Laboratory of
Computational
Systems
Biotechnology

EPFL

Introduction to Chemical Engineering

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Fridays, 14h15 - 17h00
2024-2025

Example 3: Distillation

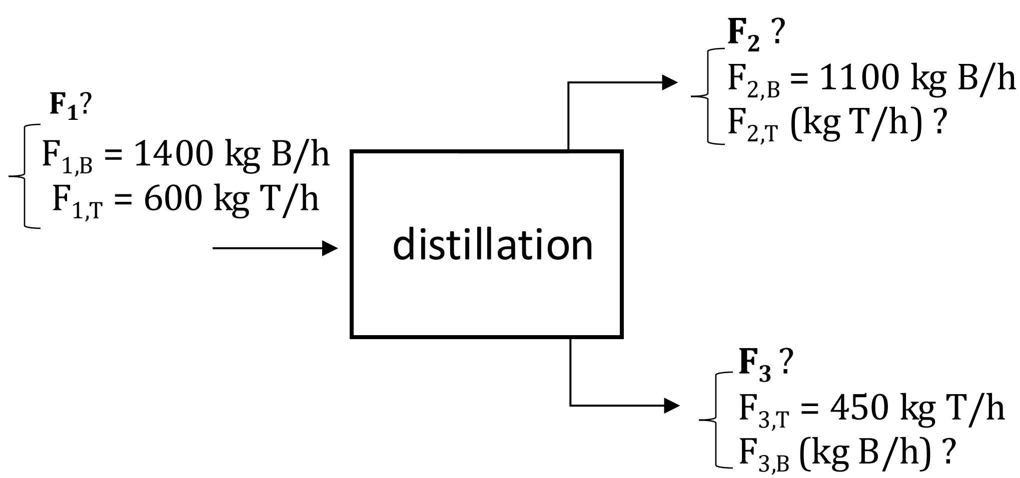
In a distillation process working at steady state, 2,000 kg/h of a binary mixture of benzene (B) and toluene (T) containing 70% B by mass is separated.
There are two output streams in this process: a top stream, which carries 1100kg B/h, and a bottom stream, which contains 450kg T/h.
What is the flow 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

3) Basis: kg/h

1)

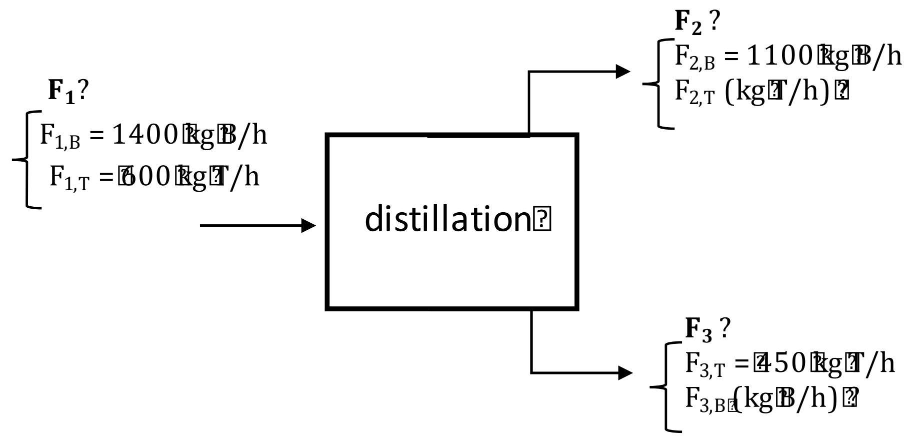


Example 3: Distillation

4) **Mass balances:**
How many equations can we write?

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

Total : 3 equations



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

Example 3: Distillation

1. **For benzene**:

$1400 - (1100 + F_{3,B}) = 0$ (steady state/st. st.)

