

Introduction to Chemical Engineering

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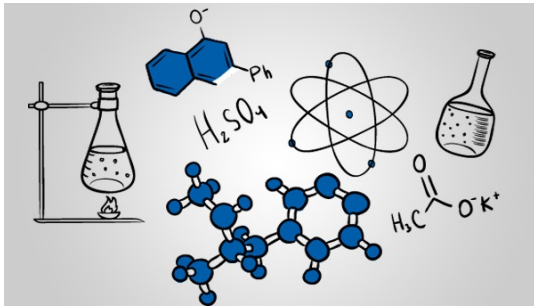
Fridays, 14 - 17h
2024-2025

Session I: Introduction

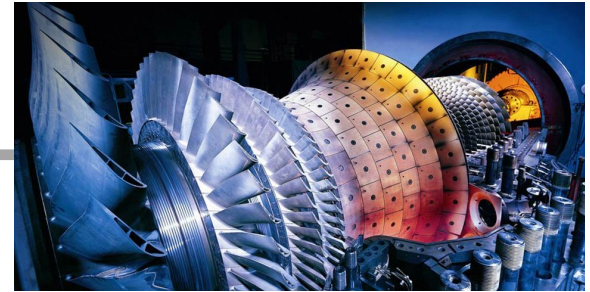
The **class today** will provide you with:

- I. An **overview of Chemical Engineering** and why we care about this course
- II. The **organization** of this course
- III. The **first steps** into the course

What is Chemical Engineering about?



Chemistry: knowledge on molecules, reactions, thermodynamics, ...



Engineering: knowledge on processes, design, handling many unknowns at a time, more in-depth mathematics, ...

Chemical Engineer

What's my definition?

- A chemist tries to understand what makes molecules happy.
- A chemical engineer manipulates molecules happiness ~~for financial gain.~~ to create new technology to solve the big problems facing humanity.

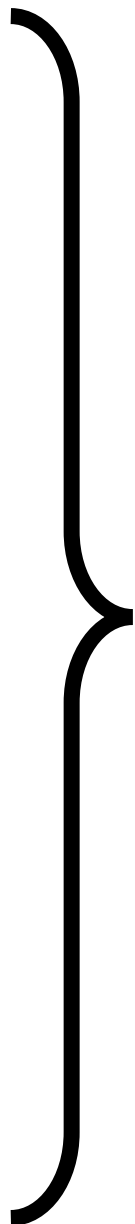
What kinds of problems can a chemical engineer solve?

- Production of chemicals, chemical processing
- Energy sector
- Environmental science and engineering, pollution control, quality control
- Pharmaceutical companies, biotechnology, bioengineering, metabolic engineering
- Food industry
- Nanotechnology and advance materials
- ...



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Commonality?

What kinds of problems can a chemical engineer solve?

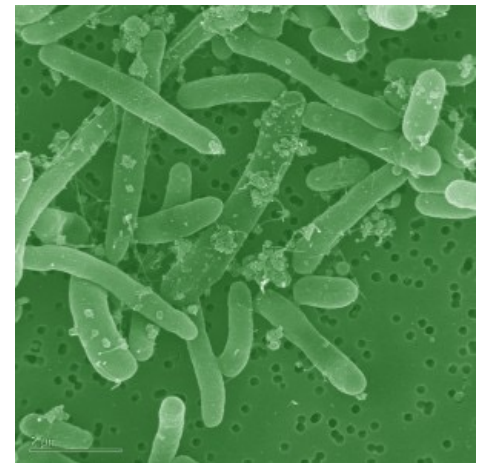
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What kinds of problems can a chemical engineer solve?

Genetic engineering

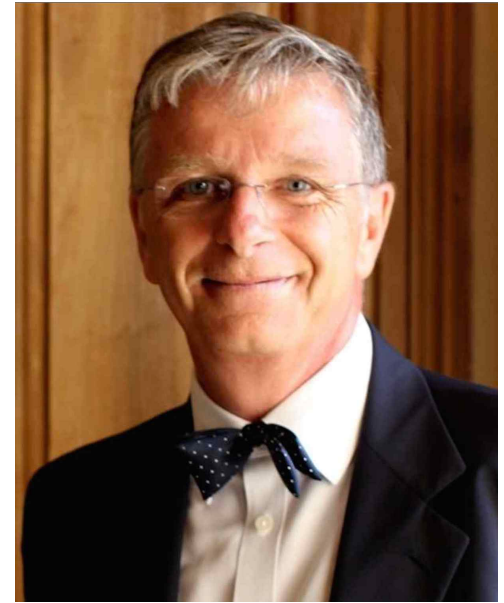
- Jay Keasling – Discover Magazine’s 2006 “Scientist of the Year”
- Bacteria as reactors
- “Reprogram” bacteria genome to make bacteria that eat cellulose and produce:
 - Artemisinin (kills malaria-carrying parasite)
 - Biodiesel for cars



What kinds of problems can a chemical engineer solve?

Electrochemistry

- Hubert Girault: Faraday medal 2006, Royal Society of Chemistry
- Hydrogen production and distribution
- Fuel cell cars



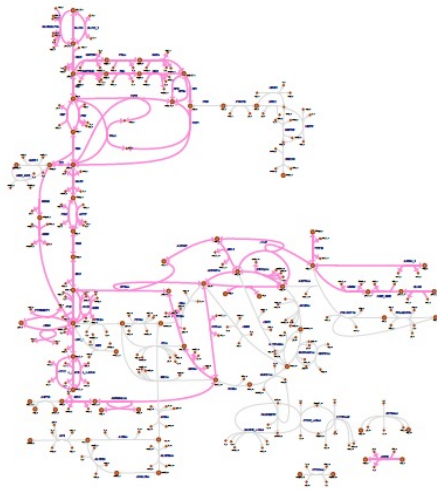
What kinds of problems can a chemical engineer solve?

