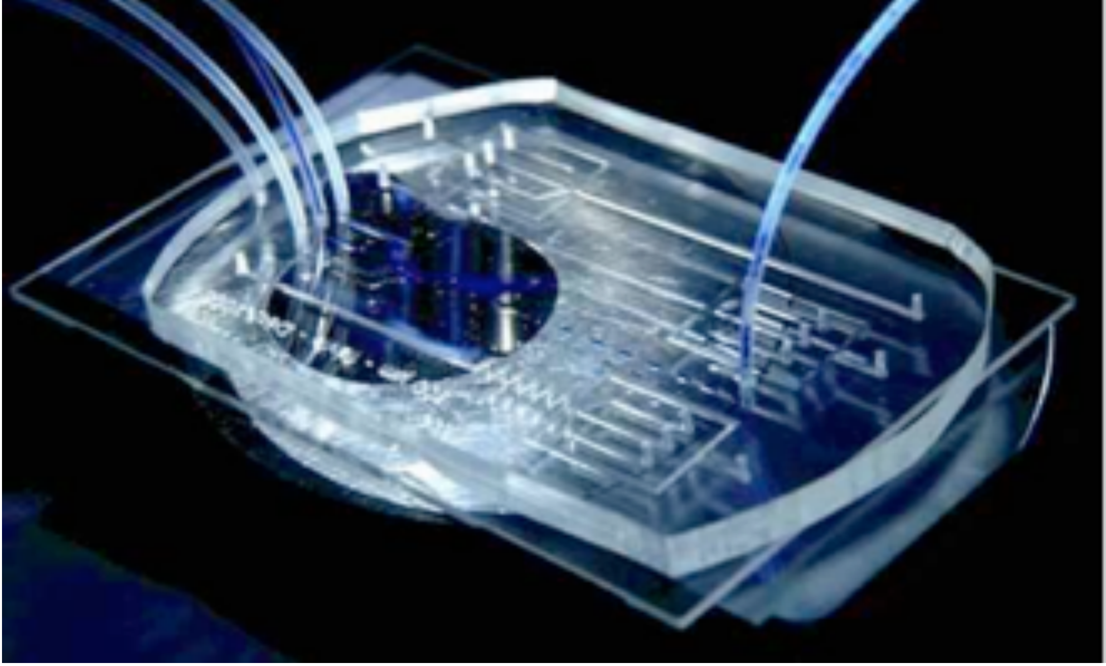

Chemical Engineering: application to environment and sustainable production (Lecture 1)

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Course Outline

7 topics

1. Introduction / Mass balance
2. Ideal reactors
3. Thermal balance
4. Vapor-liquid equilibrium; Single stage distillation (evaporation)
5. Distillation (multistage)
6. Mass transfer: Diffusion + Convection
7. Mass transfer: Design of a mass contactor

Content of a Session

- Homework (pre-work) on the Lecture before the session (slides with embedded oral explanations will be given in Edunao).

- Duration of a session 2.00 hours
  1. During 30 min: discussion about the content of the lecture, simultaneously in classroom and through MS Teams « *ST5 - 52 - Bioprocédés (2020-2021)* » (team code: **c2ouf10**). What are the main point to highlight and remember? The key points will be discussed and summarized.
  2. During 1:30: Case Study. Progressive Solving. The correction will be given at the end (available on Edunao)

Assessment

2 marks:

➢ One short project

- A case study to solve during a limited time (3 hours)
- A written report indicating the approach followed, the details of the calculations, the numerical values obtained, and comments are to be submitted in due course
- A work in group of 4 students. One group = one typing report
- September 23rd

→ 40 % of the final mark

➢ Final written exam

- 1.5 hours
- November 3rd (to be confirmed)
- Individual exam

→ 60 % of the final mark

Course Schedule: 9 sessions

Please note: Sessions start on at 9:30 AM or 2:45 PM

Occurrence	Topic	Nature	Duration (hour)	Date
1	Intro. & Mass Balance	Lecture + Case Study	2.00	Tues. 15/9 9:30 AM
2	Ideal Reactor	Lecture + Case Study	2.00	Wed. 16/9 2:45 PM
3	Ideal Reactor	Project	3.00	Wed. 23/9 8:30 AM
4	Thermal Balance	Lecture + Case Study	2.00	Fri. 25/9 2:45 PM
5	L-V Eq. Flash distillation	Lecture	2.00	Mon. 28/9 9:30 AM
6	Multistage distillation	Lecture + Case Study	2.00	Wed. 30/9 9:30 AM
7	Diffusion & Convection	Lecture + Case Study	2.00	Mon. 5/10 9:30 AM
8	Mass Transfer Contactor Design	Lecture + Case Study	2.00	Wed. 7/10 9:30 AM
9	Executive summary	Lecture	3.00	Mon. 19/10 8:30 AM

Syllabus

- Introduction – Mass and enthalpy balances, simple flow models
- An example of a unit operation: distillation, ideal stage model
- Reactor, 0D & 1D models, chemical & enzymatic kinetics
- Heat & mass transfer, influence of hydrodynamics
- Polyphasic systems

Objectives

- To know the basic notions presented in the lectures
- To analyze the running of an industrial process
- To write Heat & mass balances for an equipment or at the scale manufacturing unit
- To develop a modeling strategy for an equipment
- To use modeling for the definition / diagnosis / optimization of equipment / troubleshooting (solving problems)

Outline: Session 1

1. Chemical Engineering: Definition
2. Processes in industry – Process engineer
3. Sustainable Development: main principles
4. Towards a sustainable Process Engineering
5. Industrial Process: brief introduction
6. Mass balance
7. Bibliography

Chemical Engineering: Definition

- Chemical Engineering is the study and practice of transforming substances at large scales for the tangible improvement of the human condition
- Such transformations are executed to produce other useful substances or energy (most of the time both)
- Presence in vast segments of the industry: chemicals, petroleum-oil, cosmetics, crop science, pharmaceuticals, electronics, *etc*.

(Univ of Illinois)

Chemical Engineering: Definition

Chemical Engineering differs from Chemistry mainly in the focus on large scales

- Large Scale: How Much???