$\rightarrow F_{3,B} = 300$ kg/h

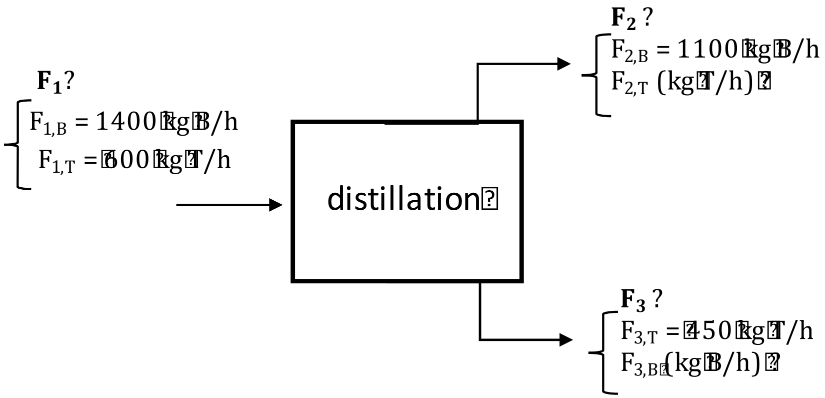
2. **For toluene**:

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

3. **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 if 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?

$$x + y = 5$$
$$2x + y = 7$$

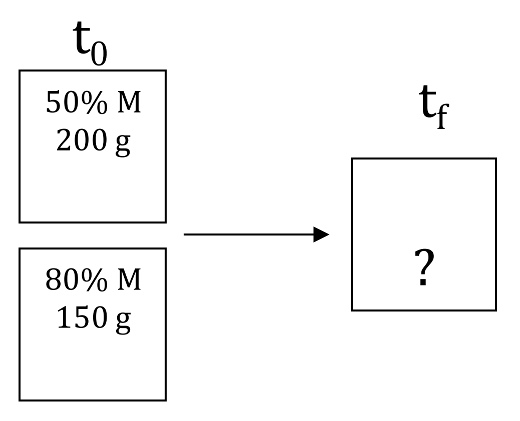
Example 4: Mixing

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?

3)Basis: total time $t_0 \rightarrow t_f$



Example 4: Mixing

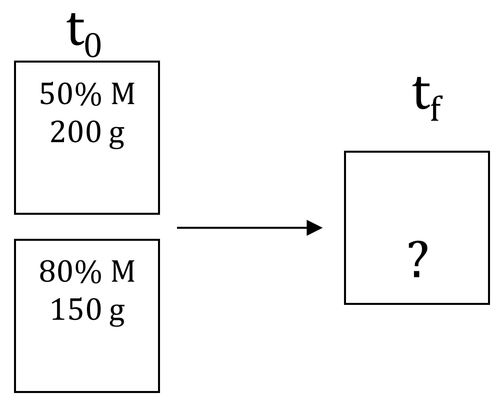
4) Mass balances

General:

Input + ~~generation~~ – ~~output~~ – ~~consumption~~ = accumulation

Specific to our problem: ?

Input = Accumulation



Methanol:

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

100 + 120 = 220 g methanol

Water:

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

100 + 30 = 130 g water

Total:

220 + 130 = 350 g

Composition of final mixture:

methanol: 220/350 = 63% kg/kg,

water: 130/350 = 37% kg/kg

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

Session II: Friday 20 September 2024

After studying this session, you will be able to:

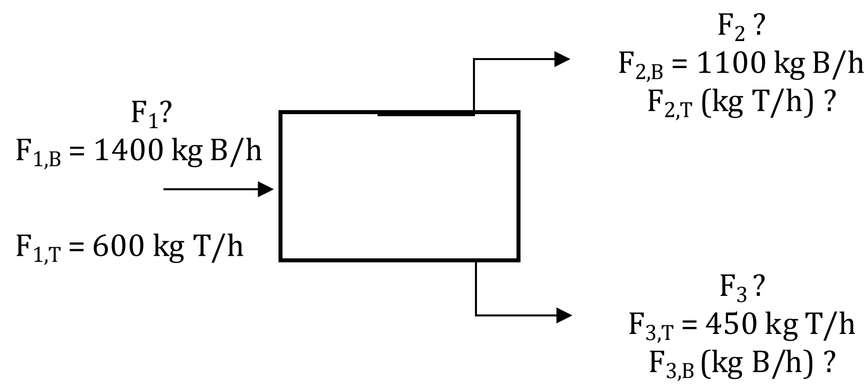
1. Perform Degree of Freedom analysis on a unit operation
2. Perform a Material Balance on a single unit process (following the general procedure)
3. Perform Mass Balances on multiple-unit processes

1. Degree of freedom

What is degree of freedom?

In chemical engineering, the number of **independent equations** that can be obtained from a non-reactive system is equal to the number of **unique molecular species** in that system

E.g.: (from Session I)



Number of equations:

- ➢ One for each molecular specie : B, T
- ➢ One for total mass: Total = B+T

Are they independent?

