Homogeneous reactor

Chapter4: Study of homogeneous isothermal chemical reactors with one reaction

Chapter 1: General

- Stoichiometry: Concept of conversion rate; Concept of advancement; Case of a single reaction; Case of several reactions.

Chapter 2: Classification of chemical reactors

- Perfectly stirred batch reactor;
- Perfectly stirred stationary continuous reactor;
- Stationary tubular continuous plug flow reactor.

Chapter 3: Material balances in ideal reactors

-Single reaction:
-Perfectly agitated closed reactor;
-Continuous perfectly stirred reactor in steady state;
-Piston reactor in steady state.

Chapter4: Study of homogeneous isothermal chemical reactors with one reaction

-R.D.P.A; R.C.P.A; R.C.P;
-Chemical Reactor Association:
=> Association of stationary continuous reactors in plug flow (series/parallel);
=> Association of perfectly stirred stationary continuous reactors (series/parallel);
-Comparative performances of ideal reactors.

Chapter 5: Study of homogeneous isothermal chemical reactors with several reactions

- Consecutive irreversible reactions;
-Competitive reactions;
-Selectivity and yield;

Chapter 6: Ideal non-isothermal reactors

-Notions of thermal balances in ideal non-isothermal reactors.

Chapter4: Study of homogeneous isothermal chemical reactors with one reaction

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IV.1. Introduction

Chemical reactors can be combined in different ways. These associations can be either in series (Figure 1) or in parallel (Figure 2).

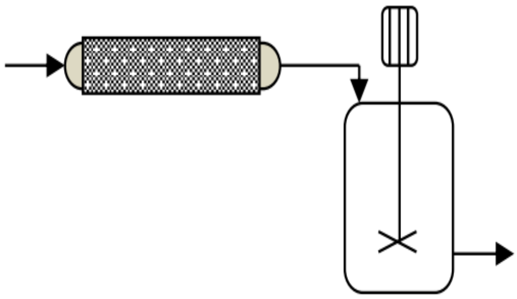


Figure 1: Serial association of a piston reactor and a continuous reactor

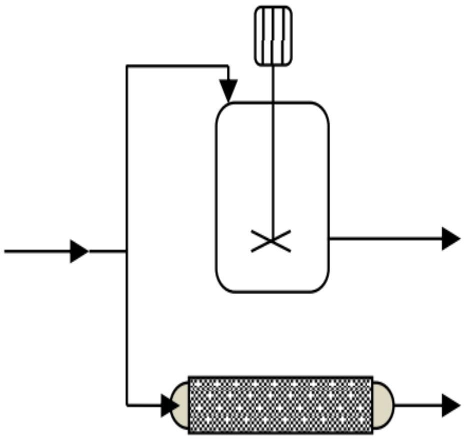
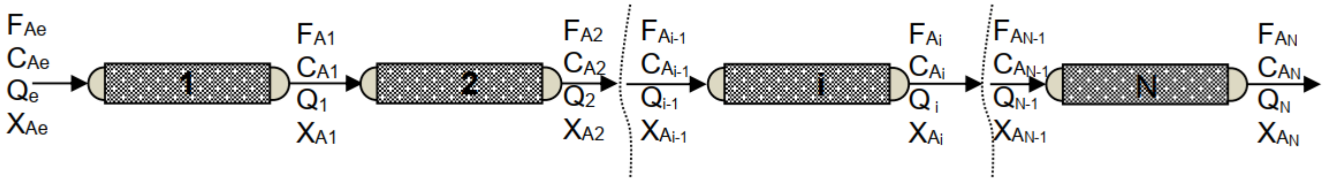


Figure 2: Parallel association of a continuous reactor and a piston reactor

- **The serial association of reactors makes it possible to increase the conversion rate.**
- **The parallel association of reactors makes it possible to increase the load to be treated, thus leading to an increase in production.**

IV.2. Association of piston reactors in series

Considering a chemical reaction taking place in a cascade of N piston reactors placed in series



The material balance relative to reagent A in the i^th reactor gives:

$$\frac{\tau_i}{C_{ie}} = \frac{V_i}{F_{ie}} = \int_{X_{Ai-1}}^{X_{Ai}} \frac{dX_A}{(-r_A)_i}$$

The overall passage time (τ_G) in this cascade is the sum of the passage times in all the reactors (same thing for the overall volume). This allows you to write:

$$\frac{\tau_G}{C_{ie}} = \frac{V_G}{F_{ie}} = \frac{\sum_{i=1}^{i=N}\tau_i}{C_{ie}} = \frac{\sum_{i=1}^{i=N}V_i}{F_{ie}} = \sum_{i=1}^{i=N}\int_{X_{Ai-1}}^{X_{Ai}} \frac{dX_A}{(-r_A)_i}$$