The definition of "large" is a bit arbitrary, of course, but is set mainly by the scale of useful commercial production

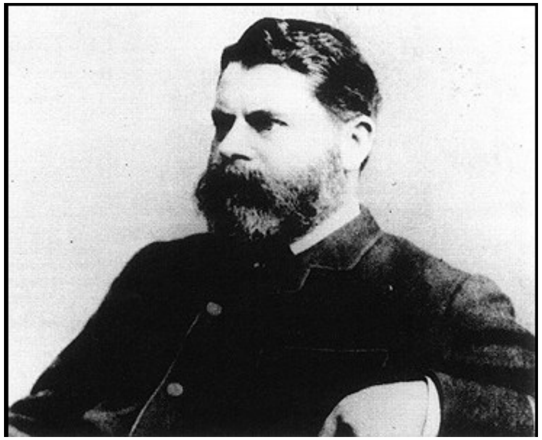
(Univ of Illinois)

Chemical Engineering: Scales

- Scales of investigation and production (in volume):
  - Lab scale: milliliter to liter → investigation of chemistry, definition of a (bio-)chemical route
  - Pilot scale: tens to hundreds of liters → validation of the chemistry, detection of some issues (heat transfer, rheological behavior of the flow, *etc*.), validation of the productivity (kg/batch or kg/hour)
  - Plant scale: thousands of liters → production

(Univ of Illinois)

Chemical Engineering: The foundations



E. Davis, founding father of chemical engineering Manchester Technical school, UK, 1888

- **Birth of Chemical Engineering in the MIT in 1902 with W. H. Walker**
- **Concept of Unit Operation (A. D. Little, MIT,1915) – 1^{rst} Paradigm**

- **<u>Foundation treaty:</u> "Principles of Chemical Engineering" by Walker, Lewis et McAdams, 1923**

Chemical Engineering: Evolution

1st paradigm: Approach by considering unit operation

- Transport of fluids: agitation-stirring, mixing
- Heating / Cooling
- Mass Transfer operations :
  - ☐ stripping, distillation (Gas / Liquid)
  - ☐ emulsification, extraction (Liquid / Liquid)
  - ☐ dissolution, crystallization, précipitation (Liquid / Solid)
  - ☐ condensation, drying, lyophilization…(Gas / Solid)
- Reactions in liquid or gas state
- Operations on powders: milling, sieving, conveying, *etc*.

In the fifties: 1 operation ⇔ 1 operator (simple automation)

From the seventies: a plant ⇔ only a few operators (development of advanced control systems)

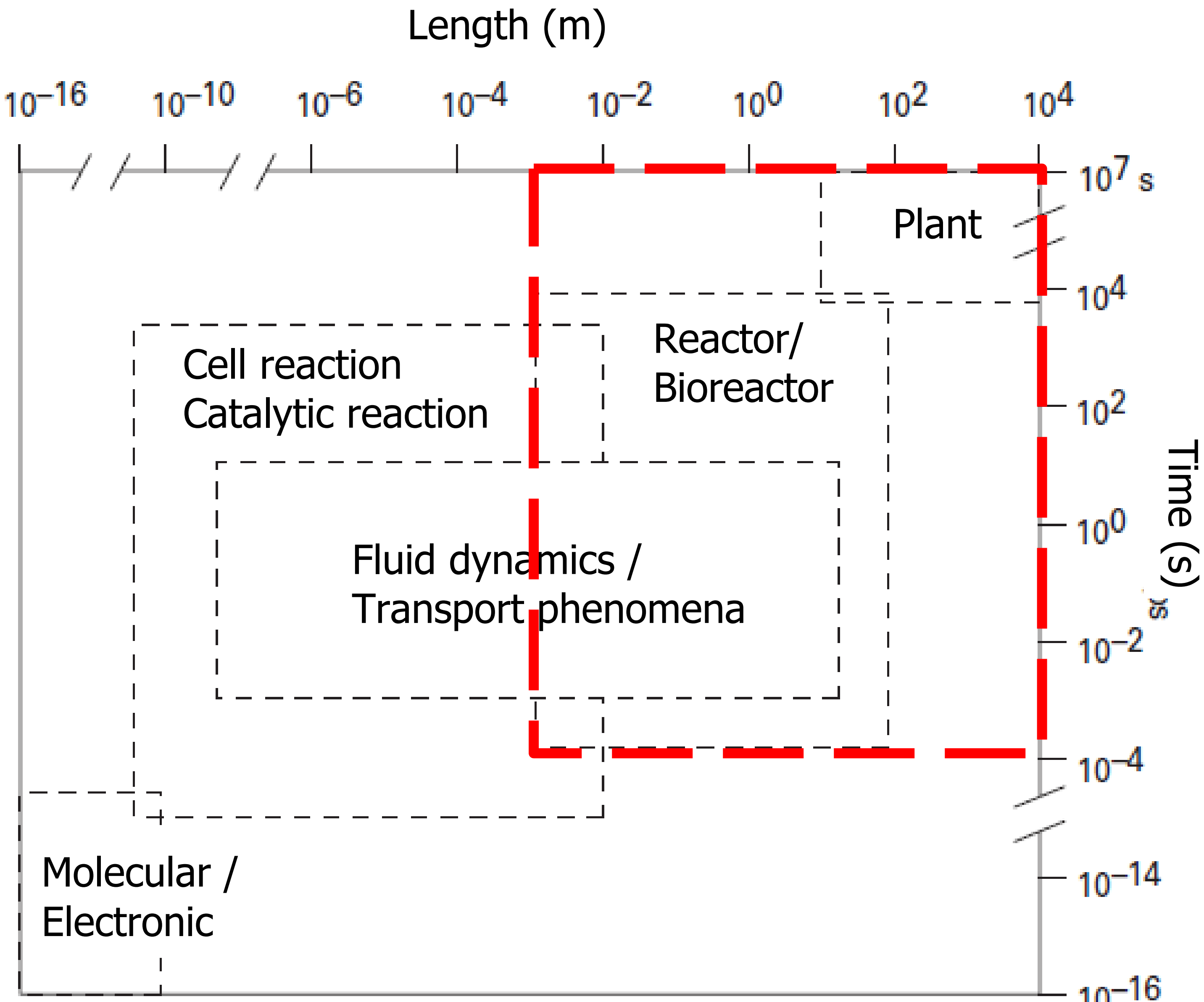
Chemical Engineering: Evolution

2^{nd} paradigm: Approach by considering mechanisms

- ➢ In the unit operations → same mechanisms involved:
  - ❑ Transfer Sciences (Mass, Heat, Flow)
  - ❑ Transport phenomena, Bird, Steward and Lightfoot, 1960
- ➢ Coupling (pairing) phenomena:

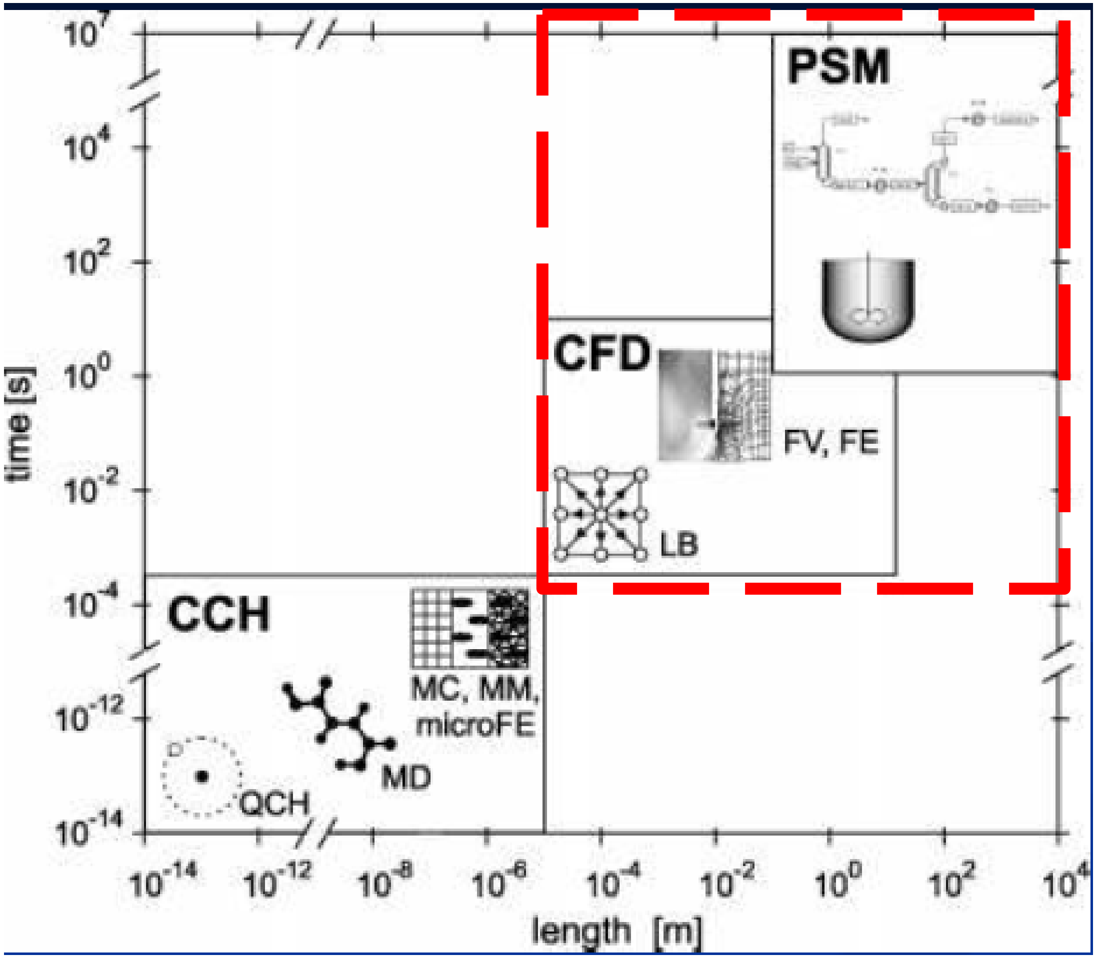
  (Heat & Mass; Mass & Flow ; Heat & Flow; Mass & Chemistry, *etc*.)
- ➢ Chemical / Biochemical Reactions:
  - ❑ Chemical Reaction Engineering, O.Levenspiel, 1999 (3rd Ed.)
  - ❑ Génie de la Réaction Chimique; J. Villermaux, 1993 (2nd Ed.)

Chemical Engineering:
What are the scale (spatial and time) to consider?



(Charpentier 2013)

Time and spatial Multiscale approach: Impact on Modelling in Chem. Eng.

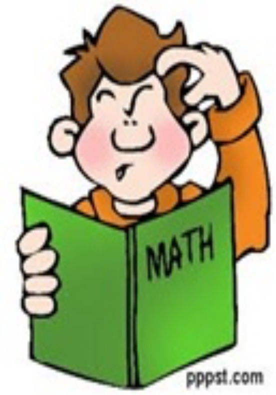


- PSM : Process System Modelling
- CFD : Computational Fluid Dynamics
- Computational CHemistry

(Charpentier 2013)

Chemical Engineering Approach

Methodology



No general result but a general methodology

Balances (Mass ; Heat)

« Nothing is lost, nothing is created, everything is transformed/converted »

Outline: Session 1

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Processes in Industry

- Objectives:
  - ☐ To transform raw materials (fossil, renewable, **waste**) in end-used products
  - ☐ To provide services to other industries

- Numerous industrial sectors (almost Endless!)
  - ☐ Chemistry, Oil/petroleum
  - ☐ Materials : metallurgy, cement, gypsum, ceramics, glass, textile, inks, adhesive, coating, painting, semi-conductor, *etc*.
  - ☐ Cosmetics
  - ☐ Pharmaceuticals, vaccine
  - ☐ Food / Feed industry
  - ☐ Environment
  - ☐ Energy Production
  - ☐ *Etc*.