Only 2 (B and T) or (B and Total) or (T and Total)

- Not all problems are solvable: problems can have too much information (unsolvable) or give not enough data (infinite solutions)
- A **<u>degree-of-freedom analysis</u>** is used to determine whether a problem is solvable with the information given

How to perform a degree-of-freedom analysis?

1. **Draw a properly labeled flowchart**: what we have and what we don't have to define the mass balance for all the species.

Each stream must have information about its total flow rate and its composition (this is equivalent to having the flow rate of each species in the stream)

2. **Count the number of unknowns:** what information is missing ?

3. **Count the number of independent equations:**

For any system, we can write exactly as many independent material balances as unique chemical species we have.

⚠ **If we write a balance equation for total mass, we should omit one of the chemical species, because a balance equation for total mass is not *independent* and can be obtained by summing all the equations for unique chemical species**

How to perform a degree-of-freedom analysis?

4. Calculate the **Degrees of freedom (DOF)**

DOF = Number of unknowns – Number of independent equations

- **If the DOF = zero, the problem is solvable, one solution (*determined*)**
- **If the DOF > zero, the problem has infinite solutions (*underdetermined*)**
- **If the DOF < zero, the problem is unsolvable** (we have too many constraints) **(???)**

Example 1: Mixing

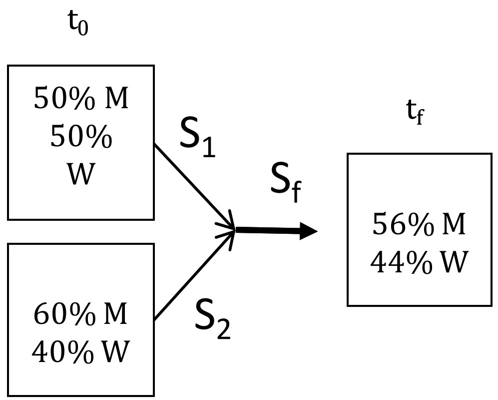
We have two different mixtures of methanol/water

1: 50 % W methanol

2: 60 % W methanol

and we want a final solution 56% W of methanol?

1. Draw the flow chart… and label it!!!!



The mass balance equations are well defined with the information from the flowchart

General:

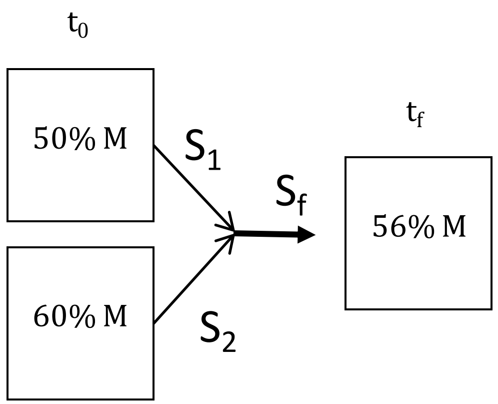
Input + generation – output – consumption = accumulation

Specific to our problem: ?

Input = Accumulation

Example 1: Mixing

We have two different mixtures of methanol/water
  1: 50 % W methanol
  2: 60 % W methanol
and we want a final solution 56% W of methanol?



Input = Accumulation

<u>Mass balance equations</u>:

Methanol: $0{,}5 \cdot S_1 + 0{,}6 \cdot S_2 + 0 - 0 = S_f \cdot X_f = S_f \cdot 0{,}56$

Water: $0{,}5 \cdot S_1 + 0{,}4 \cdot S_2 = S_f \cdot 0{,}44$

Total: $S_1 + S_2 = S_f$

DOF analysis:

2. Number of unknowns: 3 (S_1, S_2, S_f)
3. Number of independent equations: 2
4. DOF = 3 – 2 = 1

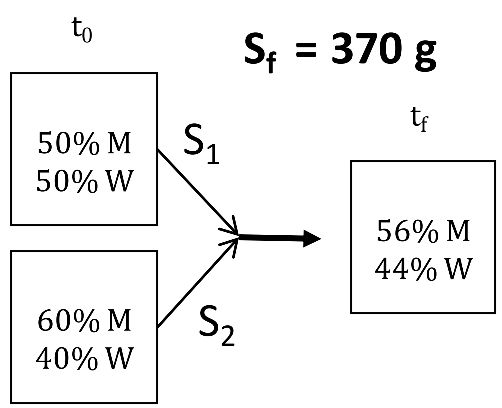
→ The problem is missing required information, it has infinitely many solutions (we can't solve it*) !