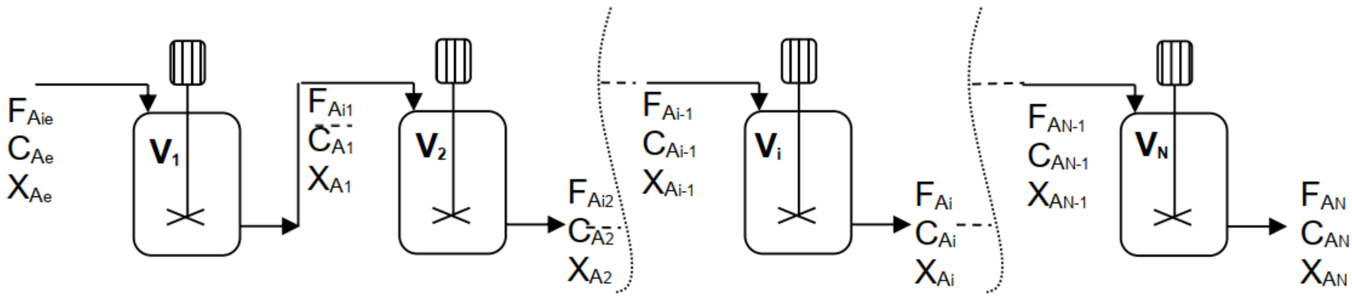
$$\sum_{i=1}^{i=N}\int_{X_{Ai-1}}^{X_{Ai}} \frac{dX_A}{(-r_A)_i} = \int_{X_{Ae}}^{X_N} \frac{dX_A}{(-r_A)}$$

$$\frac{\tau_G}{C_{ie}} = \frac{V_G}{F_{ie}} = \int_{X_{Ae}}^{X_N} \frac{dX_A}{(-r_A)} \qquad (17)$$

According to this relationship, a cascade of N piston reactors placed in series is equivalent to a single reactor piston whose volume is equal to the sum of the volumes of the reactors of the cascade and operating in the same conditions (F_{Ae}, X_{Ae} and X_{AN}).

IV. 3. Association of continuous reactors in series

Considering a chemical reaction taking place in a cascade of N continuous reactors perfectly stirred placed in series.



Material balance in relation to reagent A in the i^th reactor:

$$\frac{V_i}{F_{Ae}} = \frac{\tau_i}{C_{Ae}} = \frac{X_{Ai} - X_{Ai-1}}{(-r_A)_i} \quad \text{.....18}$$

Remarks

- According to this equation, if we are interested in the output of the i^th^ reactor, we must calculate beforehand the output quantities of all the reactors placed upstream.

IV. 3.1. Case where the volumes of the reactors are identical ($V_1 = V_2 = ... =V_N$)

Consider that the reaction is of order 1 with α'= 0 ($Q_e= Q_1 = Q_2 = ...= Q_N$)

$$X_{Ai} = \frac{F_{Ae} - F_{Ai}}{F_{Ae}} = \frac{C_{Ae}Q_e - C_{Ai}Q_i}{C_{Ae}Q_e} = \frac{C_{Ae} - C_{Ai}}{C_{Ae}} = 1 - \frac{C_{Ai}}{C_{Ae}}$$

We have: $X_{Ai-1} = 1 - \frac{C_{Ai-1}}{C_{Ae}}$ and: $(-r_A)_i = kC_{Ai} = kC_{Ae}(1-X_{Ai})$

Replacing X_{Ai}, X_{Ai-1} and $(-r_A)_i$ by their expressions in equation (18):

$$\frac{V_i}{F_{Ae}} = \frac{\tau_i}{C_{Ae}} = \frac{X_{Ai} - X_{Ai-1}}{(-r_A)_i} = \frac{\frac{C_{Ai-1}}{C_{Ae}} - \frac{C_{Ai}}{C_{Ae}}}{kC_{Ai}} = \frac{C_{Ai} - C_{Ai-1}}{kC_{Ae}C_{Ai}}$$

$$\text{D'où} \quad \frac{C_{Ai-1}}{C_{Ai}} = 1 + k\tau_i \quad ou \quad \frac{C_{Ai}}{C_{Ai-1}} = \frac{1}{1+k\tau_i}$$