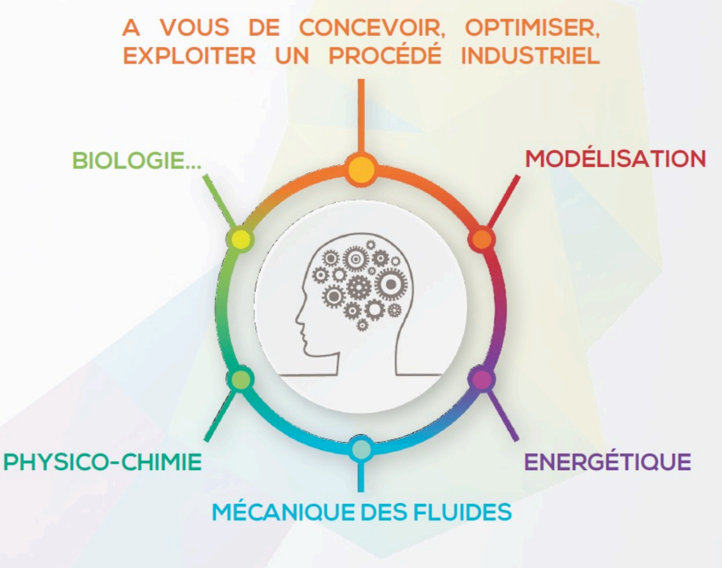
Process Engineer: his/her job

- DESIGN / RUN / UPGRADE-OPTIMIZE / TROUBLESHOOT

- **To Design** **plants for manufacturing several qualities and quantities of well-defined products**

- **Identify**
  - **Inlets & outlets of Mass, Energy and Wastes**
  - **Essential equipment / setups**
  - **Connection between them**

- **Design equipment / setups**



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Sustainable Development: Definition

Most frequently quoted definition :

"Sustainable development is development that meets the needs of the present without compromising the ability of future generations to meet their own needs"

(from the World Commission on Environment and Development's (the Brundtland Commission) report Our Common Future (Oxford: Oxford University Press, 1987)

- It contains within it two key concepts:
  - ☐ the concept of **needs**, in particular the essential needs of the world's poor, to which overriding priority should be given
  - ☐ the idea of **limitations** imposed by the state of technology and social organization on the environment's ability to meet present and future needs

Sustainable Development: Main Principles

Acting on 3 Pillars (Social/Environment/Economy)

Sustainable Development

3 requirements:

Cost-effective manner

Socially fair

Environmentally sustainable

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Last Century : No Sustainable Development in Industry

Only 25 % mass of the inlet in the tube is converted into products and services

Need to enhance the process efficiency by:

- **Factor 4 (Von Weizsacker, 1998)**
- **Fractor 10 (Schmidt-Bleek, 1993)**
- **Factor 20 (AllChemE, 2001)**

Source:
World Research Institute
(2005)

Towards a Sustainable Process Engineering

- Several road maps published
  - Green chemistry: 12 principles
  - Green Engineering: 12 principles
  - Other recommendations published in the open literature

- Practically:
  - CO_2 sequestration
  - Low carbon energy (consumption/emission) process
  - Reduction of wastage of natural resources
  - Substitute fossil energies by renewable energies
  - Main resources of materials = wastes
  - *Etc.*

Towards a Sustainable Process Engineering

How to balance social and economic constraints?

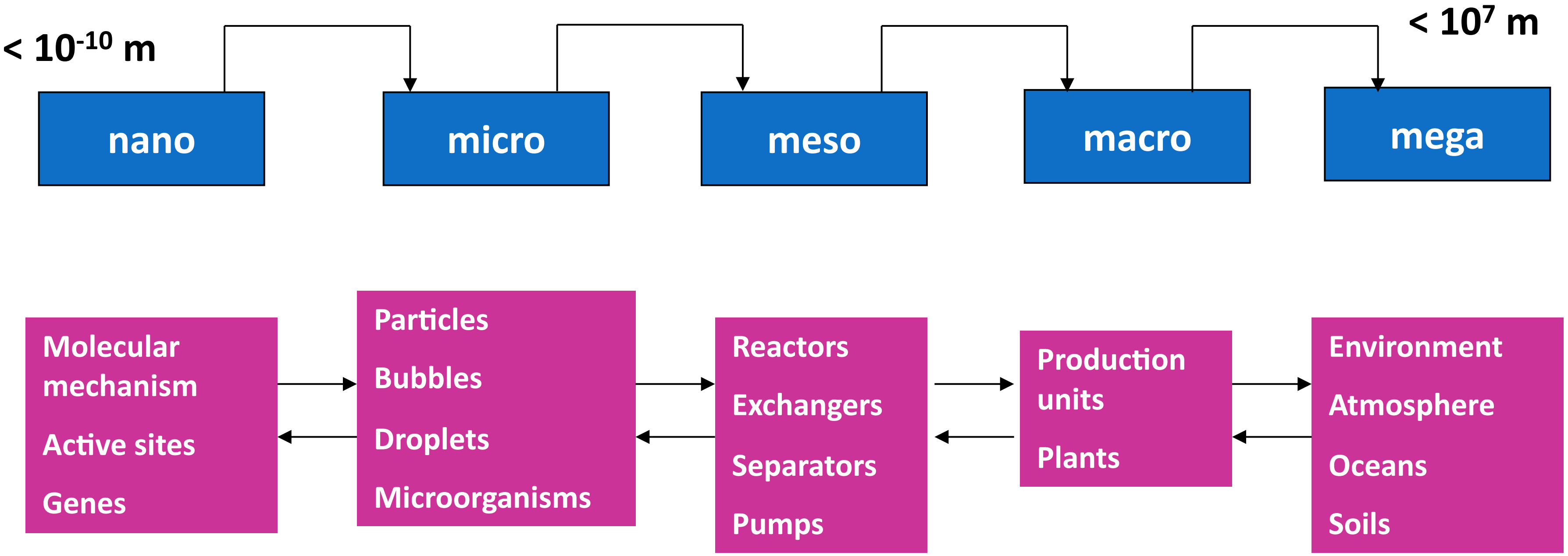
Low carbon / Safe & clean process

↓

- Better control of the Process (time and space):
  - ☐ To know the time and spatial dynamics of the involved phenomena
  - ☐ To understand and to describe the relationships between events at NANO and MICRO Scales to better convert MOLECULES to USEFUL PRODUCTS at the PROCESS-scale

