Course 1:
Fundamental notions

1. Introduction:

The principles of conservation of three physical quantities: matter (or mass), energy and momentum are generally used to solve process engineering problems. Systematic assessments are essential for calculating installations, but also for providing the engineer with information on the correct operation of a piece of equipment.

Industrial process concepts are based on material assessments. The assessments cover the entire process and specify the optimum quantities of raw materials and the quantities of finished products produced. The data on the individual process units dictate the flows and compositions of the system and set out the basic equations for equipment sizing.

A good understanding of material assessments calculations is essential in process design.

2. What is a mass assessment:

The mass assessment or material assessment is a calculation which consists of evaluating the quantities of products to be produced in the chemical and/or physical transformations of a process. This calculation gives the input and output flow rates for each unit operation.

3. What is the assessment used for?

Assessments are used to calculate all the data needed to size and optimise an installation. They enable us to make technical and economic assessments of the process and the process units, based on knowledge of the consumption of materials and energy and the yield of the products obtained.

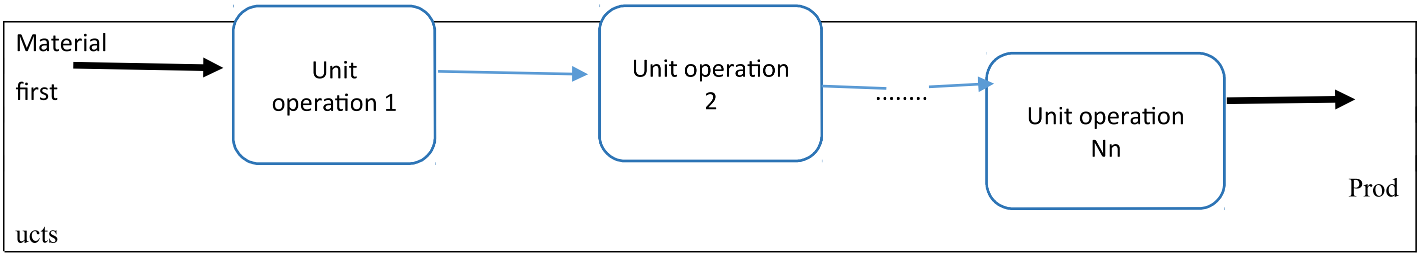
The material assessment approves and solves and/or validates the optimum operating conditions of a unit by :

- Calculate certain quantities (composition and quantities of material flows) ;
- Calculates certain ratios characteristic of a chemical process (conversion rate, recycling rate, yield, etc.) or a physical process (number of stages in a distillation operation).

The aim of the energy assessment is to determine, by calculation, the quantities of energy and, in particular, the quantities of heat, in order to choose the equipment best suited to the energy evolution and to reduce energy expenditure and estimate the manufacturing cost.

4. What is a process

This is the integration of unit operations illustrating the transformation of raw materials or reagents into products and/or by-products.



<u>Classification of processes</u>

before writing a material assessment, you need to identify the type of process involved

4.1. Discontinuous:

these are systems in which there is no exchange of matter between the system and the external environment during operation. The masses are charged before the start of the operation and are discharged when the device is stopped. (example: distillation batch).

4.2. Continuous system open system:

These are systems in which there are flows of materials entering and leaving the system during the operation. Example: pumping liquid at a constant rate through a distillation column to draw off product streams at the top and the bottom of the column.

4.3. Semi-continuous system or semi-open system:

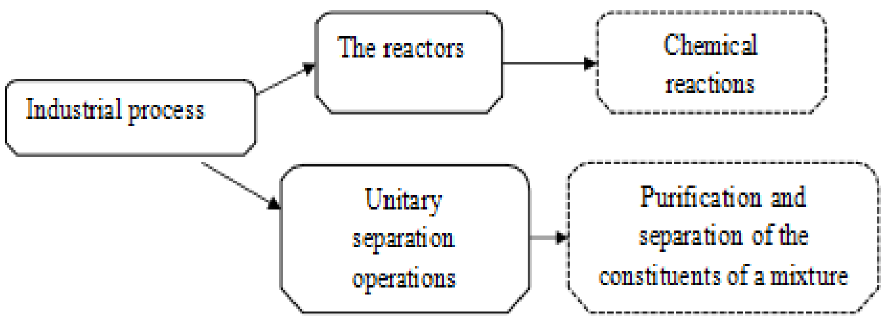
These are systems in which there is simultaneous entry and exit of matter during the operation and loading and unloading of masses at the beginning and the end of the operation. Example: washnig a gas in a column, filling a flask with air at a constant flow rate of 3 g/min.

