



Homogeneous reactor

Chapter 2: Classification of chemical reactors

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.

Chapter 4: 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.

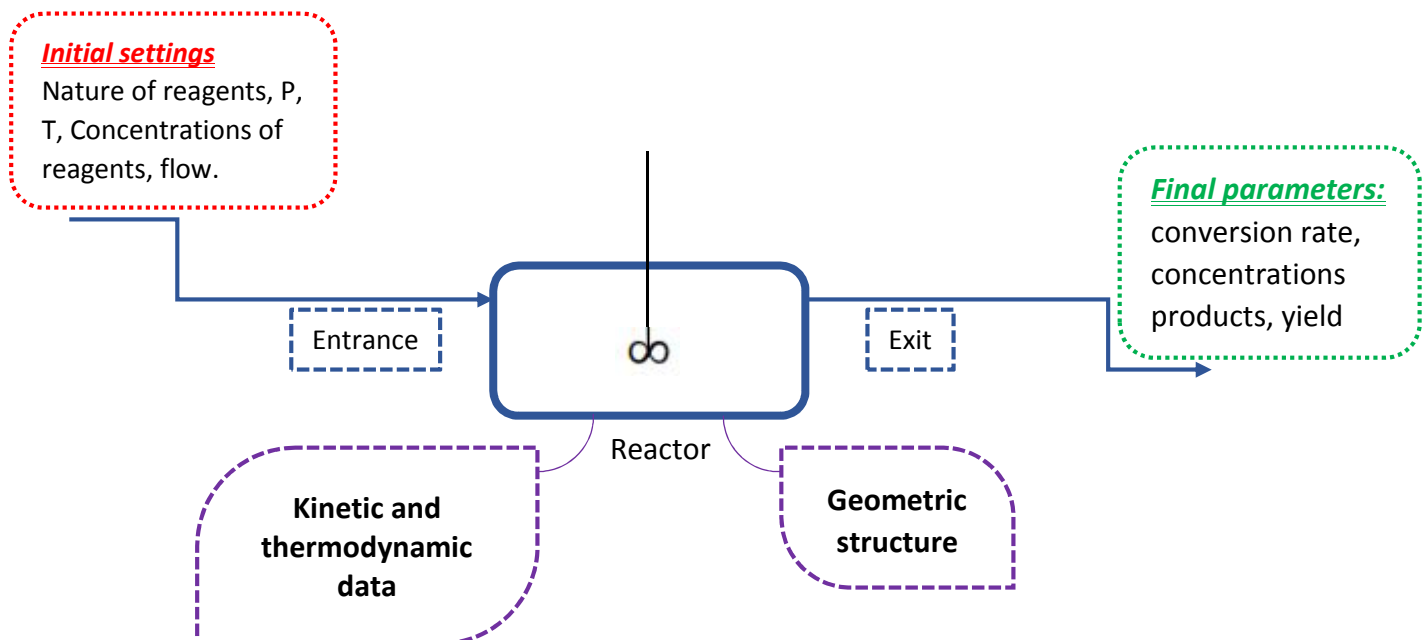


Chapter 2: Classification of chemical reactors

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