Metabolic exploration

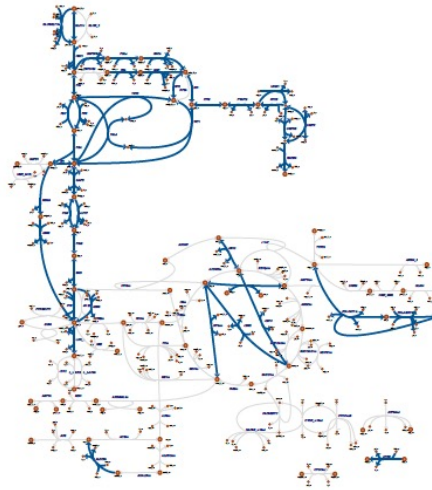
- Former PhD student of LCSB
- Exploring the metabolism of human cancers



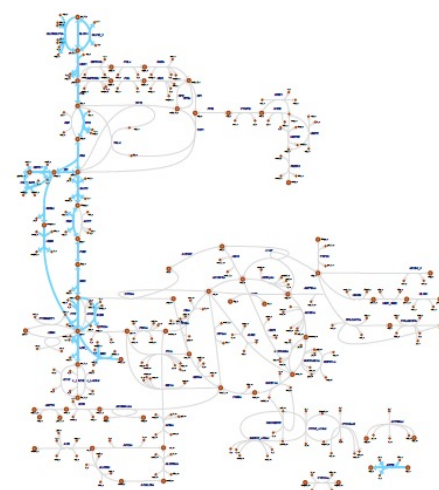
Minimal networks to study the Warburg effect



Breast cancer



Colon cancer



Ovarian cancer

What kinds of problems can a chemical engineer solve?



- Swiss agro-chemical company
- \$16.7 Bio. Revenue
- 53.000 people employed
- Main business divisions
 - Crop protection
 - Pesticides
 - Fungicides
 - Herbicides
 - Insecticides
 - Seeds



Headquarters in Basel, Switzerland

Why do we need ICE?

This course is an introduction to the tools used in Chemical Engineering

You will learn systematic approaches to the solution of problems faced by chemical engineers (and not only by chemical engineers)

You will learn how to understand the inherent value of the problem and to apply general rules that serve for all processes

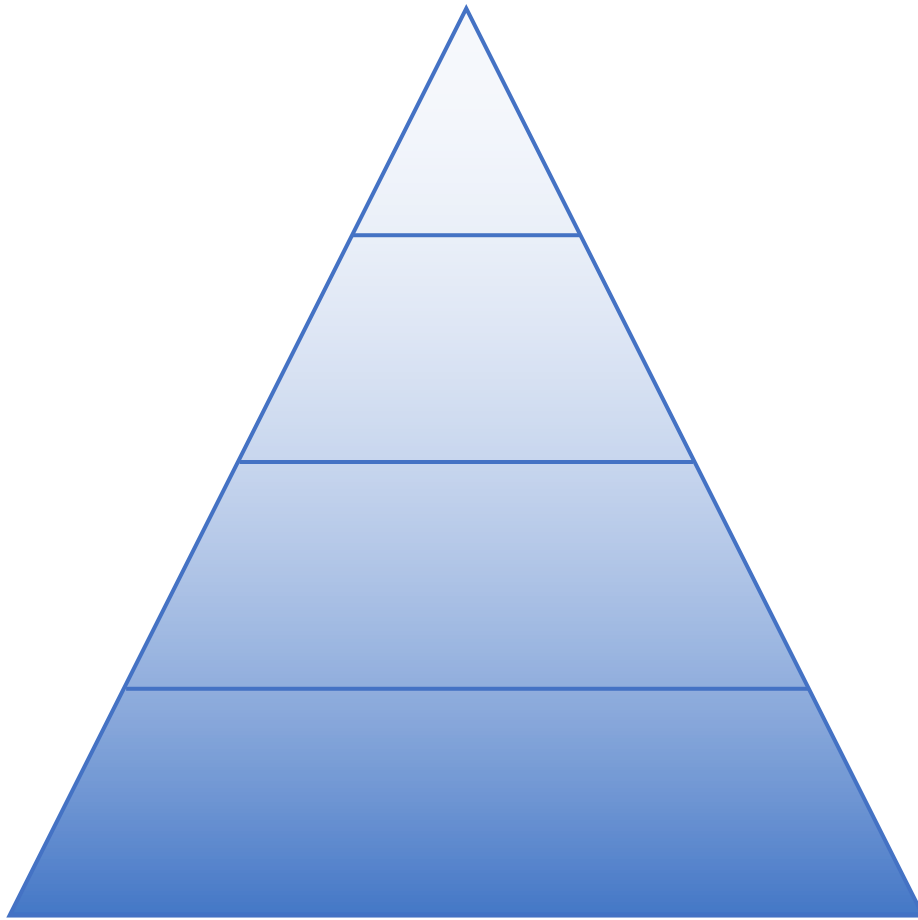
You will learn how to adapt general equations to your specific problem

Course Schedule

Date	Subject
13-Sep	1. Fundamentals of Material Balances 1.1. Process definition and classification 1.2. Material balance calculations
20-Sep	1.3. Balances on multiple-unit processes 1.4. Chemical reaction stoichiometry
27-Sep	1.5. Balances on reactive processes
04-Oct	Review on Mass Balances
11-Oct	1.5. Balances on multiple unit reactive processes
18-Oct	2. Energy and Energy Balances 2.1. Energy balances on closed systems 2.2. Open systems at steady state
01-Nov	3. Balances on Non-Reactive Processes 3.1. Energy balance calculation 3.2. Changes in Pressure, Temperature, Phases 3.3. Mixing and Solution
08-Nov	4. Balances on Non-Reactive Processes Problems: Mass and Energy Balances on non-Reactive Systems
15-Nov	Midterm Exam: Mass & Energy Balances non-Reactive Systems
22-Nov	Review Midterm
29-Nov	5. Balances on Reactive Processes 5.1. Heats of reaction/combustion 5.2. Combustion reactions 5.3. Enthalpy of reaction 5.4. Energy balance calculation
06-Dec	6. Energy balances on mixing processes Review
13-Dec	Review and Study Session

Recommended textbook:
Elementary Principles of Chemical Processes
Richard M. Felder & Ronald W. Rousseau

Building on top of Acquired Knowledge



Energy Balance reactive

Energy Balance Non-Reactive

Mass Balance Reactive

Mass Balance Non-Reactive

Midterm & Exam ?