4.4. **Stationary:** operating parameters (T, P, V, flow rates) do not vary with time.

4.5. **Transient:** process variables vary over time.

5. <u>Units operations</u>

Equipments in which one of the characteristics operations of a mechanism takes place. In an industrial process, the reactors in which the unit operations take place and the chemical reactions used to select and purify the components of a mixture evolve are generally characterised.

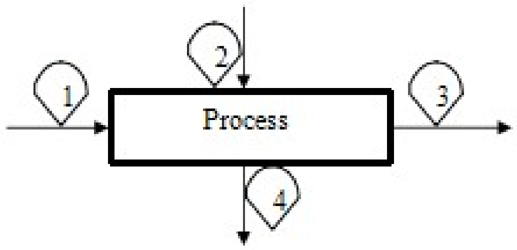


The most popular unit operations are:

- **Distillation:** separation of homogeneous liquid mixtures at different temperatures by evaporation.
- **Absorption:** movement of a gaseous solute towards a liquid phase.
- **Adsorption: liquid or gaseous particles** attach themselves to a solid surface.
- **Liquid-liquid extraction:** separation of substances from a miscible liquid-liquid mixture.
- **Sieving:** classifying solid particles according to their size.
- **Filtration:** removal of solid particles mixed with a liquid or gas.
- **Drying:** the dissipation of moisture or other liquids from a solid by evaporation

6. Flow of a process:

It is a movement of material and/or energy characterized by an origin, a destination and a path.



Each flow is characterized by a given or yet to be determined quantity of matter or heat. We can also find masses, volumes, concentrations, flow rates, etc. It all depends on the data for the process under study.

7. <u>Process variables:</u>

In a process, material flows are characterized by variables of various kinds (volume flow, temperature, pressure, composition, pH, electrical conductivity, etc)

Table I.1: The different balance sheet variables

en masse						
quantity	mass	mass flow rate	mass fraction	specific enthalpy	heat, work	heat output
symbol	m	$m^{\cdot}$	w	$\hat{H}$	$\boldsymbol{Q}$	$\boldsymbol{Q}^{\cdot}$
unit	kg	kg - s^{-1}	-	J - kg^{-1}	J	W
in mole						
quantity	number of moles	molar flow	mole fraction	molar enthalp y	heat, work	heat output
symbol	n	$n^{\cdot}$	x	$\bar{H}$	$\boldsymbol{Q}$	$\boldsymbol{Q}^{\cdot}$
unit	$mole$	$mole$ - s^{-1}	-	J - mol^{-1}	J	W

- **Mass fraction**

The quantity which expresses the mass composition of a mixture (the mass ratio of each constituent in the mixture) is the mass fraction noted **w**, or the mass percentage **(w%)**

$$W_i = (\text{mass of i}) / (\text{total mass}) = m_i/m$$

- **Molar fraction**

Is the *molar* composition of a mixture (i.e. the molar measurements of each component in the mixture). The *molar* ratio noted **x**, or the *molar percentage* (**x %**) is a measure for expressing the molar fraction of an element **i** and is equal to the ratio of the number of moles of this element $\mathbf{n_i}$ to the total number of moles **n** in the mixture.

$$x^i = \frac{\text{number of moles of i}}{\text{total number of moles}} = \frac{n_i}{n}$$

- Volume fraction of i : $\nu_i = V_i/V$
- Partial density of i: $\varrho_i = m_i/V_i$ (Kg/m^3)
- Molar concentration by volume of i: $C_i = n_i/V$ (kmol/m^3)
- The average molar mass of the mixture : $M\hat{} = \Sigma M_i x_i$ (Kg.kmol^{-1})
- The molar concentration by volume of the mixture $\Sigma C_i = \varrho / M$ (kmol.m^{-3}

- **the concept of accumulation**

accumulation can be positive in the case of material gain, or negative in the case of material loss by system