II.1. Introduction

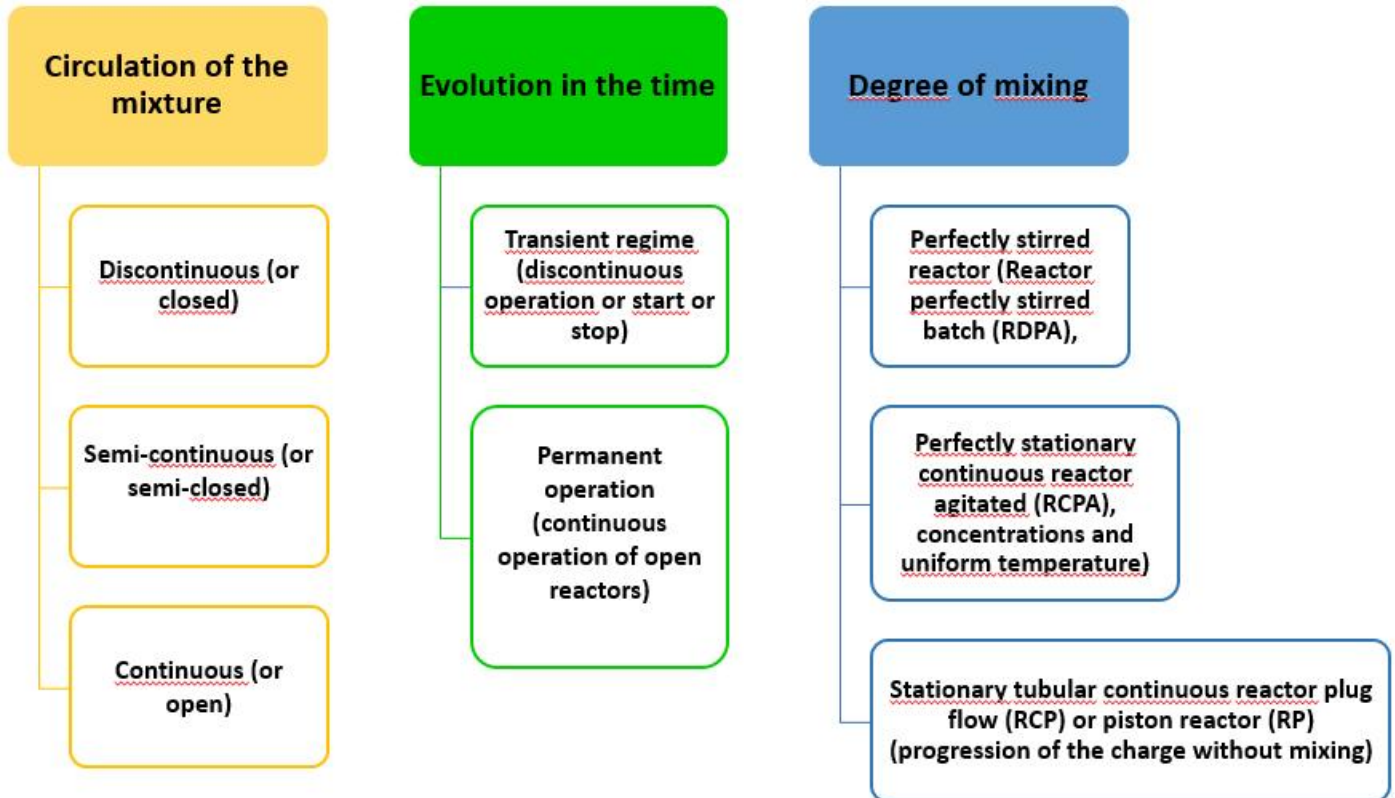
A chemical reactor is a container in which, chemical reactions and matter transformation processes can be carried out and optimized. The volume of the reactor is by definition the volume of the reacting species (and not the volume of container used).