Session I: Friday 13 September 2024

After studying this session, you will be able to:

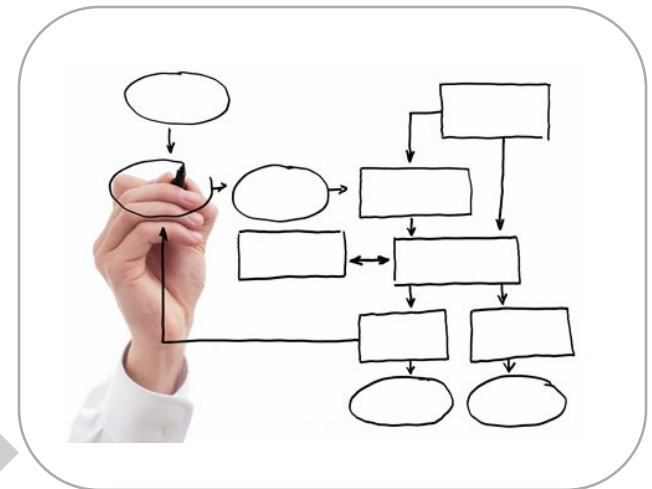
1. Understand and apply the principles of material balances
 - What is a process and how to define it
 - Classification of processes
2. Know the main equation on Material Balances and how to apply it to the different processes
3. Solve a mass balance in a simple process

1. Principles of Material Balances

Objectives

- What is a process?
- Understanding the main types of processes

- Describing a process :



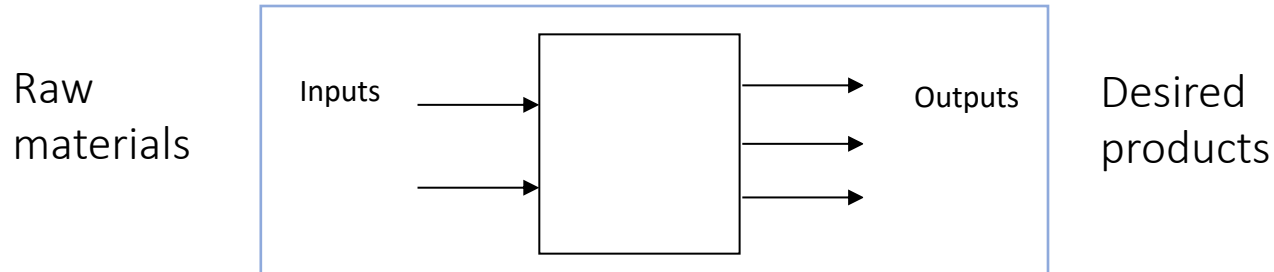
- With Diagrams (conceptually)

- Mathematically

$$\begin{aligned}
 & \dots, X_{i,j}, U_{i,j=1}, \dots, U_{i,j=I} \} \\
 & \sum_{v=\Delta}^{Y_r} \sum_{i=1}^I \sum_{z=v+\lambda \epsilon \alpha \delta_i}^{v+\lambda \epsilon \alpha \delta_i + \lambda \epsilon_i} p_z (1+r)^{-(z-v)} L_{i,z,v} \theta_{i,z,v} a_{m,i} a_{l,i} \cdot 8760 \\
 & \cdot \sum_{v=\Delta}^{Y_r} \sum_{i=1}^I \sum_{z=v+\lambda \epsilon \alpha \delta_i}^{v+\lambda \epsilon \alpha \delta_i + \lambda \epsilon_i} C_{fuel,i,z,v} (1+r)^{-(z-v)} L_{i,z,v} \theta_{i,z,v} a_{m,i} a_{l,i} \cdot 8760 \\
 & \cdot \sum_{v=\Delta}^{Y_r} \sum_{i=1}^I \sum_{z=v+\lambda \epsilon \alpha \delta_i}^{v+\lambda \epsilon \alpha \delta_i + \lambda \epsilon_i} C_{fom,i,z} (1+r)^{-(z-v)} L_{i,z,v} \\
 & \cdot \sum_{v=\Delta}^{Y_r} \sum_{i=1}^I C_{l,i,v} X_{l,i,v} \\
 & \cdot \sum_{v=\Delta}^{Y_r} \sum_{i=1}^I \sum_{z=v+\lambda \epsilon \alpha \delta_i}^{v+\lambda \epsilon \alpha \delta_i + \lambda \epsilon_i} L_{i,z,v} \theta_{i,z,v} a_{m,i} a_{l,i} \cdot 8760 \cdot \frac{f_{CO_2}}{e f f_i} \cdot (1+r)^{-(z-i)} \cdot p_{CO_2} \\
 & \cdot \sum_{v=\Delta}^{Y_r} \sum_{i=1}^I \sum_{z=v+\lambda \epsilon \alpha \delta_i}^{v+\lambda \epsilon \alpha \delta_i + \lambda \epsilon_i} L_{i,z,v} \theta_{i,z,v} a_{m,i} a_{l,i} \cdot 8760 \cdot em_{mix} \cdot (1+r)^{-(z-i)} \cdot p_{CO_2}
 \end{aligned}$$

Basics of Process

Process is a transformation, involving **inputs, outputs and a system**

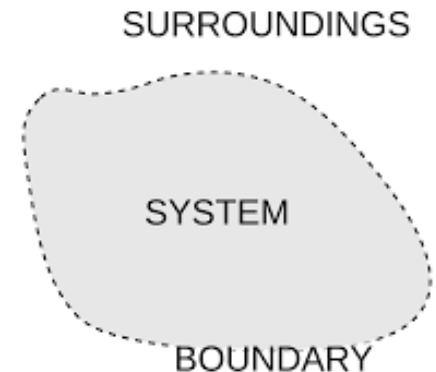


A system is defined by its **boundaries and its content**

Definition of boundaries, inputs and outputs

A system with the time of operation:

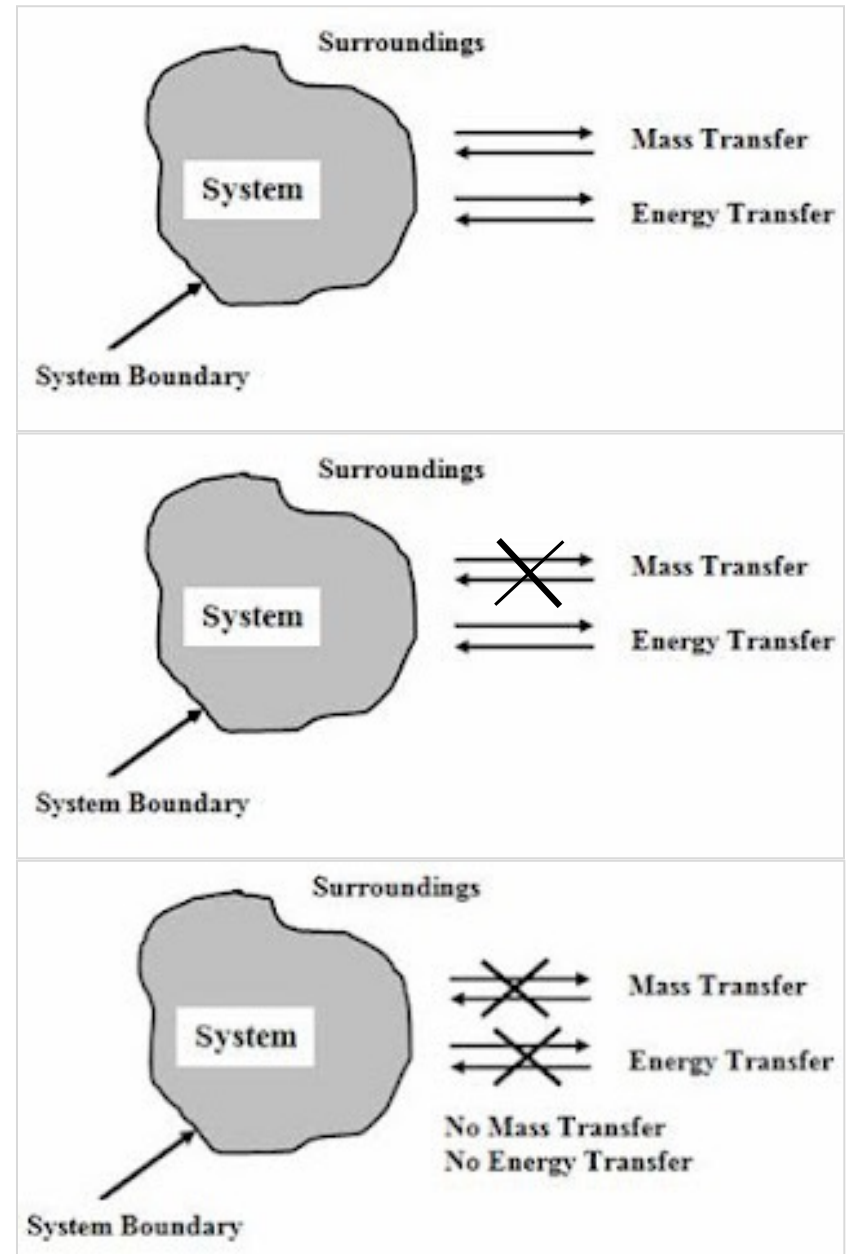
- Inputs, contents and outputs are functions of time
- **Boundaries are not functions of time**



Types of systems

The system is:

- Open or Closed:
When mass flows or not
(input and output of mass)
- Diathermic or Adiabatic:
When heat flows or not
(input and output of energy)
- Closed + adiabatic =?



Process classification

A process can work in two forms:

- **Steady-state:** NO change in the rates (e.g. flows, dC/dt) with time
- **Transient:** varying rates with time

Basic concepts: 1) Change, 2) Time

Example: Wastewater treatment during a day

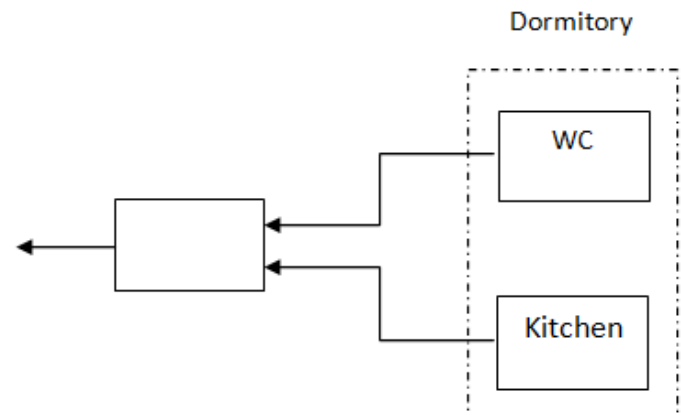
6:00-7:30: all getting ready “steady flow”.

8:15-12:00: classes-no flow or occasional

6:45-7:00: fluctuations

Time of observation

Relative fluctuation



Process classification

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Process classification

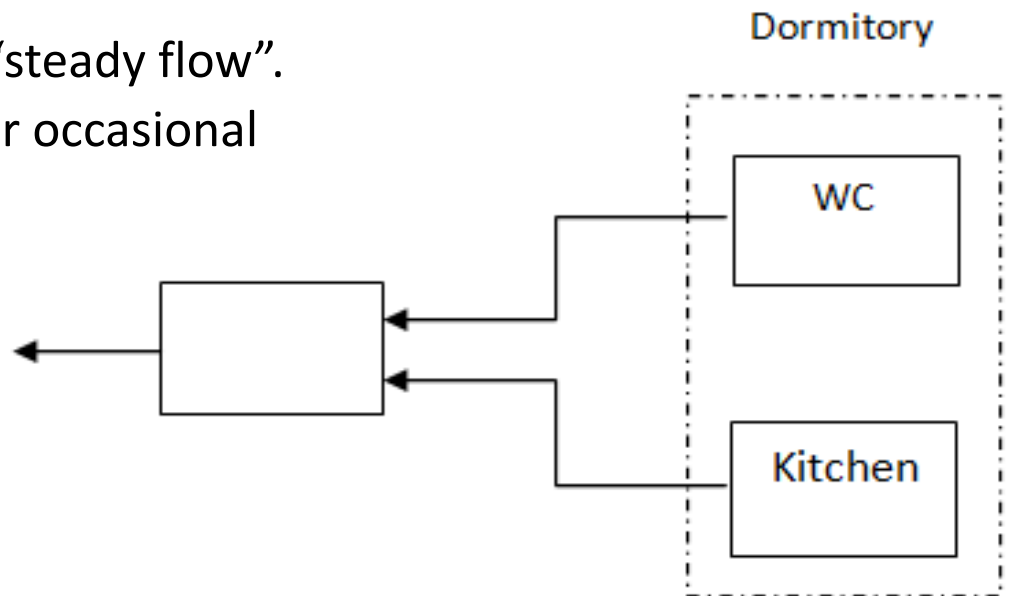
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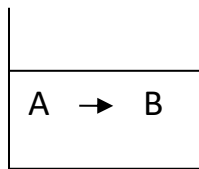
Time of observation
Relative fluctuation