Example 1: Mixing, continued…

(we can't solve it*) ? → We can define one more unknown:

If we define that we want 370 g of the final 56% W solution…

Mass balance equations:



Methanol: $0{,}5 \,.\, S_1 + 0{,}6 \,.\, S_2 = \mathbf{370} \,.\, 0{,}56$

Water: $0{,}5 \,.\, S_1 + 0{,}4 \,.\, S_2 = \mathbf{370} \,.\, 0{,}44$

Total: $S_1 + S_2 = \mathbf{370}$

… we can calculate the mass of the stream 1 and 2:

$S_1 \approx 148$g and $S_2 \approx 222$g

- In this case, the mass of the final solution has been defined as the calculation basis

General procedure for Single-Unit Process Material Balance Calculations (in non-reactive processes)

How to solve mass balance questions

0) Check given units. Make sure that you understand the system.

Problem set up

1) **Draw flowchart and label:**

- Stream flow (rate): volumetric/mass (rate)
- Stream composition: mass/mol fraction for each component
- Identify the units (to be converted if they don't match)
- Identify information given or needed for each stream
- Identify possible given relations between streams

2) **Choose a basis:** Unit, time or numerical convenience (m = 100 kg/min, t = 1 h…) → problem specific

3) **Reformulate the problem** as list of known/unknowns and check units (Remember not to apply a volumetric balance!)

How to solve mass balance questions

4) **Formulate equations**. Can be :

- Material balances:
  - Molecular species
  - Elemental balances

- Process specifications:
  - Relation between streams
  - Distribution of species

- Physical constrains:
  - Mole/mass fractions
  - Is it not a liquid? Is it a gas stream?

- Physical properties

How to solve mass balance questions

5) Perform a **degree-of-freedom analysis**

- Degrees of freedom (DOF) = Number of unknowns – Number of equations
- Minimize/eliminate dependent equations
- Identify equations with less unknowns
- Highlight unknowns

6) **Solve** equations

Always outline outline solution procedure

7) **Calculate** required/asked quantities

8) **Rescale**

Example 2: Material Balance on a Distillation Column

A liquid mixture containing 45.0% benzene (B) and 55.0% toluene (T) by mass is fed to a distillation column.

A product stream leaving the top of the column (the overhead product) contains 95.0 mole % B, and a bottom product stream contains 8.0 % of the benzene fed to the column (meaning that 92% of the benzene leaves with the overhead product).

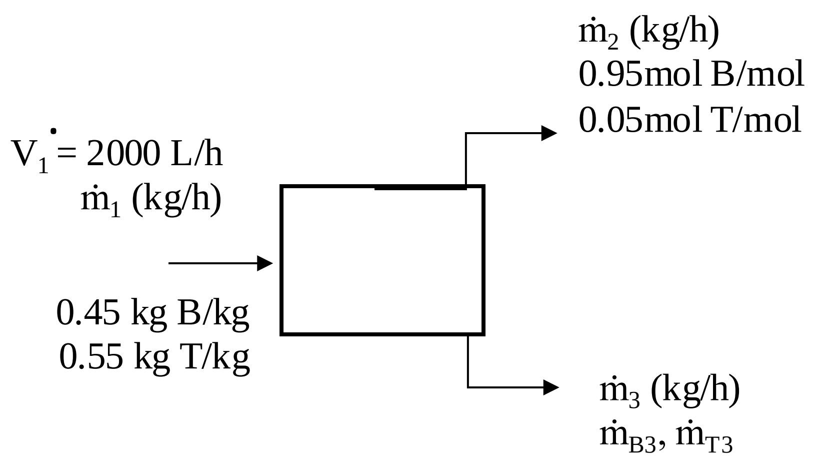
The volumetric flow rate of the feed stream is 2000 L/h and the density of the feed mixture is 0.872. Determine:

- the mass flow rate of the overhead product stream ?
- the mass flow rate and composition (mass fractions) of the bottom product stream?

0) Check the units

mass/volume/mol???