II.2. Classification of chemical reactors

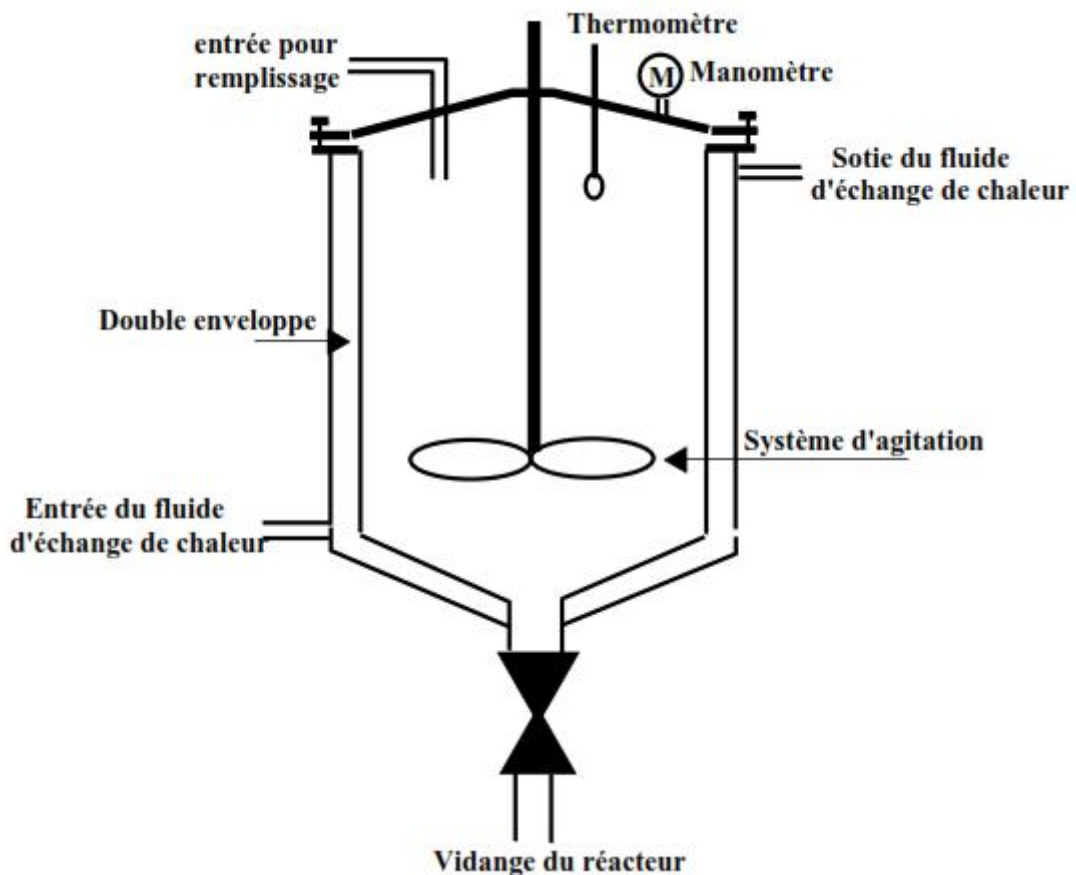
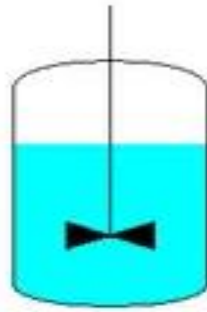
Chemical reactors occupy a central place in companies in the chemical and life sciences sector. By bringing together reagents under suitable conditions, they make it possible to combine and transform raw materials into useful products by chemical(s) reaction(s).

Reactors can be classified according to several criteria:



II.2.1. Perfectly stirred discontinuous reactor:

- ⇒ Commonly known as “*Batch reactor*” or Simply “*closed reactor*”.
- ✓ Corresponds to a system which does not exchange matter with the external environment ($E = E = 0$).
- ✓ They are very often used in the liquid phase.
- ✓ They are made up of:
 - A tank with a rounded bottom;
 - A stirring system;
 - A heat exchanger;
 - Inlet and outlet for filling and emptying
 - Accessories (manometer, thermometer, pH meter).
- ✓ The reagents are initially introduced into the reactor, although mixed, and left in the apparatus so that the reaction takes place for a certain time. The resulting mixture is then discharged;
- ✓ This is a non-stationary operation where the composition of the mixture changes over time but remains uniform at all times in the device;
- ✓ A homogeneous mixture at the molecular scale with an identical temperature in the entire reaction medium;
- ✓ Volume and density are constant.