- Process Intensification

Multi-length scale approach



< 10^{-10} m

< 10^{7} m

nano → **micro** → **meso** → **macro** → **mega**

Molecular mechanism
Active sites
Genes

Particles
Bubbles
Droplets
Microorganisms

Reactors
Exchangers
Separators
Pumps

Production units
Plants

Environment
Atmosphere
Oceans
Soils

(Charpentier 2013)

Process Intensification

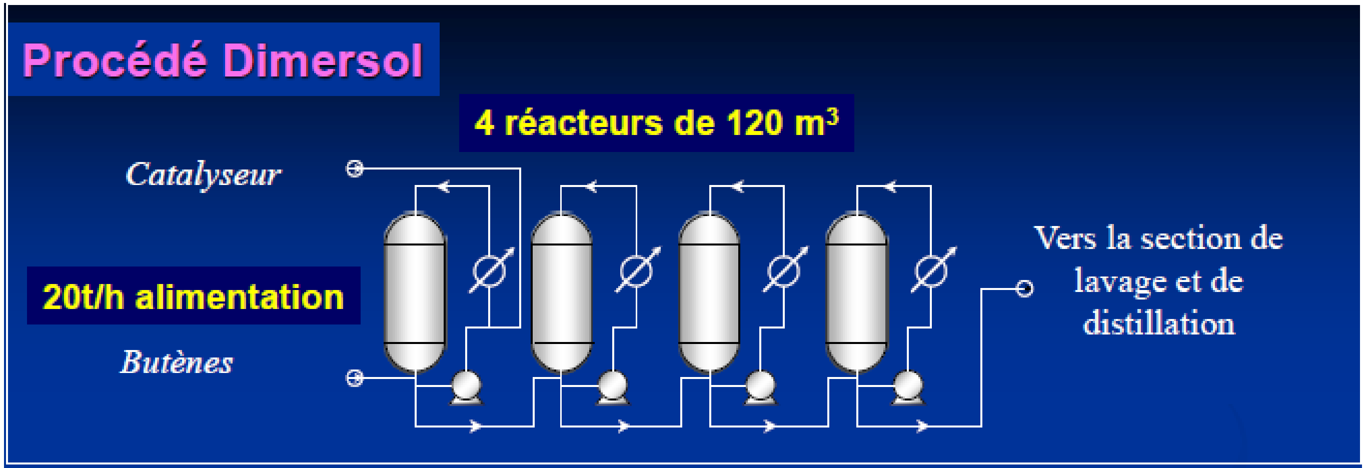
“producing much more and better with using much less”

3 areas of improvement:

1. To Develop multifunctional equipment (“Technology Push”)
2. To use new operating modes
3. To use microengineering and microtechnology

Process Intensification:
1 – Multi-functional equipment

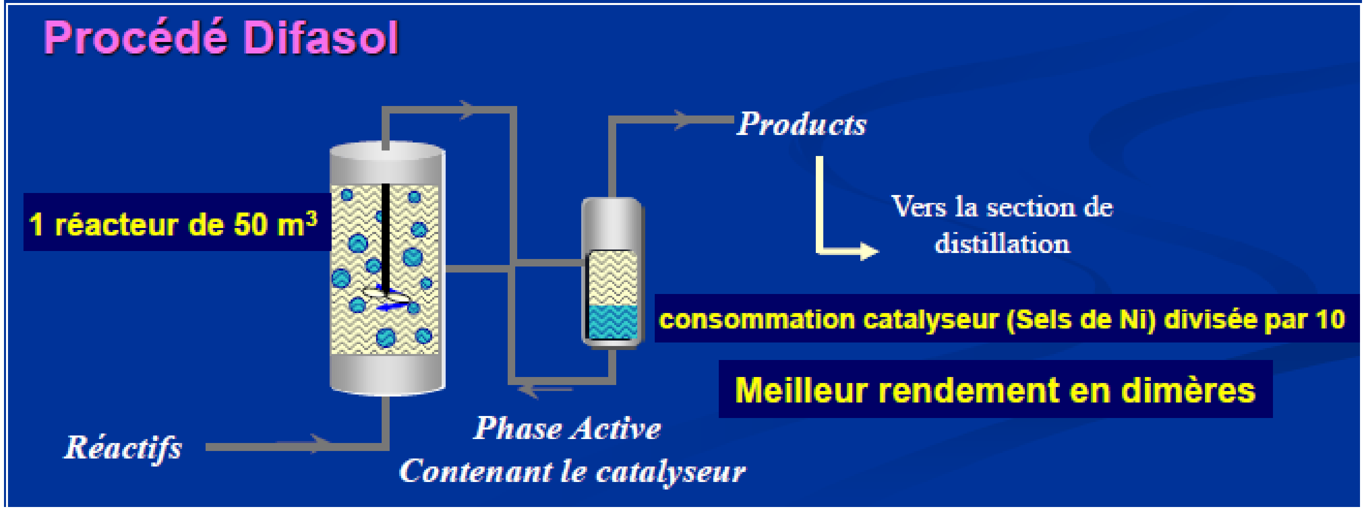
- **Ex.: Implementation of a Liquid-Liquid Biphasic Catalysis**
  (Dimersol process : Dimerization of olefins)