1) Draw and label the flowchart



Example 2: Material Balance on a Distillation Column

2) Choose a basis:

Time= 1 hour

3) Reformulate the problem as a list of known/unknowns :

Knowns:

Unknowns:

4) Formulate equations:

Example 2: Material Balance on a Distillation Column

5) DOF analysis

- 4 unknowns ($\dot{m}_1$, $\dot{m}_2$, $\dot{m}_{B3}$, $\dot{m}_{T3}$)

4 equations:
- Mass balances (for both species)
- One relation for the density (physical relation)
- Derived one relation for benzene (8% down, 92% up) (process specs)

→ DOF=0

6) Set up and solve equations

The volumetric flow rate for the conversion:

$$\dot{m}_1 = (2000\ L / h) \times (0.872\ kg / L) \rightarrow \dot{m}_1 = 1744\ kg / h$$

Relationship information for benzene:

$$\dot{m}_{B3} = 0.08 \times (0.45 \times \dot{m}_1) \rightarrow \dot{m}_{B3} = 62.8\ kg\ of\ B / h$$

Example 2: Material Balance on a Distillation Column

Benzene balance :

$$0.45 \times \dot{m}_1 = \dot{m}_2 \times y_{B2} + \dot{m}_{B3} \rightarrow \dot{m}_2 \approx 766 \text{ kg of benzene / h}$$

Another way to find $\dot{m}_2$:

a bottom product stream contains 8.0 % of the benzene fed to the column (meaning that 92% of the benzene leaves with the overhead product).

$$0.92 \times 0.45 \times \dot{m}_1 = \dot{m}_2 \times y_{B3} \rightarrow \dot{m}_2 \approx 766 \text{ kg of benzene / h}$$

Toluene balance :

$$0.55 \times \dot{m}_1 = 0.058 \times \dot{m}_2 + \dot{m}_{T3} \rightarrow \dot{m}_{T3} = 915 \text{ kg of toluene / h}$$

Total mass balance to verify the calculations ?

The additional calculations:

$\dot{m}_3 = \dot{m}_{B3} + \dot{m}_{T3} = 62.8$ kg / h + 915 kg / h ≈ 978 kg / h

$y_{B3} = \dot{m}_{B3} / \dot{m}_3 = 62.8$ kg de B / (978 kg / h) = 0.064 kg of B / kg