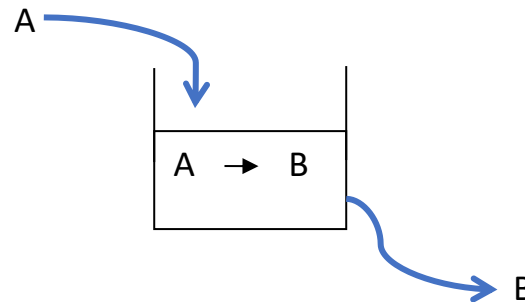
Main types of processes

Processes, as a function of time (of observation), can be classified taking into account the quantity or activity of materials that enter or exit into the system during this time

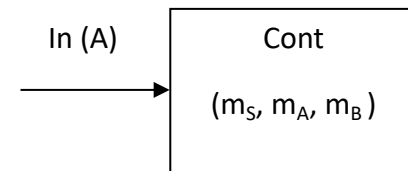
Batch



Continuous



Semi-batch Fed-batch

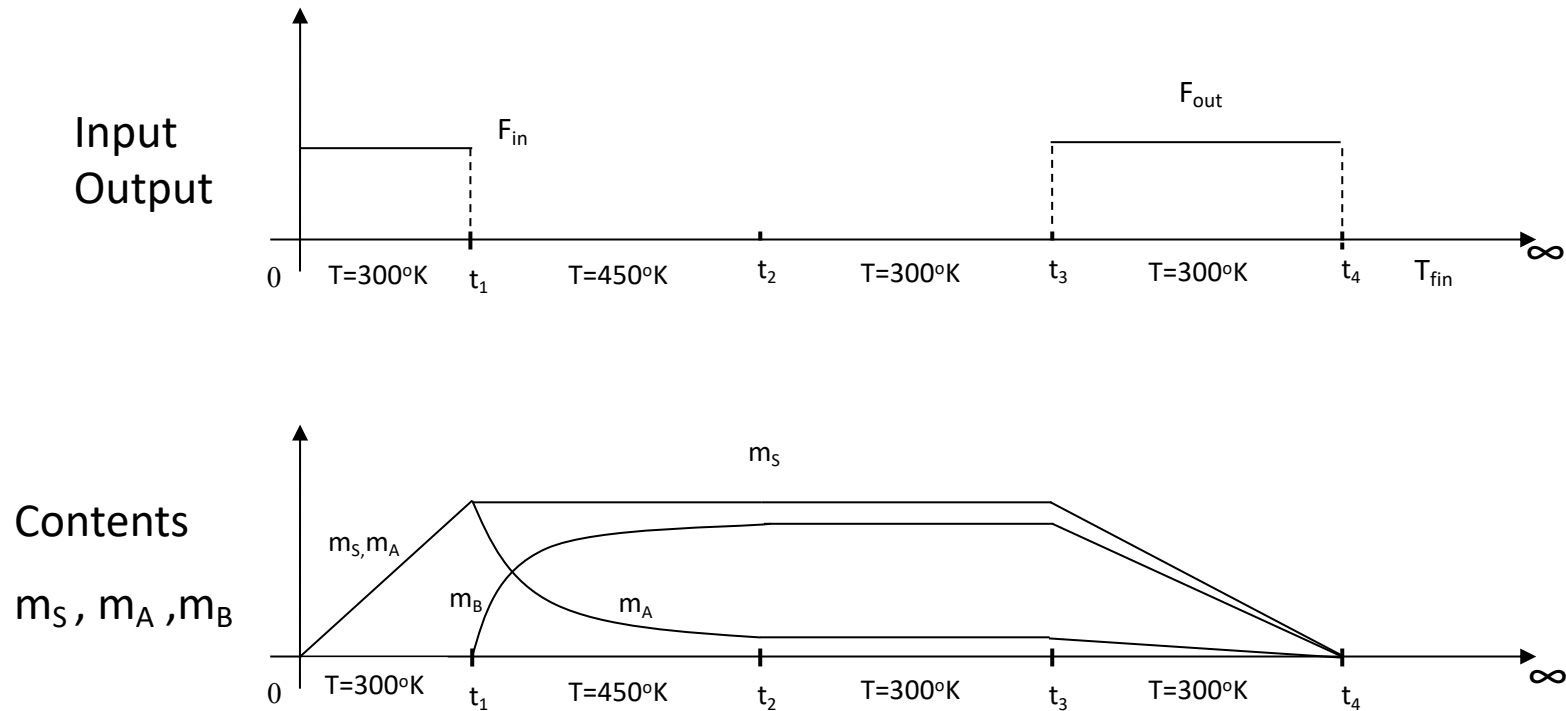


- **Important concept:** Inputs, outputs and contents will be defined always in terms of a calculation basis

(e.g. the observation time defines the time as a base, so we can define the production of B for a given time)

Example 1

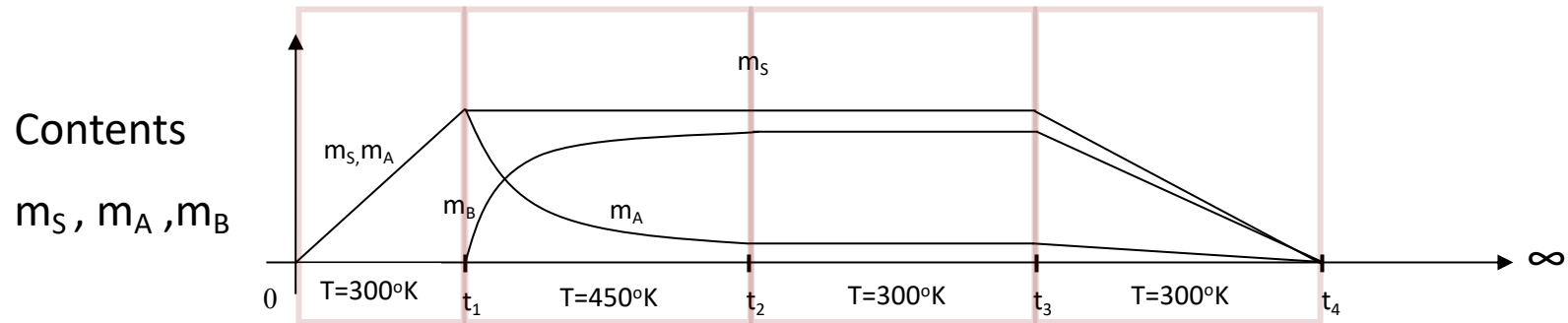
Example: How can we characterize this process?



