_A}{1 + 0.5 \cdot C_A} \qquad (r \text{ in mol·L}^{-1}\text{·h}^{-1} \text{ and } C_A \text{ in mol/L})$$

In order to characterise the reactor, a pulse tracer test was performed, after which it was obtained that the tracer concentration measured versus time can be fitted to the following equation:

$$C(t) = 2\exp(-2t) \qquad (C \text{ in mg/L and } t \text{ in h})$$

a) Calculate E(t) and the mean residence time in the reactor t_m.
b) Calculate F(t). Which fraction of the effluent will remain in the reactor after the first hour after injection of the tracer?

c) Calculate the conversion to be obtained in the reactor with the corresponding approximation of the reaction rate if the initial concentration of A is low (C_{A0} = 0.001 mol/L).
d) Calculate the expected conversion limits in case of having a high initial concentration of A (C_{A0} = 1 mol/L).
e) Compare the results of parts c) and d) with the conversion to be obtained using the ideal CSTR model with the initial concentrations indicated in those parts.

Suggestion: use time increments of 0.1 h.

58.- *(exam sep'07)* Consider the following 2 liquid-phase reactions taking place in parallel:

$$A \to B \qquad \therefore \quad r_B = k_1 C_A^2$$
$$A \to (1/2)C \quad \therefore \quad r_C = k_2 C_A$$

For a feeding stream containing only the reactant A, determine the concentrations of this compound according to the following models:

a) Ideal CSTR.
b) Ideal PFR.
c) Completely segregated flow with an E(t) identical to that obtained with a model of tanks in series for n = 2.
d) Maximum mixedness model with the same E(t) used in the previous part.
e) For the four previous cases, determine also the concentration of B, its yield (R) and selectivity (S).

Data:

C_{A0}=2.5 mol/L
k_1=3 L/(mol·s)
k_2=0.4 s^{-1}
τ=1 s

Suggestions:

- Present the model equations in terms of C_A instead of X_A. In this case, for the complete segregation model $X_A(t), \overline{X_A}$ can be replaced by $C_A(t), \overline{C}_A$ in the equation describing the model.
- In the maximum mixedness model consider a value of $\lambda \to \infty \equiv \lambda_\infty = 10\tau$.

59.- *(exam feb'07)* We have a reactor in which the elementary reaction $A \to 2B$ takes place in liquid phase with k = 0.15 min^{-1}. The theoretical volume of the reactor is 430 L. In order to characterise the behaviour of the reactor a pulse tracer test has been performed with a volumetric flow rate of 50 L/min. The concentrations measured at the exit of the reactor are the following ones:

t (min)	0	1	2	3	4	5	6	7	8	9
C (mg/L)	0	0	0	0	0	10	190	161.5	123.5	95

t (min)	10	11	12	13	14	15	16	17	18
C (mg/L)	76	58.9	43.7	20.9	7.6	1.9	0.38	0.095	0.0019

a) Calculate and plot the corresponding curves *E(t)*, *F(t)* and *E(θ)*.
b) Calculate the conversion for the reaction with the segregation model.
c) Repeat the previous part using the maximum mixedness model.
d) In view of the curves E and F, indicate a possible model which represents reasonably the behaviour of the reactor. Determine the parameters of the model, compare the model with the actual behaviour of the reactor and calculate the conversion using this model.

60.- *(exam jul'08)* Consider a tubular reactor with residence time $\tau = 10$ s, where an irreversible first-order reaction $A \rightarrow products$ takes place in liquid phase, and whose rate constant (referred to the reaction rate r_i) is known, $k = 0.1\ s^{-1}$.

a) The behaviour of this reactor can be approximated to a PFR with laminar flow regime whose residence time distribution function is as follows:

$$E(t) = \begin{cases} 0 & t < \dfrac{\tau}{2} \\ \dfrac{1}{2}\dfrac{\tau^2}{t^3} & t \geq \dfrac{\tau}{2} \end{cases}$$

Calculate the average conversion using the segregation model.

b) Compare the result in a) with the conversion that would result from the segregation model if the behaviour of the reactor approaches an ideal CSTR and an ideal PFR.
c) Plot the cumulative distribution function F(t) for a laminar PFR, an ideal CSTR and an ideal PFR, and according to these curves comment on the appropriateness of approximating the residence time distribution of a laminar PFR with that corresponding to an ideal CSTR or an ideal PFR.