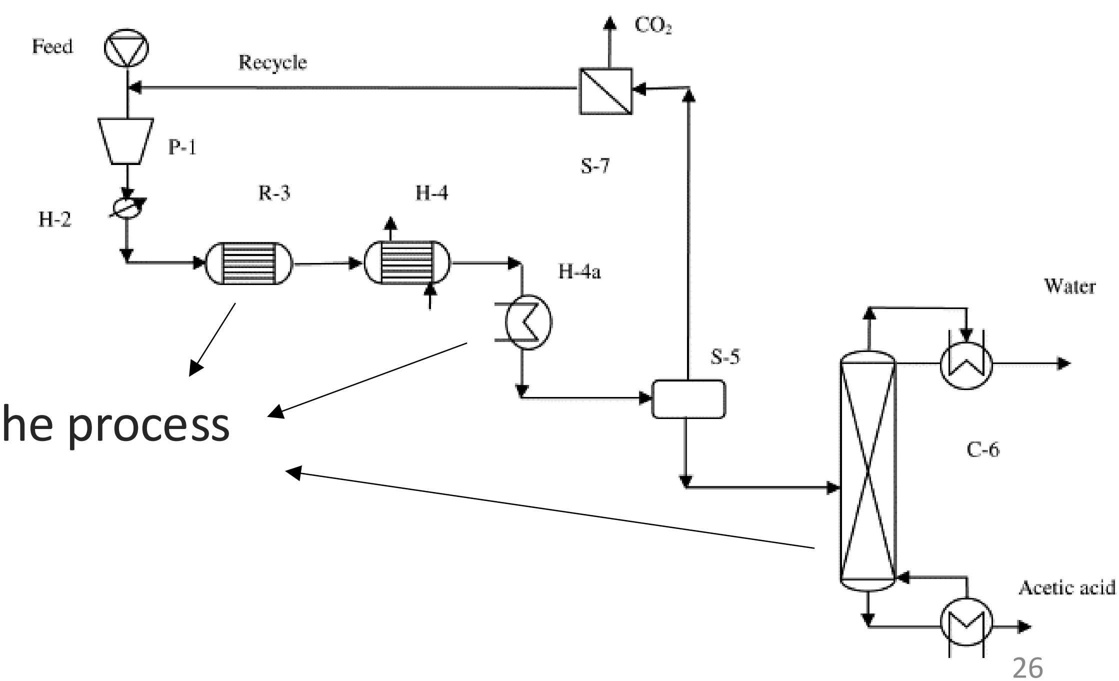
$y_{T3} = 1 - y_{B3} = 0.936$ kg T / kg

3. Mass balance on multiple-unit processes

Multiple-unit processes

- In the vast majority of real chemical processes, there will be:
  - more than one raw material (feed) entering the system AND
  - more than one unit operation through which the product must pass in order to achieve the desired result

  - Examples:
    - mixing reactants before going to reactor
    - blending products
    - separating products
    - recycling



  - Universal icons to show the process units on the paper

How to do mass balance for multiple-unit systems?

Multiple-unit processes are tougher to solve, but it is doable!

1) Label a flowchart completely with all the relevant unknowns

2) Perform a degree of freedom analysis **on each unit operation**

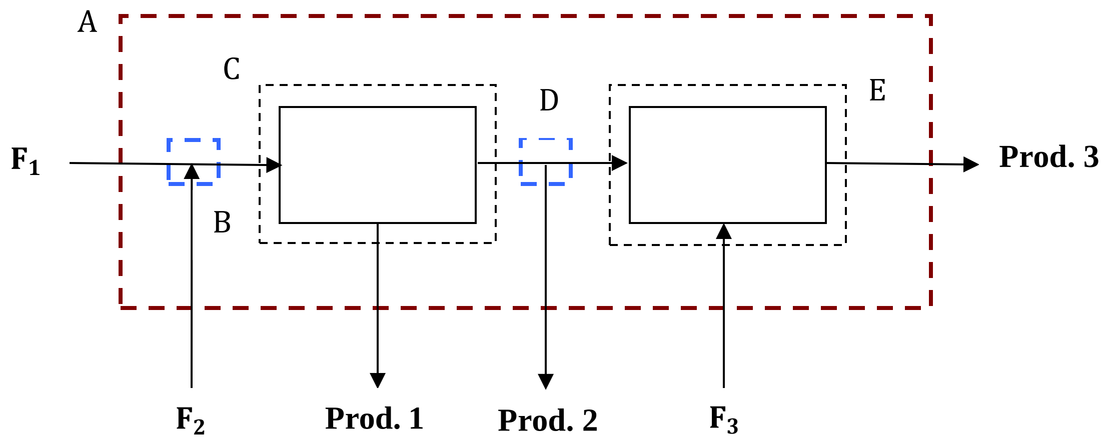
3) **Find and extract with dashed line a unit operation or combination of unit operations (subsystems) for which the degrees of freedom is zero**

4) Calculate all of the unknowns involved in this combination

5) Recalculate the degrees of freedom for each process, treating the calculated values as known rather than as variables