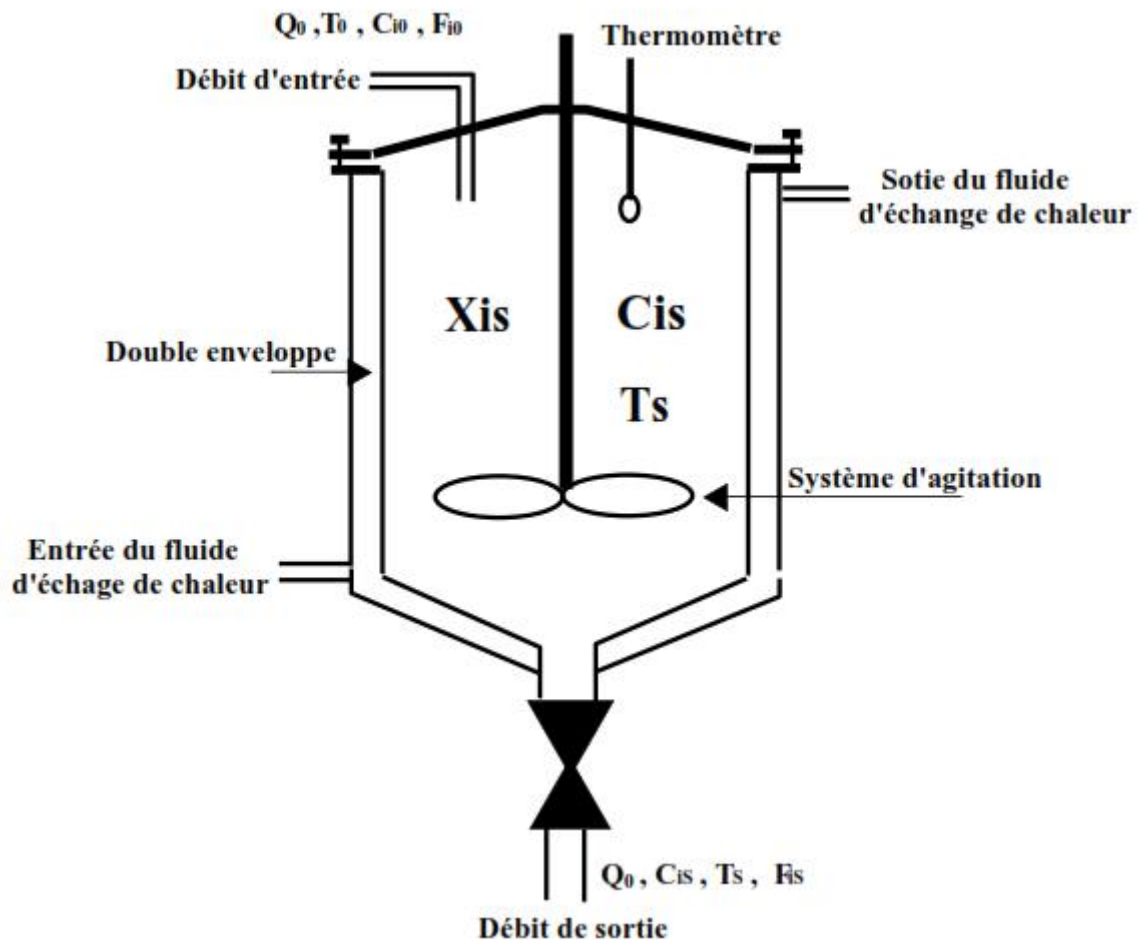
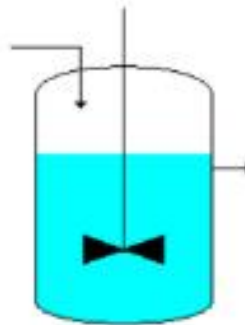
Schematization of closed reactor

<i>Advantages</i> 😊	<i>Disadvantages</i> ☹️
<ul style="list-style-type: none">+ Simple installation and offering great versatility.+ Allows reactions requiring variations in operating conditions (in particular change in temperature).	<ul style="list-style-type: none">- Works at high reagent concentrations at the start of the reaction (safety issue, poorer conversion in case of inhibition by the substrate).- Requires downtime between each operation (emptying, cleaning, filling) which affects performance.