Procédé Dimersol

4 réacteurs de 120 m^3

20t/h alimentation



Procédé Difasol

1 réacteur de 50 m^3

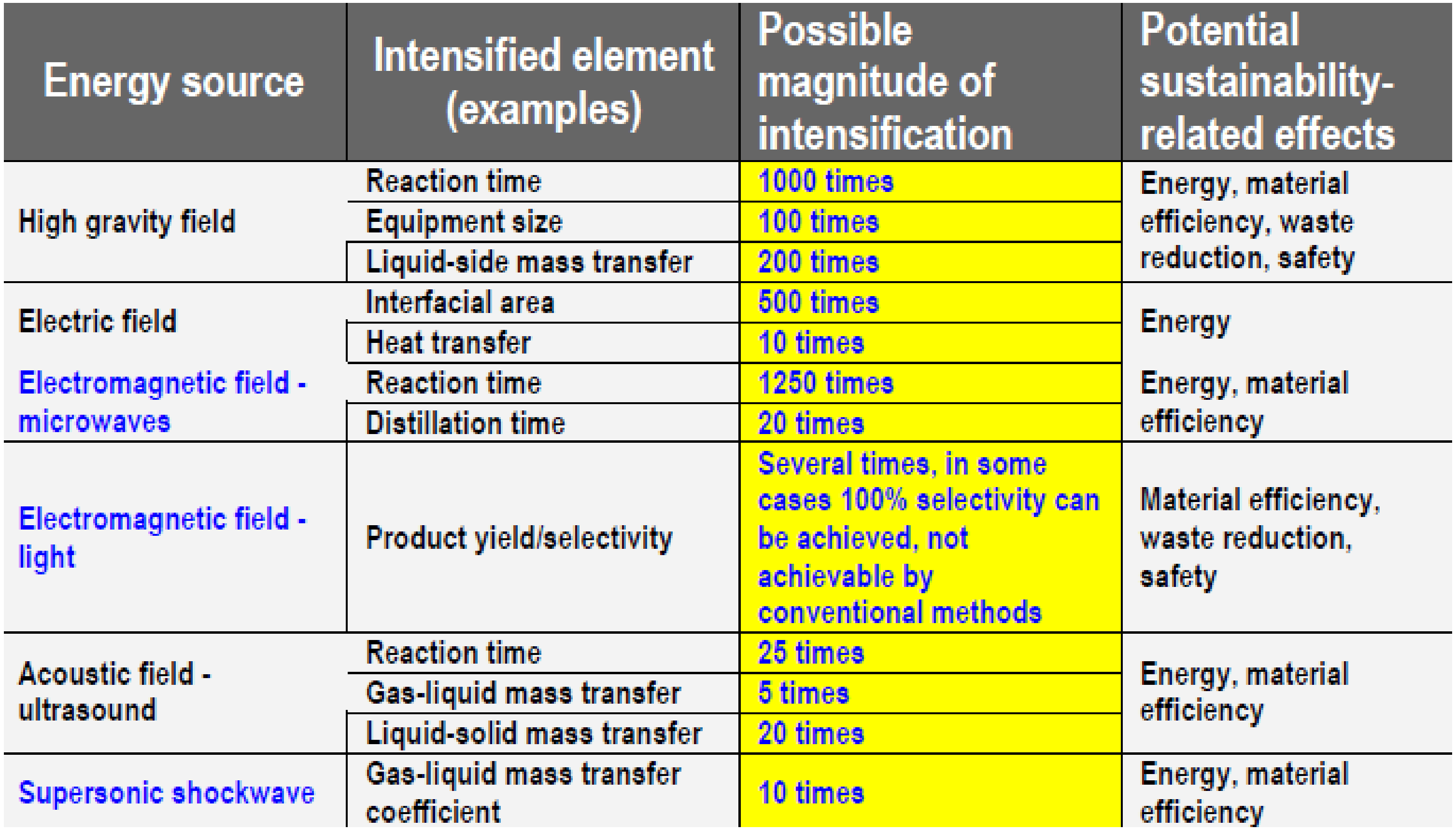
consommation catalyseur (Sels de Ni) divisée par 10

Meilleur rendement en dimères

Process Intensification:

2 - New Operating Modes

- **Ex.: Use of External driving forces in order to enhance mass transfer**

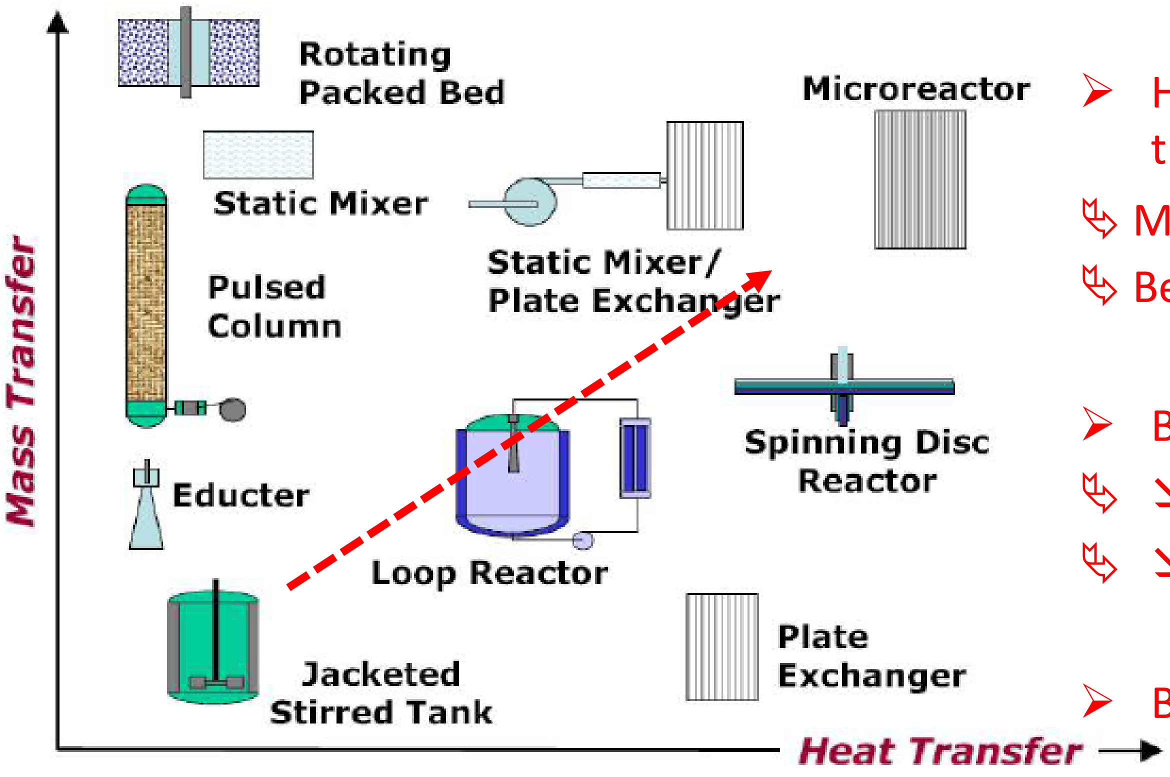


Energy source	Intensified element (examples)	Possible magnitude of intensification	Potential sustainability-related effects
High gravity field	Reaction time	1000 times	Energy, material efficiency, waste reduction, safety
	Equipment size	100 times	
	Liquid-side mass transfer	200 times	
Electric field	Interfacial area	500 times	Energy
	Heat transfer	10 times	
Electromagnetic field - microwaves	Reaction time	1250 times	Energy, material efficiency
	Distillation time	20 times	
Electromagnetic field - light	Product yield/selectivity	Several times, in some cases 100% selectivity can be achieved, not achievable by conventional methods	Material efficiency, waste reduction, safety
Acoustic field - ultrasound	Reaction time	25 times	Energy, material efficiency
	Gas-liquid mass transfer	5 times	
	Liquid-solid mass transfer	20 times	
Supersonic shockwave	Gas-liquid mass transfer coefficient	10 times	Energy, material efficiency

Beware : applicability at large volume

(Stankiewicz, ChERD, 2006, 84, 511)

Process Intensification:
3 - Using micro-devices

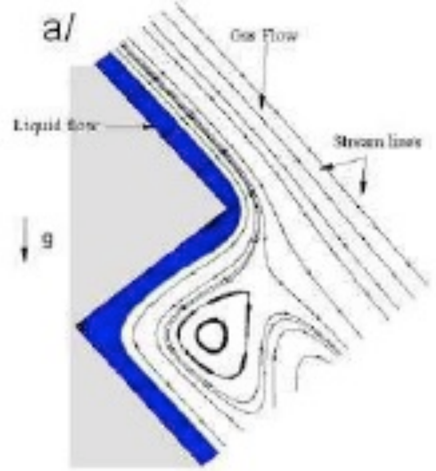


- ➢ Higher surface/volume ratio and turbulent flow :
  - ↳ Mass transfer ↗
  - ↳ Better heat control ↗
- ➢ Better chemical selectivity
  - ↳ ↘ need in reactants
  - ↳ ↘ waste volume
- ➢ Better safety
- ➢ ONLY for valuable products ☹ !!

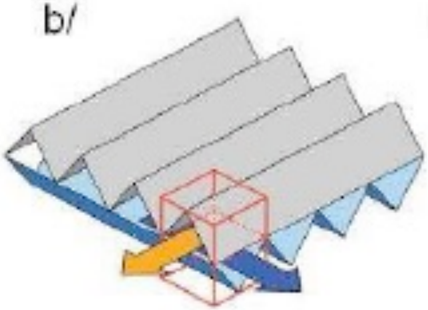
Process Intensification :
3 - Using micro-structured elements embedded in conventional technologies

a) **Liquid Film flowing on a folded surface & sheared by a gas**
b) **Elementary cell of a microstructured packing**
c) **Packing Element**
d) **Mass transfer column**

a/



b/



c/

d/

(Sulzer ChemTech)

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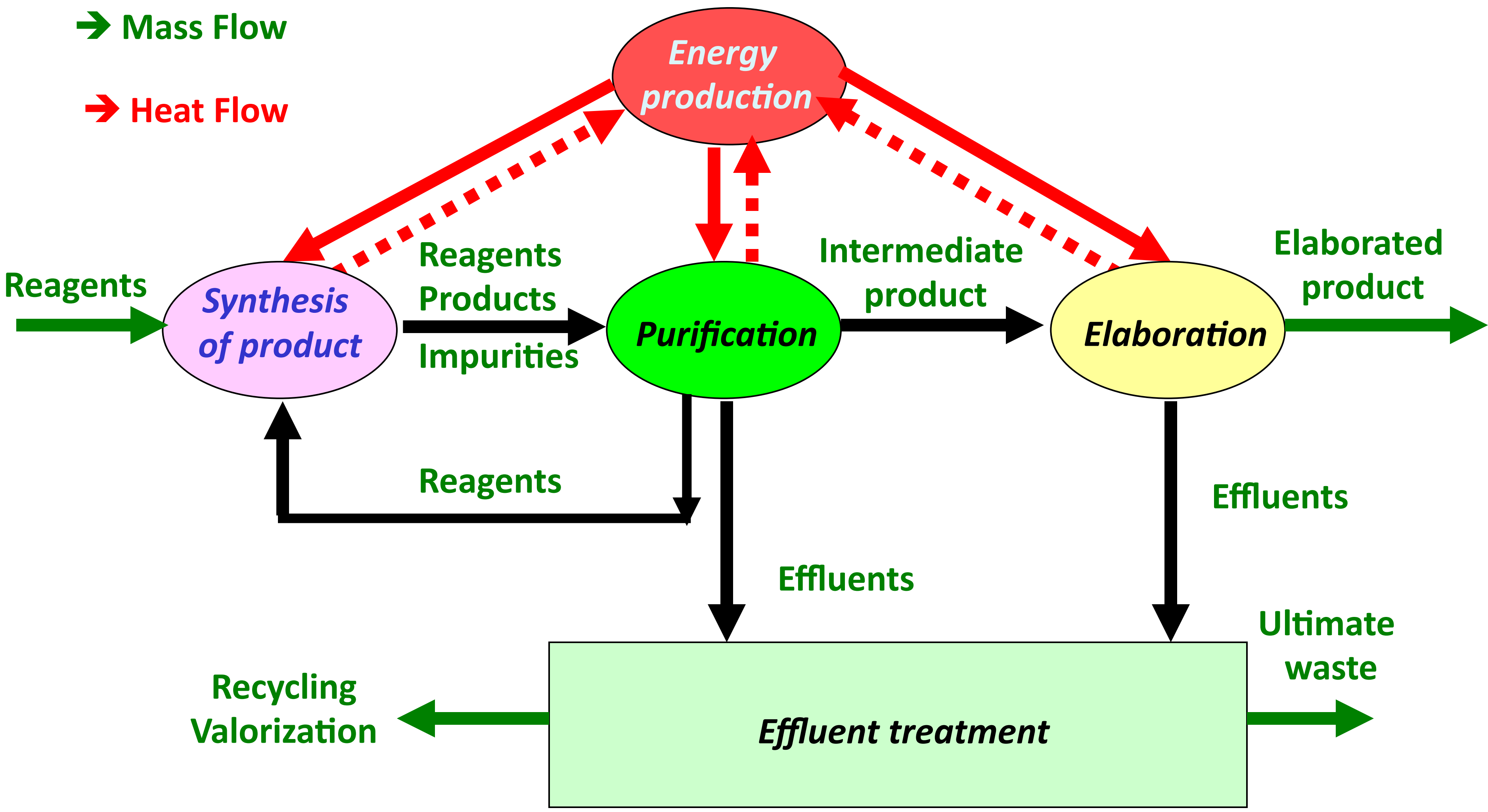
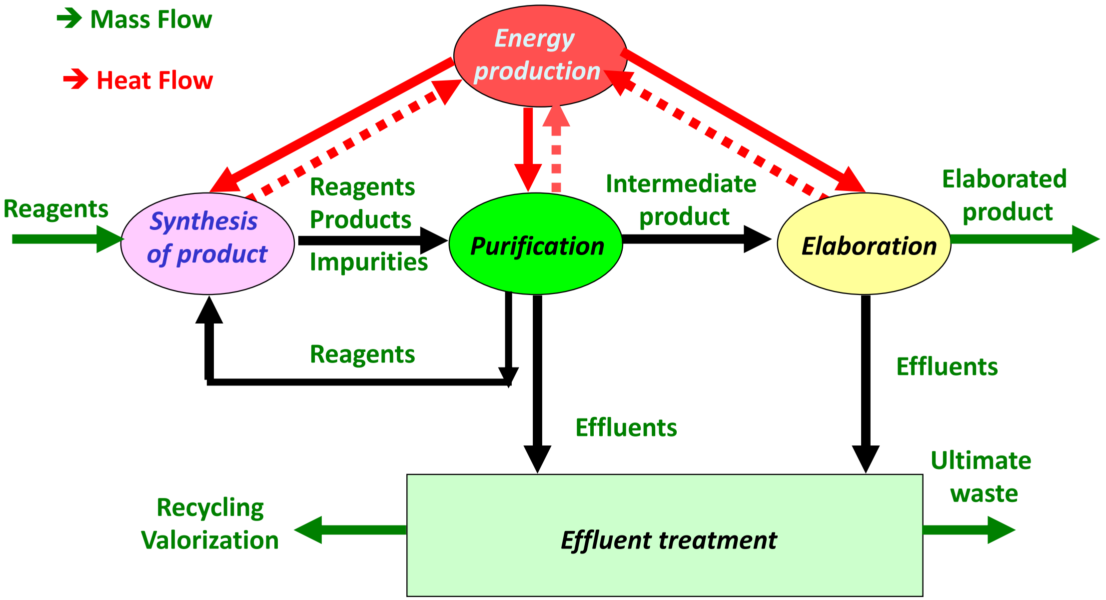
Process flowsheet (diagram)