6) Repeat these steps until everything is calculated

Mass balance on multiple units



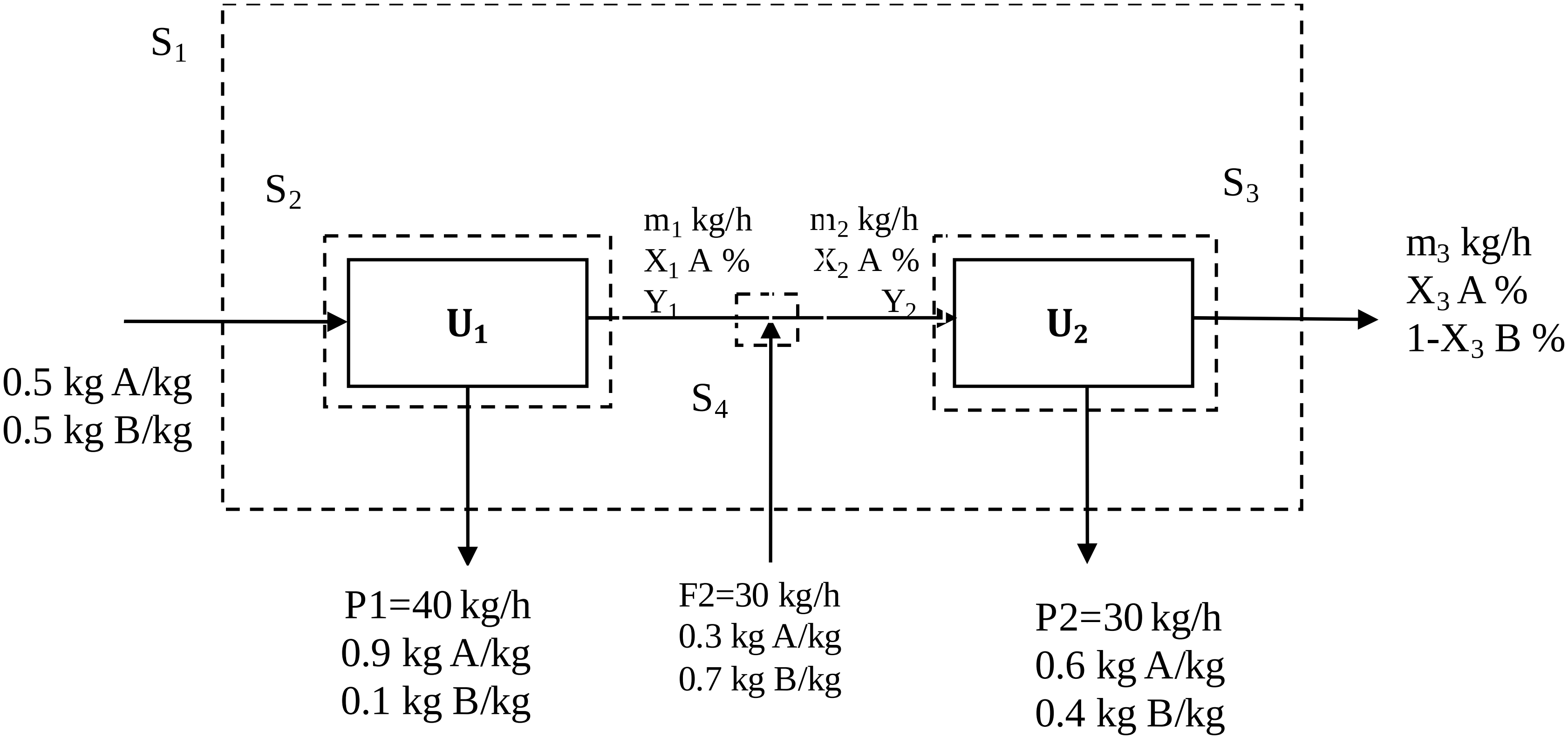
How many systems do we have?

We have 5 systems:

- The overall system : A
- Mixing and splitting points are also systems: F_1 and F_2 are mixing (point B) and D is splitting (point D)
- The internal units: C, E

We have to define the mass balances for each system and start with the unit with **DOF=0**