II.2.2. Perfectly stirred stationary continuous reactor:

- ⇒ Otherwise called CSTR: “*continuous stirred tank reactor*” or simply “*open reactor*”.
- ✓ This is a stationary type reactor with ideal flow whose contents are well mixed and uniform;
- ✓ The output flow has therefore the same composition as the fluid in the reactor;
- ✓ A homogeneous mixture at the molecular scale with an identical temperature in the entire reaction medium;
- ✓ Volume and density are constant.



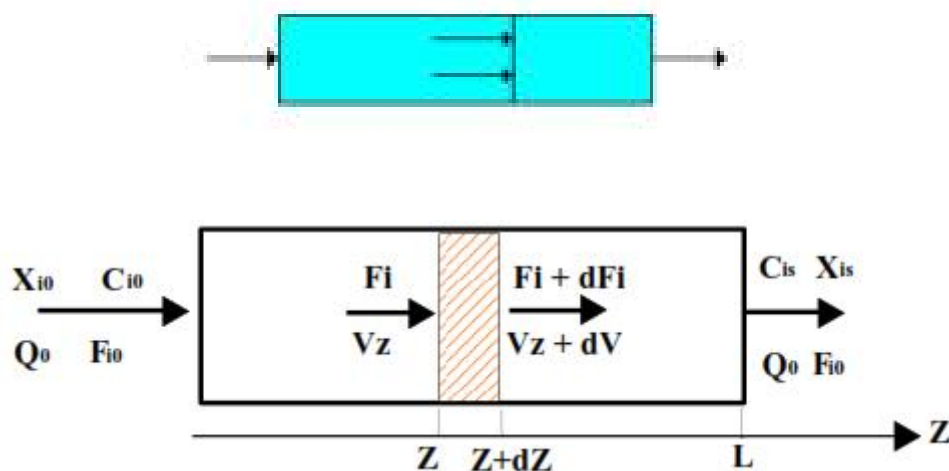
Schematization of open reactor



Advantages 😊	Disadvantages 😞
<ul style="list-style-type: none"> + Little variation in the quality of a product over a long period of time; + High performance; + Good for kinetic studies; + Works at low concentrations of reagents (better conversion rate or in case of inhibition by the substrate). 	<ul style="list-style-type: none"> - Less good conversion for reaction orders greater than one. - Requires excellent flow control (entrance and exit). - Does not allow reactions requiring variations in operating conditions.

II.2.3. Stationary tubular continuous plug flow reactor

- ⇒ Otherwise called PFTR: “Plug Flow Tubular Reactor” it is also a “piston reactor”.
- ✓ It is also an ideal flow stationary reactor;
- ✓ They are most often used for reactions in the gas phase in the presence of a catalyst;
- ✓ It is characterized by the fact that the flow of fluid through the reactor is orderly, with no element mixing with or overtaking another;
- ✓ Lateral diffusion is permitted, but axial mixing (in the direction flow) is assumed to be zero. The necessary and sufficient condition for the existence of a piston-type flow in the reactor is that the residence time in the reactor is the same for all elements of the fluid;
- ✓ The reactor is considered in a stationary state, but has a temperature and concentration profile depending on its axis;
- ✓ We do not consider the reactor in its entirety, but we divide it into thin sections;
- ✓ Density is constant.



Schematization of piston reactor



Advantages 😊

- + Little variation in the quality of a product over a long period of time.
- + High performance.

Disadvantages 😞

- Requires excellent flow control (input and output)

- **NOTE:**

- We will deal here with the case of these three homogeneous ideal reactors where the reaction takes place in a single liquid or gas phase.
- We will see the case of a simple reaction, then the case of multiple reactions.
- The reaction can be irreversible or reversible. It could be endo or exo-thermal ($\Delta H > 0$ or $\Delta H < 0$ respectively).
- In fluid mechanics, a fluid is said to be ideal (perfect) if it is possible to describe its movement without taking into account the effects of viscosity, as well as thermal conductivity in opposite of real fluid.