Example: stock back

- **Production and consumption**

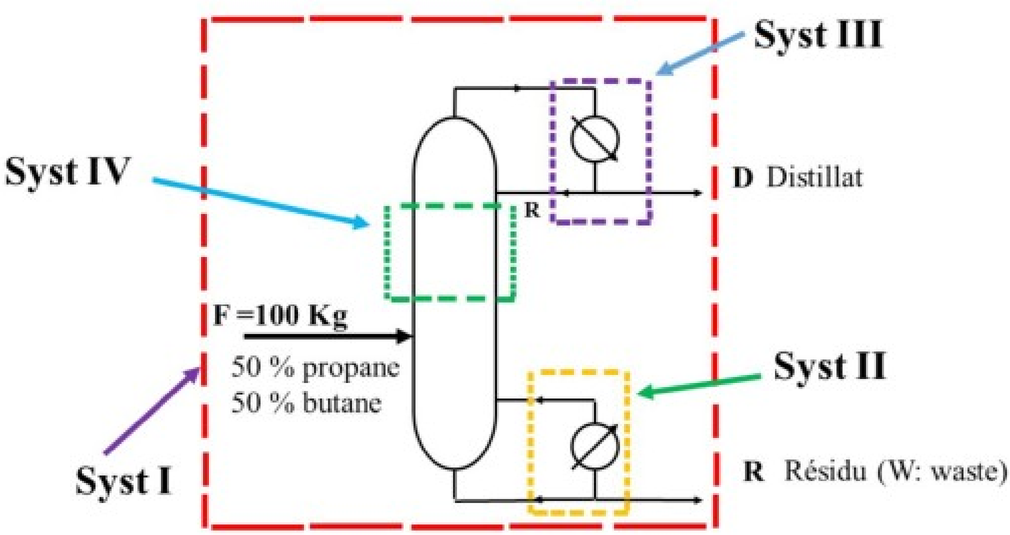
In the case of chemical reactions, we have the production of some particles, are called **"Products"** , and consumption of others is called **"Reactants".**

If we balance a reactant we use the consumption term in the balance equation, and if we balance a product we use the production parameter.

- **System**

it is always necessary to define the system on which we are making our material assessment. A system is a part of a process or the entire process on which we are making the assessment.

Example : Distillation Column



- **General equatEquation of a balance**

The assessment (balance) equation is written as follows:

Accumulation = Input – Output + Production – Consumption

Acc = I - O + P - C

in simplified terms, models are considered as black boxes containing transfer functions to input variables to produce a result (output variables)

Models are a simplified representation of reality. Simplifying assumptions must be made to help represent a complex reality. To be acceptable, the errors caused by the simplification of reality must be less than the accuracy of the phenomenon that we want to estimate.

3- Macroscopic assessment models

macroscopic models try to describe systems in term of the assessment of phenomena in batch, the production of a forest, the production of a chemical reactors, and the needs for irrigation water, among other examples.

The main models that we must use can be represented by macroscopic models. The evolution of the water level of a batch, in a dam or in a lake is the most typical case where a macroscopic model can be used to simulate reality.

4- Distillation column assessment :

- **Presentation of the conservation of matter (or mass)**

the law of conservation of matter, also known as the law of conservation of mass, states that the mass of a closed system will remain constant over time and will not be destroyed as a result, no matter what process is taking place inside the system.

An analogous statement is that mass cannot be created or destroyed, but it will be reorganized in space and transformed into different types of particles.

This implies that for any chemical process in a closed system, the mass of the reactants must be equal to the mass of the products. This is also the main idea of the first law of thermodynamics.

Lavoisier: " Nothing is lost, Nothing is created, everthing is transformed"

5- General equations:

The general form of the equation that translates the conservation of matter in a chemical engineering process is:

Input = Output + Mass accumulation

in our case, we will assume in each exercise that the accumulation in the system is zero.

Mathematically, the translation of the conservation of matter for a system without chemical reaction therefore becomes the following:

Input = Output

6- Yield (ŋ):

distillation yield: the aim of distillation is to obtain the maximum of the most volatile product in the distillate, so ŋ is equal to the quotient of the mass of the pure volatile product collected in the distillate by the mass of the same product in the feed.

$$Xd * D \Big/ Xf * F$$

7. Material balance for unit processes

This chapter should enable you to :

1- understand how the unit operations most commonly used in chemical engineering work.

2. draw a diagram of a fully documented process.

3. Calculate the number of degrees of freedom of a problem to ensure that it has a unique solution, given the available data.

4. Draw up the material balances for the problem.

Distillation is a separation method based on the differences in volatility between the constituents of a liquid mixture.

the distillation column operates in such a way that the more volatile constituents are recovered in the distillate at the top of the column, and the less volatile constituents remain at the bottom of the column in the reboiler.