61.- *(exam jul'10)* In a 10 L reactor we want to carry out the elementary reversible reaction $A \underset{2}{\overset{1}{\rightleftarrows}} B$ in liquid phase at constant temperature, with a feeding stream containing only reactant A. Previously, the behaviour of this reactor is going to be characterised, for which a tracer is introduced by a pulse signal, and the variation of tracer concentration with time at the reactor exit is measured. The data collected in the tracer experiment are the following:

t (min)	C(t) (mg/L)
0	0
0.5	60
1	70
1.5	86
2	91
2.5	84
3	78
3.5	76
4	67
4.5	57
5	47

t (min)	C(t) (mg/L)
6	36
7	25
9	12
11	5.7
13	2.2
15	0.98
17	0.43
19	0.16
21	0.07
23	0.03
25	0.01

a) Plot the normalised function of the residence time distribution E(θ) and the normalised function of the cumulative distribution F(θ). Which fraction of tracer remains inside the reactor at 6 minutes?

Calculate the conversion achieved in the reactor with the following models:

b) Tanks-in-series model.
c) Maximum mixedness model.

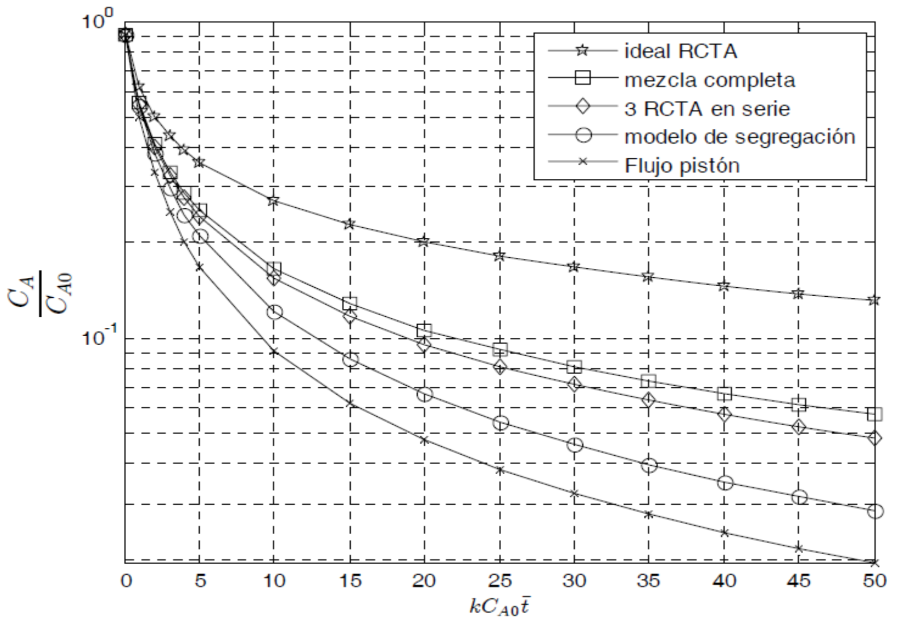
Note: for part c) use the expression of E(t) corresponding to the tanks-in-series model used in part b), and use time increments no longer than 0.5 minutes.

Data of kinetic constants:

k_1 (direct reaction) = 2 min^{-1}

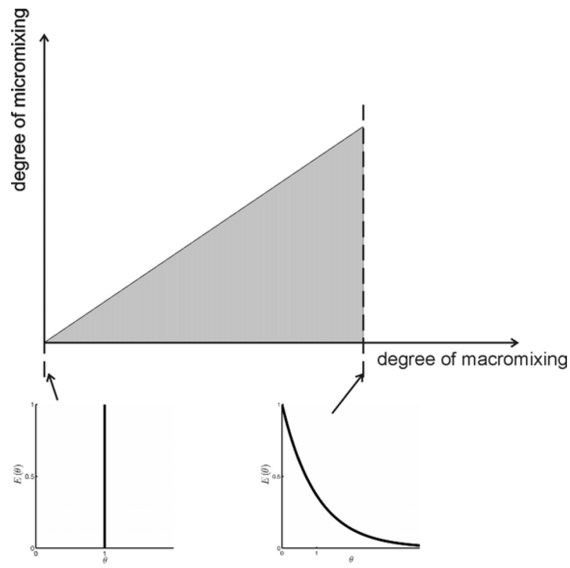
k_2 (reverse reaction) = 0.6 min^{-1}

62.- *(exam jan'10)* A second-order reaction in liquid phase with a single reagent ($\alpha_A = -1$) is carried out in a reactor whose RTD is $E(\theta)=\frac{27}{2}\theta^2 e^{-3\theta}$. We have studied the behaviour of this reactor using various models for a range of values for the parameter $R = kC_{A0}\tau$, obtaining the following plot:



Obtain the values of $\frac{\bar{C}_A}{C_{A0}}$ for the largest possible value of the parameter $R = kC_{A0}\tau = 50$ using the following models:

a) Ideal CSTR
b) Ideal PFR
c) Segregation model
d) Maximum mixedness model
e) 3 CSTR in series
f) Each of the above models assumes a certain degree of both micromixing and macromixing. Place a point for each model in the shaded area in the following figure. Explain the answer.



Suggestions:

-A normalised time *(θ)* value equal or beyond 4 can be assumed as infinite.

-Part c)
This part can be solved numerically but it is faster if it is done analytically using the following recommendations:

1- For the general equation of the segregation model, $\overline{X_A}$ and $X_A(t)$ can be replaced by $\frac{\bar{C}_A}{C_{A0}}$ and $\frac{C_A(t)}{C_{A0}}$, respectively.

2- The approximation $\int_0^{\infty} \frac{1}{1+R\theta} d\theta \approx \int_0^{\infty} \frac{1}{R\theta} d\theta$ is valid for $R > 40$.

3- Integration by parts is useful for an integrand with the following expression: xe^{-ax}. Choose $u = x$ and $dv = e^{-ax}dx$.

-Part d)

1- The following expression can be used: $\frac{E(\theta)}{1-F(\theta)} = \frac{\frac{27}{2}\theta^2}{\frac{9}{2}\theta^2 + 3\theta + 1}$.

2- The following expressions can transform the differential equation of the maximum mixedness model in terms of the normalised time *(θ)*:

-for the conversion degree of the key component: $\frac{dX_A}{d\lambda} = f(\lambda, X_A) \rightarrow \frac{dX_A}{d\theta} = \tau f(\lambda, X_A)$, and also: $\frac{E(\lambda)}{1-F(\lambda)} = \left(\frac{E(\theta)}{1-F(\theta)}\right)\frac{1}{\tau}$.

3- This part can be solved using Excel, but it is also solved faster using Matlab.

4- If we solve the ordinary differential equation by using Excel, you must take an increment of the independent variable small enough, $|\Delta\theta| \leq 0.02$.

63.- *(exam jan'11)* In a reactor of volume V = 10 L you want to carry out the reaction $2A \rightarrow B$ in liquid phase at constant temperature. The feeding is introduced with a volumetric flow rate Q_v of 2.5 L/min and it contains only reactant A, with C_{A0} = 0.2 mol/L. In order to characterise previously the behaviour of the reactor, and suspecting that it behaves like a tank reactor with dead volume, a pulse tracer test is performed using the above Q_v and we measure the variation of tracer concentration with time at the output of the reactor. The results obtained are shown in the following table:

t (min)	C(t) (mg/L)
0	15.37
0.4	15.10
0.8	12.15
1.2	11.93
1.6	9.60
2.0	9.43
2.4	7.59
2.8	7.46
3.2	6.00
4.0	5.24

t (min)	C(t) (mg/L)
4.8	3.75
5.6	3.27
6.8	2.08
8.0	1.62
9.2	1.03
10.8	0.71
12.8	0.36
16.8	0.12
20.8	0.034
24.0	0.001

a) Calculate and plot E(θ) and F(θ). Which fraction of tracer will be out at 4 minutes?
b) Which is the dead volume of the tank?

Calculate the conversion achieved in the reactor using the following models:

c) Ideal CSTR with dead volume
d) Segregation model
e) Maximum mixedness model
f) Compare the conversion values obtained with the above three models

Notes:

For parts d) and e) use the analytical expression of E(t) from the model of an ideal CSTR with dead volume.

Kinetic equation of the reaction:

$r = kC_A^2$, being k = 2.5 $L\cdot mol^{-1}\cdot min^{-1}$, with r in $mol\cdot L^{-1}\cdot min^{-1}$ and C_A in $mol\cdot L^{-1}$