- We have to define **basis of time**

Example 1

Solution:

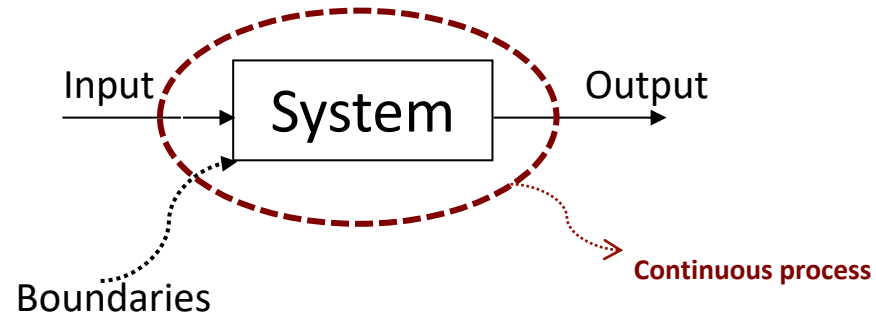


Basis tactic: We decompose process into batch and continuous choosing the basis

- t_0 - t_1 : **semi batch** (open and transient)
- t_1 - t_2 : nothing crosses the borders. The system is closed and transient (concentrations change) : **Batch**
- t_2 - t_3 : nothing crosses the borders. The system is closed and steady state: **Batch**
- t_3 - t_4 : **semi batch** (open and transient)
 - And if we consider t_0 - t_1 and t_3 - t_4 together, the process is continuous and transient

Describing a process

- ✓ Process
- ✓ System



Material balance : Balance on a conserved quantity in a system

- the mass balance concept is based on the fundamental physical principle that matter can neither be created nor destroyed
- the mass of inputs to a process balances the mass of outputs as products

2. The Equation on Material Balances

The mother of all equations

$$\begin{array}{ccccccccc} \textbf{Input} & + & \textbf{generation} & - & \textbf{output} & - & \textbf{consumption} & = & \textbf{accumulation} \\ \left(\begin{array}{c} \text{Entering} \\ \text{through} \\ \text{boundaries} \end{array} \right) & & \left(\begin{array}{c} \text{Produced} \\ \text{in the} \\ \text{system} \end{array} \right) & & \left(\begin{array}{c} \text{Leaving} \\ \text{through} \\ \text{boundaries} \end{array} \right) & & \left(\begin{array}{c} \text{Consumed} \\ \text{within} \\ \text{system} \end{array} \right) & & \left(\begin{array}{c} \text{Build up} \\ \text{within} \\ \text{system} \end{array} \right) \end{array}$$

Common assumptions on the general equation

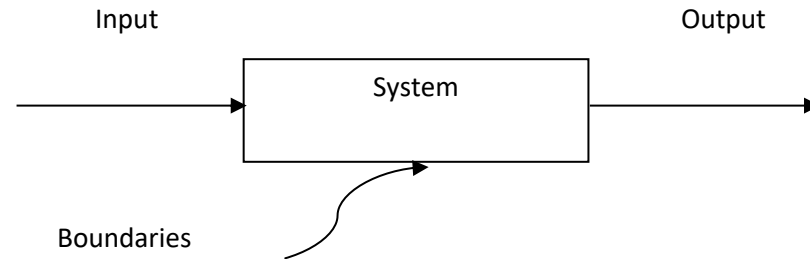
The general balance equation might be simplified according to the process at hand

Examples :

- 1) for steady-state continuous process
- 2) for closed system
- 3) for a system with no generation

1. Describing a steady-state continuous process

Balance on a conserved quantity in a system:



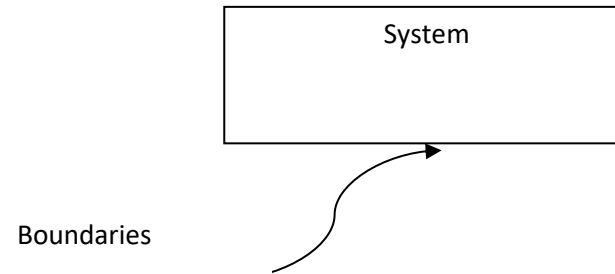
The mother of all equations:

$$\begin{array}{ccccccccc} \text{Input} & + & \text{generation} & - & \text{output} & - & \text{consumption} & = & \text{accumulation} \\ \left(\begin{array}{c} \text{Entering} \\ \text{through} \\ \text{boundaries} \end{array} \right) & & \left(\begin{array}{c} \text{Produced} \\ \text{in the} \\ \text{system} \end{array} \right) & & \left(\begin{array}{c} \text{Leaving} \\ \text{through} \\ \text{boundaries} \end{array} \right) & & \left(\begin{array}{c} \text{Consumed} \\ \text{within} \\ \text{system} \end{array} \right) & & \left(\begin{array}{c} \text{Build up} \\ \text{within} \\ \text{system} \end{array} \right) \end{array}$$

The equation is crossed out with a large red X, indicating it is incorrect for a steady-state process.

2. Describing a closed system

Balance on a conserved quantity in a system:



The mother of all equations:

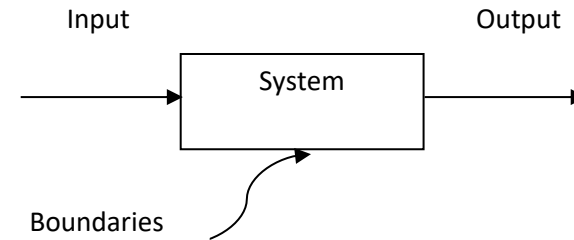
$$\begin{array}{ccccccc} \text{Input} & + & \text{generation} & - & \text{output} & - & \text{consumption} & = & \text{accumulation} \\ \left(\begin{array}{c} \text{Entering} \\ \text{through} \\ \text{boundaries} \end{array} \right) & & \left(\begin{array}{c} \text{Produced} \\ \text{in the} \\ \text{system} \end{array} \right) & & \left(\begin{array}{c} \text{Leaving} \\ \text{through} \\ \text{boundaries} \end{array} \right) & & \left(\begin{array}{c} \text{Consumed} \\ \text{within} \\ \text{system} \end{array} \right) & & \left(\begin{array}{c} \text{Build up} \\ \text{within} \\ \text{system} \end{array} \right) \end{array}$$

The diagram shows the general balance equation for a conserved quantity in a system. The terms "Input" and "output" are crossed out with large red X's, indicating they are not applicable for a closed system. The equation simplifies to: generation minus consumption equals accumulation.