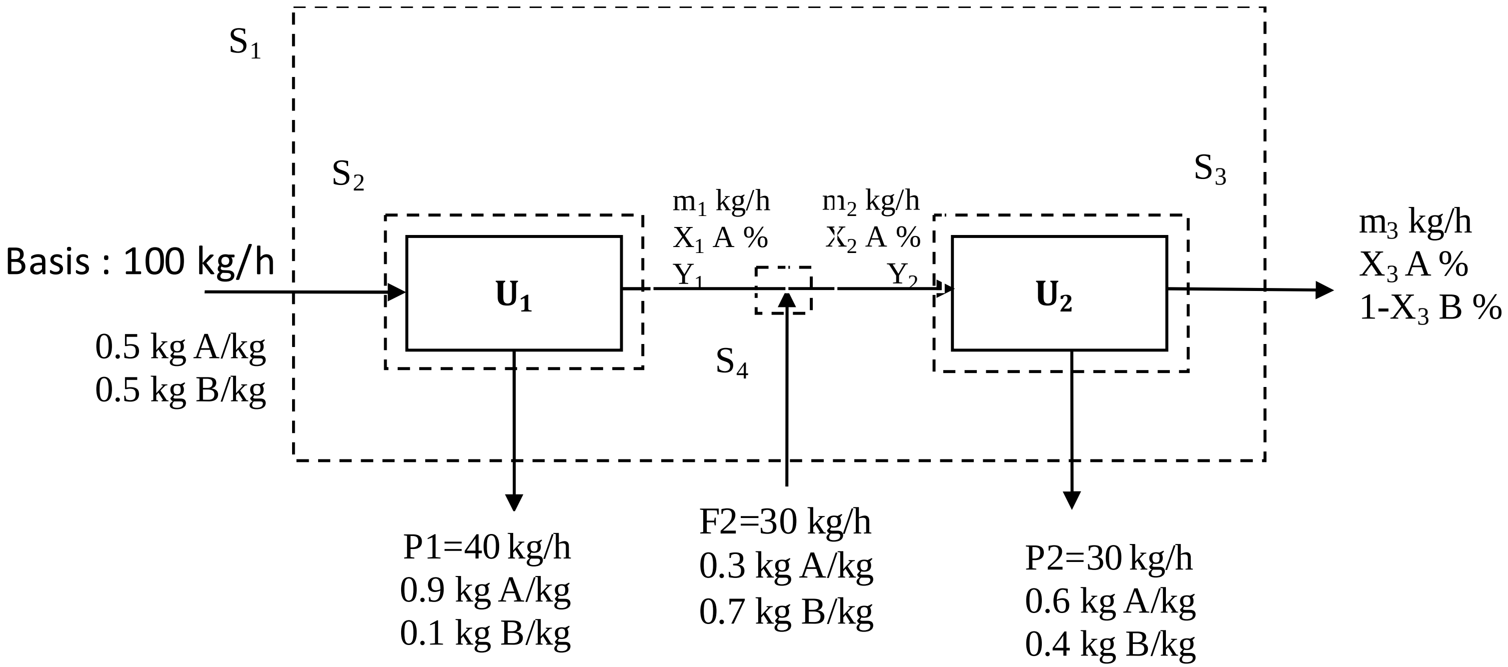
Example 3: Mass balance on 2 unit operations



- Units
- Flowchart
- How many systems?

Basis : 100kg/h feed

Example 3: Mass balance on 2 unit operations



- S_1 (global system): 2 mass balances // 2 unknowns (m_3, x_3)
- S_2 (U_1): 2 mass balances // 2 unknowns (m_1, x_1)
- S_3 (U_2): 2 mass balances // 4 unknowns (m_2, x_2 , m_3, x_3)
- S_4 (System mixing): 2 mass balances // 4 unknowns (m_1, m_2, x_1, x_2)

Example 3: Mass balance on 2 unit operations

Basis : 100kg feed

Mass balance on $\mathbf{S_1}$ (global system):

$\mathbf{S_1}$: In – Out = 0 → 100 + 30 – 40 – 30 – m_3 = 0 → m_3 = 60 kg / h

$\mathbf{S_1}$ (specie A): 50 – 36 + 9 – 18 – $60x_3$ = 0 → x_3 = 0.0834, y_3 = 0.9166

→ $m_{3,A}$ = 5 kg A / h, $m_{3,B}$ = 55 kg B / h

Unknowns left to find : m1,x1,m2, x2

Mass balance on $\mathbf{S_2}$ (U_1):

$\mathbf{S_2}$ (U_1): 100 – 40 – m_1 = 0 → m_1 = 60 kg / h

$\mathbf{S_2}$ (specie A): 50 – 36 – $60x_1$ = 0 → x_1 = 0.23, y_1 = 0.77

→ $m_{1,A}$ = 13.8 kg A / h, $m_{1,B}$ = 46.2 kg B / h

Unknowns left to find : m2, x2

Example 3: Mass balance on 2 unit operations

Mass balance on S_3 (U_2)**:**

S_3 (U_2): $m_2 – (30 + 60) = 0 \rightarrow m_2 = 90$ kg / h

S_3 (specie A): $90x_2 – 18 – 5 = 0 \rightarrow x_2 = 0.256$, $y_2 = 0.744$

$\rightarrow m_{2,A} = 23.04$ kg A / h, $m_{2,B} = 66.96$ Kg B / h

We have found all the unknowns without having to use S4 **-> not all units have to be used.**

But if we wanted to write the mass balances anyway:

Mass balance on S_4 (Mixing)**:**

S_4 : $m_1 + F_2 – m_2 = 0$

S_4 (specie A) : $m_1 x_1 + 0.3\ F_2 – m_2 x_2 = 0$

S_4 (specie B) : $m_1 y_1 + 0.7\ F_2 – m_2 y_2 = 0$

Example 3: Mass balance on 2 unit operations

DONE ☺