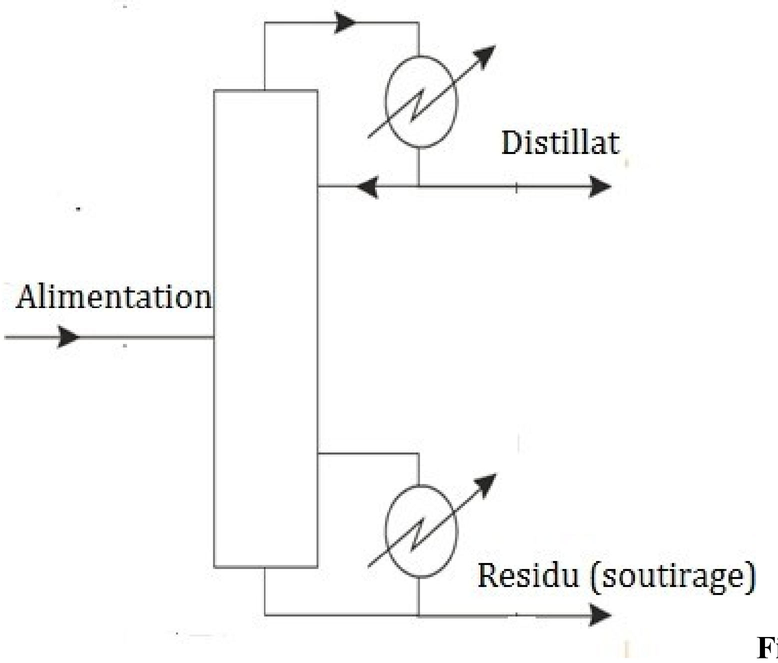
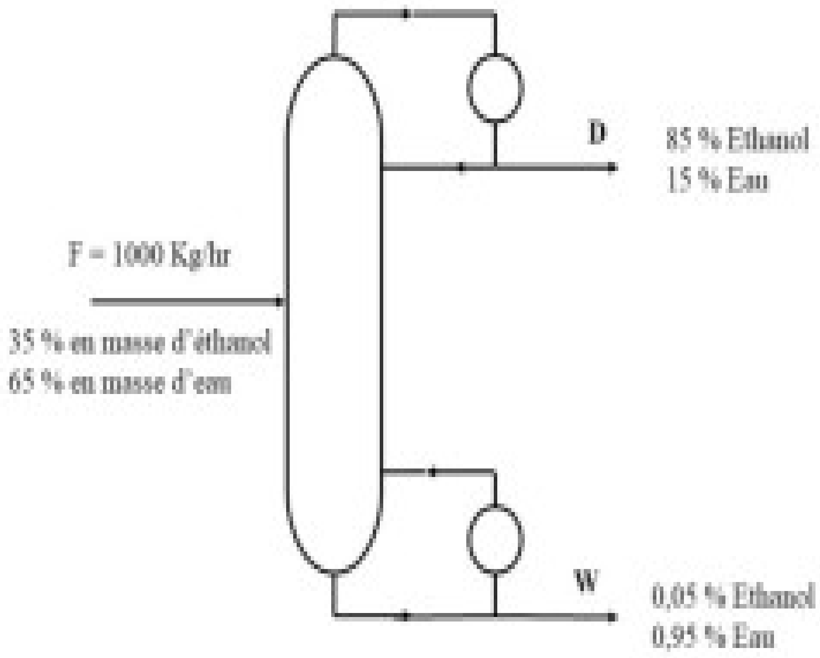


Figure 1: Distillation Column

- **Example 1:** Material assessment on a distillation column. Calculate D and W? And the distillation yield.



D: Distillate , W: Waste.

7.2. absorption column

Absorption is a physical process that consists of bringing a gaseous component into contact with a liquid phase in which it is soluble.

The purpose of this operation is to absorb a component contained in a feed gas.

The yield of the adsorption is the highest fraction in the enriched solution (E) by the fraction of the same elemnent in the feed