3. Describing a system with no generation

Usually applies to systems without reaction

Balance on a conserved quantity in a system:



The mother of all equations:

$$\begin{array}{ccccccc} \text{Input} & + & \text{generation} & - & \text{output} & - & \text{consumption} & = & \text{accumulation} \\ \left(\begin{array}{c} \text{Entering} \\ \text{through} \\ \text{boundaries} \end{array} \right) & & \left(\begin{array}{c} \text{Produced} \\ \text{in the} \\ \text{system} \end{array} \right) & & \left(\begin{array}{c} \text{Leaving} \\ \text{through} \\ \text{boundaries} \end{array} \right) & & \left(\begin{array}{c} \text{Consumed} \\ \text{within} \\ \text{system} \end{array} \right) & & \left(\begin{array}{c} \text{Build up} \\ \text{within} \\ \text{system} \end{array} \right) \end{array}$$

The diagram shows the general balance equation with terms in parentheses. The terms "generation" and "consumption" are crossed out with large red X's, indicating they are zero for a system with no reaction.

Procedure for Material Balance Calculations

For setting up a problem:

1. Translate problem into a flowchart

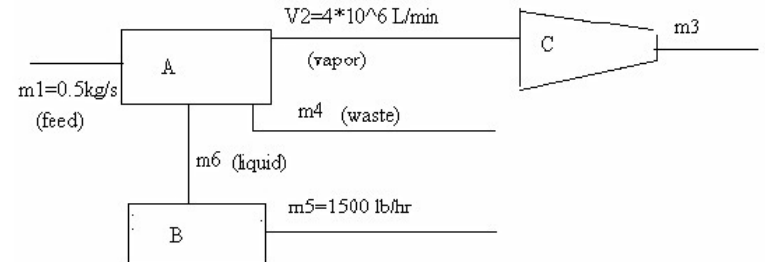
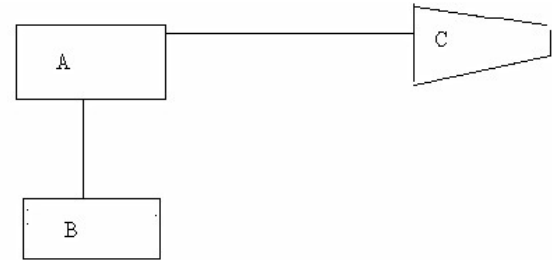
2. Label flowchart

Make sure your units are consistent

3. Define basis [scale quantities]

4. Set-up and solve mass balance equations

✓ you will usually be given a description of a process



Why do Units Matter?



The Mars Climate Orbiter

- The software calculated the force that the thrusters needed to exert in pounds of force.
- A second piece of code that read this data assumed it was in the metric unit—"newtons per square meter".

\$125 millions of losses

Example 2: Population

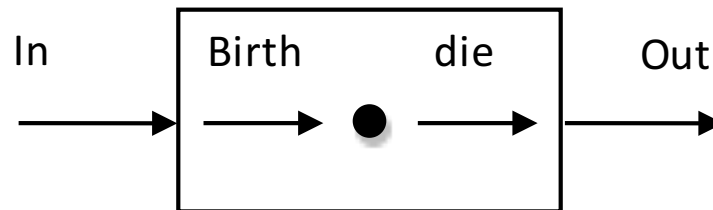
In the last 5 years, 10,000 people moved in the city of Lausanne and 8,500 person left this city. During this period, 7,000 babies were born, and 5,000 person died per year. **Find the growth of the population per year during this period.** Consider the entrance and exit of people to be equal each year.

0) Understand the problem! Type of process?

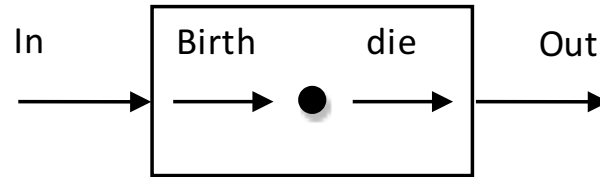
Open or closed? Continuous or Batch? Transient or steady state?

1) Translate the problem into a flowchart: draw the system and the exchanges of mass and energy with the environment

2) Label the flowchart: rates of mass exchange



Example 2: Population



3) Define basis: time AND mass units

Basis: people/year

4) Mass balance:

How should we modify the mother of all equations to describe our process?
(consider the process classification)

General: **Input + generation – output – consumption = accumulation**

Specific to our problem: ?

In + Birth – out – die = growth of the population

$10,000/5 + 7,000 - 8,500/5 - 5,000 = 2,300$ people/year

CHECK OUT: All flows should be in the same units: people/year!

Example 3: Distillation

In a distillation process working at a steady state, 2,000 kg/hr of a binary mixture of benzene (B) and toluene (T) containing 70% B by mass is separated.

There are two output streams in this process: a top stream, which carries 1100kg B/h, and a bottom stream, which contains 450kg T/h.

What is the flow rate and composition of all streams in this process?

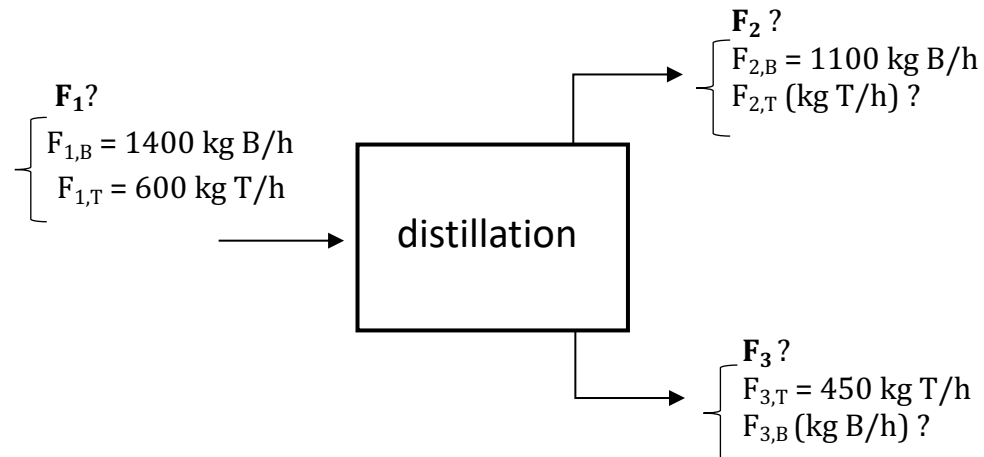
0) Understand the problem! Any new concept? Type of process?