By applying this last equation to the set of reactors in the cascade, we obtain:

$$1^{er}\ \text{RCPA}: \frac{C_{A1}}{C_{Ae}} = 1 + k\tau_1$$

$$2^{ème}\ \text{RCPA}: \frac{C_{A2}}{C_{A1}} = 1 + k\tau_2$$

$$i^{ème}\ \text{RCPA}: \frac{C_{Ai}}{C_{Ai-1}} = \frac{1}{1+k\tau_i}$$

$$N^{ème}\ \text{RCPA}: \frac{C_{AN}}{C_{AN-1}} = \frac{1}{1+k\tau_N}$$

By multiplying all of the equations side by side, we obtain:

$$\frac{C_{AN}}{C_{Ae}} = \frac{1}{(1+k\tau_i)^N} \qquad (19)$$

Equation (19) relates the concentration of A at the outlet of the reactor cascade, the flow time (or volume) in an individual reactor and the number of reactors in the cascade (N).

If we want to find a parameter, we must have the other two:
Knowing C_{AN} (or X_{AN}) and V_i (or τ_i), the number of reactors N is given by:

$$N = \frac{ln\left(\frac{C_{Ae}}{C_{AN}}\right)}{ln(1+k\tau_i)} \qquad (20)$$

Knowing C_{AN} (or X_{AN}) and N, the passage time τ_i (or the volume V_i) is given by:

$$\tau_i = \frac{V_i}{Q_e} = \frac{1}{k}\left[\left(\frac{C_{Ae}}{C_{AN}}\right)^{1/N} - 1\right] \qquad (21)$$

Remark:
The overall passage time τ_G is:

$$\tau_G = \sum_1^N \tau_i = \frac{\sum_1^N V_i}{Q_e} = \frac{N}{k}\left[\left(\frac{C_{Ae}}{C_{AN}}\right)^{1/N} - 1\right] \qquad (22)$$

Mathematically:

$$N \to \infty, \left(\frac{C_{Ae}}{C_{AN}}\right)^{1/N} \to 1 + \frac{1}{N}\ln\frac{C_{Ae}}{C_{AN}}$$

$$\tau_G = \frac{1}{k} ln\left(\frac{C_{Ae}}{C_{AN}}\right) \qquad (23)$$

Remark:
Relation (23) is exactly the same obtained if we do a material balance in a piston reactor operating under the same conditions as the cascade of continuous reactors (C_{Ae}, C_{AN}, $Q_e = Q_s$), with a volume equal to the sum of the volumes of the continuous cascade. Which means that a cascade of N firm reactors placed in series is equivalent to a single piston reactor operating in the same conditions as the cascade, but for N tending towards infinity (N →∞).

IV.3.2. Case where the volumes of the reactors are different ($V_1 \neq V_2 \neq .... \neq V_N$)

In this case, to obtain X_{AN}, it is necessary to solve equation (18) of the material balance step by step from the first reactor. This resolution can be done:
• Analytically (if the order of the reaction is simple),
• Numerically (if the order of the reaction is high),
• Or graphically.
For resolution graphically, equation (18) of the balance sheet is rearranged as follows:

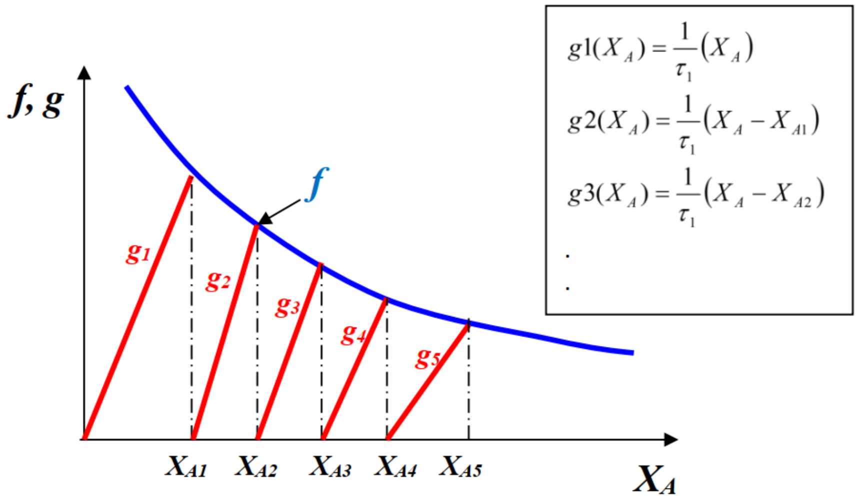
$$\frac{(-r_A)_i}{C_{Ae}} = \frac{1}{\tau_i}(X_{Ai} - X_{Ai-1})$$