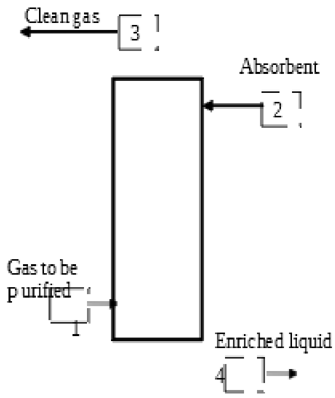
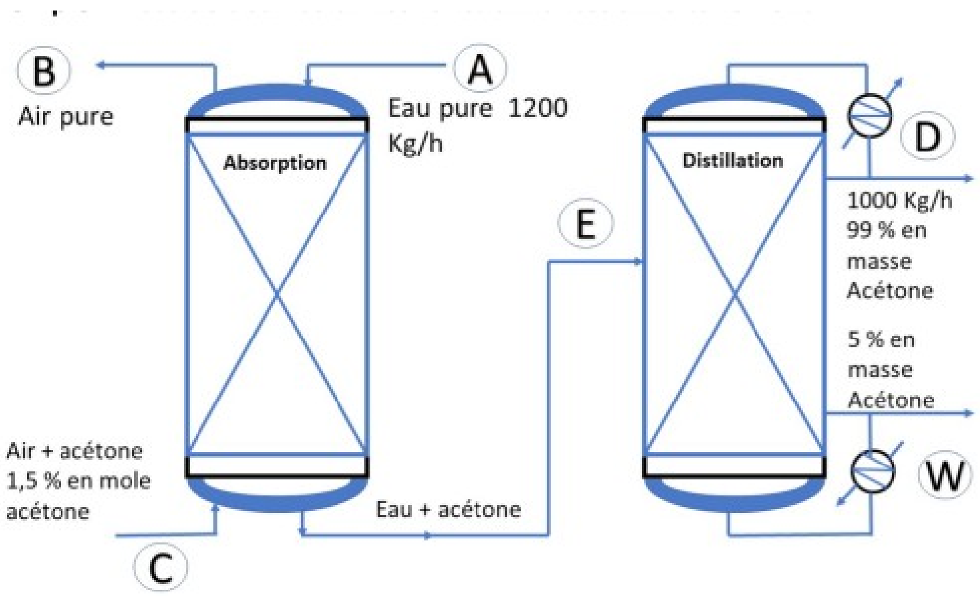


Figure 2: Absorption Column

- **Example 2:** case of two columns operating simultaneously



Determine the composition of E (the distillation column feed)

- to make an assessment we must proceed in stages:

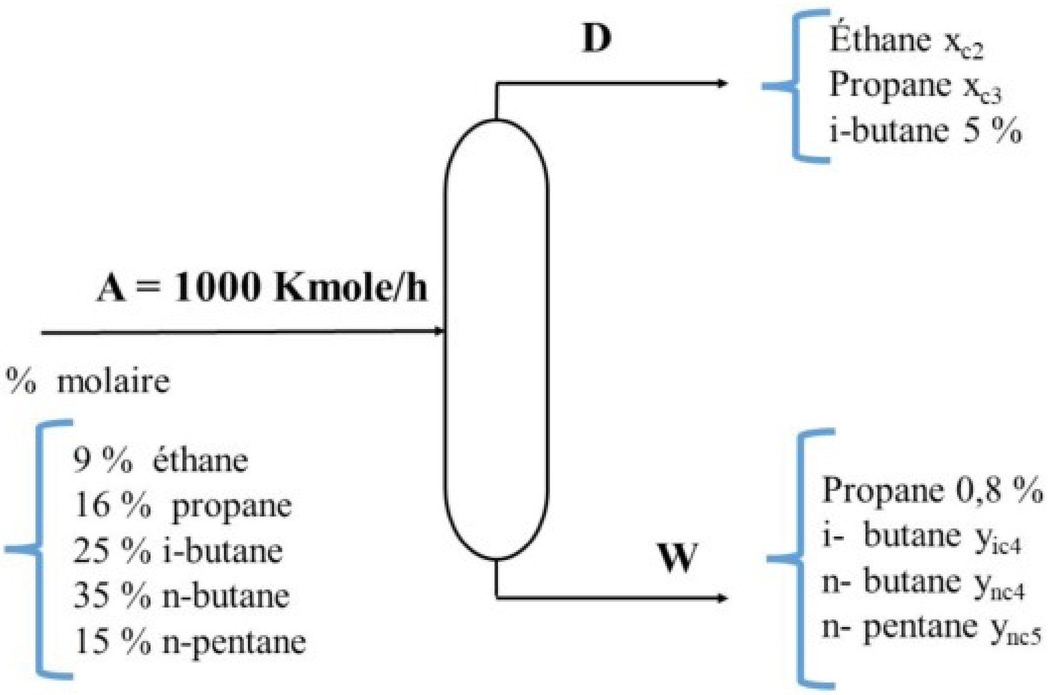
1- make a diagram of the process

2- Name all fluids

3- Put all the information next to the name

4- Choose a control surface (arround the 2nd column in our case)

- **Example 3:** Distillation of a complex mixture



- calculate the composition in D and W?