1) Translate the problem into flowchart: draw the operation unit and the streams

2) Label the flowchart: total flow rates and individual flow rates

3) Define basis: time AND mass units

Basis: kg/h

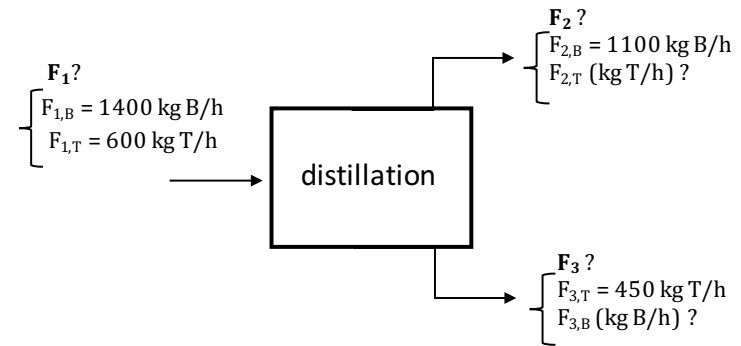


Example 3: Distillation

4) Mass balance

How many equations can we write?

- One for each molecular species
- One for each element
- One for total mass



How should we modify the mother of all equations to describe our process?
(consider the process classification)

General: **Input + generation – output – consumption = accumulation**

Specific to our problem?

Input – output = 0

For benzene:

$$1400 - (1100 + F_{3,B}) = 0 \text{ (steady state or st. st.)} \rightarrow F_{3,B} = 300 \text{ kg/h}$$

For toluene:

$$600 - (450 + F_{2,T}) = 0 \text{ (st. st.)} \rightarrow F_{2,T} = 150 \text{ kg/h}$$

Example 3: Distillation

Total mass balance :

In – out = 0

$$2000 - (1100 + 150 + 450 + 300) = 0$$

We have defined 3 mass balances, but ...

How many mass balances do we need to solve the problem?

Clues: In this problem, what is the...

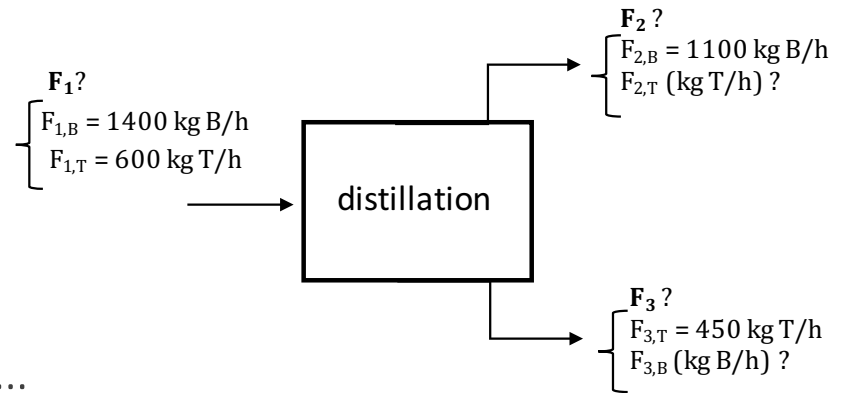
Number of molecular species?

Number of unknowns?

Number of linearly independent equations?

Which mass balances shall we choose?

Any combination as long as they are linearly independent



REMINDER: A linear independent system of equations

Two equations are linearly dependent, if:

- one can be obtained from the other by scaling it by a factor
- both equations produce identical graphs
- both equations provide the same information

Is the following system of equations linearly independent?

$$2x + 2y = 4$$

$$x + y = 2$$

$$x - y = 0$$

And the following one?

$$x + y = 5$$

$$2x + y = 7$$

Example 4: Mixing

We are working with two different binary mixtures of methanol/water. The first one contains 50 %-kg/kg (weight) methanol and the second one 80 %-kg/kg (weight) methanol.

We mix 200 g of the first one and 150 g of the second one. **What is the composition of final mixture?**

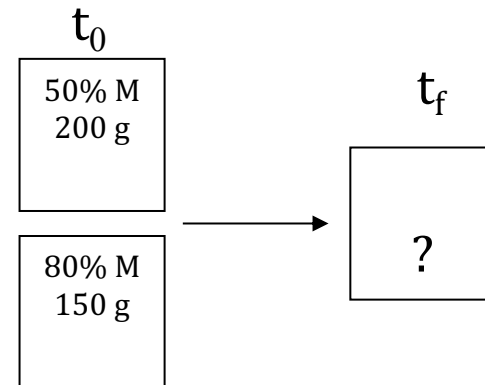
0) Understand the problem! Any new concept? Type of process?

1) Translate the problem into flowchart: draw the process

2) Label the flowchart: mass and compositions

3) Define basis: time? mass units?

Basis: total time $t_0 \rightarrow t_f$



Example 4: Mixing

4) Mass balances

How should we modify the mother of all equations to describe our process?
(consider the process classification)

General: Input + generation – output – consumption = accumulation

Specific to our problem: ?

Input = Accumulation

Methanol:

$$(0,5 \cdot 200 + 0,8 \cdot 150) = M_{\text{methanol}}$$

$$100 + 120 = 220 \text{ g methanol}$$

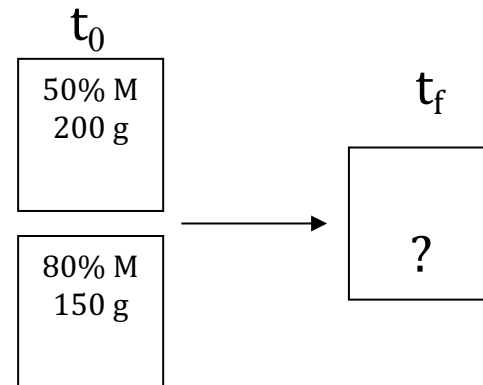
Water:

$$(0,5 \cdot 200 + 0,2 \cdot 150) = M_{\text{water}}$$

$$100 + 30 = 130 \text{ g water}$$

Total:

$$220 + 130 = 350 \text{ g}$$



Composition of final mixture:

methanol: $220/350 = 63\% \text{ kg/kg}$,

water: $130/350 = 37\% \text{ kg/kg}$