The XAi solutions are the points of intersection between the function:

$$f(X_{Ai}) = \frac{(-r_A)_i}{C_{Ae}}$$

and the rights represented by the function:

$$g(X_{Ai}) = \frac{1}{\tau_i}(X_{Ai} - X_{Ai-1})$$

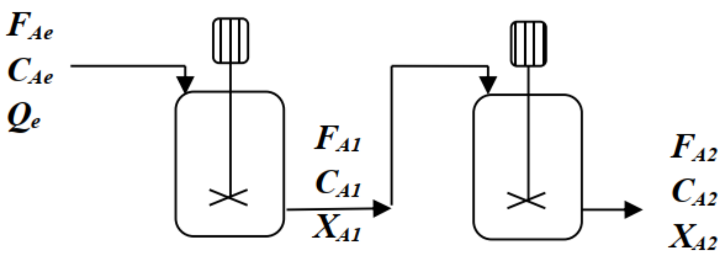


Noticed

The lines $g(X_A)$ become parallel when the passage times (τ_i) are identical (reactors of the same volume).

IV.3.3. Determining the optimal size of two continuous reactors placed in series

Or two continuous reactors of different volumes placed in series. We want to achieve a conversion rate X_{A2} (relative to reagent A) at the outlet of the second reactor. What should be the optimal volumes of the two reactors to reach X_{A2}?



$$\textbf{Réacteur 1:}\ \frac{V_1}{F_{Ae}} = \frac{X_{A1}}{(-r_A)_1} \quad (24)$$

$$\textbf{Réacteur 2:}\ \frac{V_2}{F_{Ae}} = \frac{X_{A2} - X_{A1}}{(-r_A)_2} \quad (25)$$

Answer:

The optimal volumes of the two reactors are those which ensure an overall volume (VG = V1 + V2) minimal. The latter (Vmin) can be determined either analytically or graphically.

Analytical resolution

$$V_G = V_1 + V_2 = F_{Ae}\left(\frac{X_{A1}}{(-r_A)_1} + \frac{X_{A2} - X_{A1}}{(-r_A)_2}\right) = f(X_{A1})$$

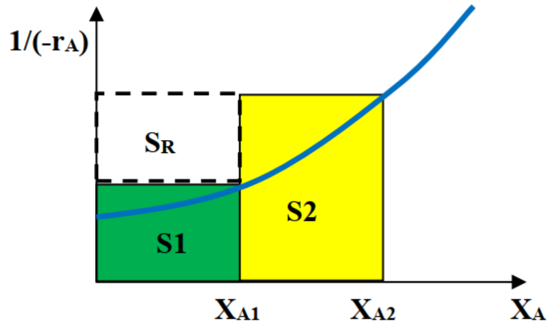
X_{A2} est donné

$$V_{G,\,min} \rightarrow \frac{dV_G}{dX_{A1}} = 0$$

This makes it possible to obtain the value of $X_{A1,\,opt}$ for which the overall volume is minimal. By substituting X_{A1} by $X_{A1,\,opt}$ in equations (24) and (25), we can determine the optimal volumes of the two continuous reactors placed in series.

Graphical resolution

- **1^er RCPA** $\frac{V_1}{F_{Ae}} = \frac{X_{A1}}{(-r_A)_1} = Surface - S1$
- **2^ème RCPA** $\frac{V_2}{F_{Ae}} = \frac{X_{A2} - X_{A1}}{(-r_A)_2} = Surface - S2$

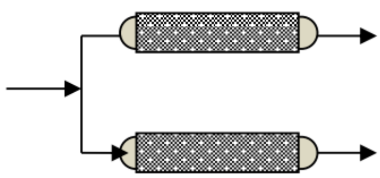


IV.4. Association en parallèle de réacteurs

Generally speaking, when reactors are placed in parallel, they are arranged so that the conversion rates at the outlet of the reactors are identical. This means that the times of passage are also identical. In this way, if the volumes of the reactors are known, we can then determine the volume flow rates circulating in each reactor.

RP1 : $\frac{\tau_1}{C_{ie}} = \frac{V_1}{F_{ie}} = \int_{X_{Aie}}^{X_{As}} \frac{dX_A}{(-r_A)_i}$

RP2 : $\frac{\tau_2}{C_{ie}} = \frac{V_i}{F_{ie}} = \int_{X_{Ai-1}}^{X_{Ai}} \frac{dX_A}{(-r_A)_i}$



$\tau_1 = V_1/Q_1$
$\tau_2 = V_2/Q_2$

Or, $\Longrightarrow$ $Q_1/Q_2 = V_1/V_2$

D'où $Q_1/Q_2 = V_1/V_2$
$Q_1+Q_2 = Qe$