Process Flowsheet



Equipment

Transformation → **Reactor** (chemical)
& Bioreactor (biochemical)

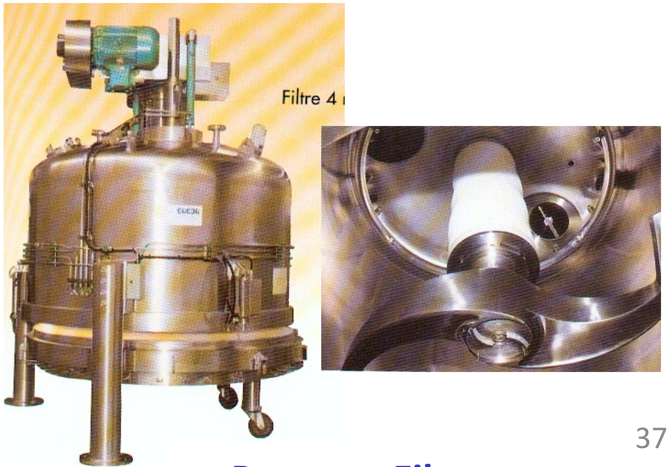
Separation / Blending (mixing) → **Column, Crystallizer, Filter, Dryer, Mixing devices, etc.**

Equipment
(main and surrounding)

Reactor $192m^3$

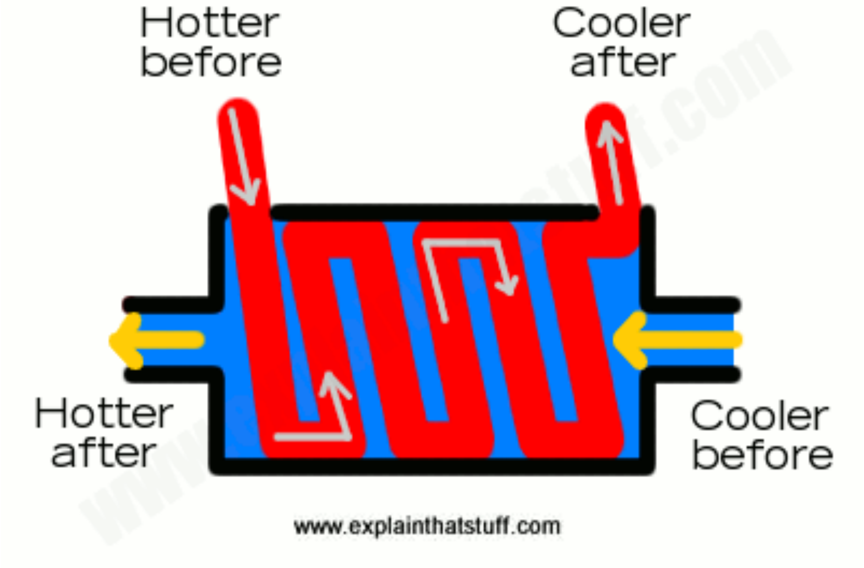
- **Chemical reactor**
  - **Two phase separator :**
    - **Without mass transfer between phases (filters, *etc*.)**
    - **With mass transfer between phases (distillation column, extraction device, *etc*.)**

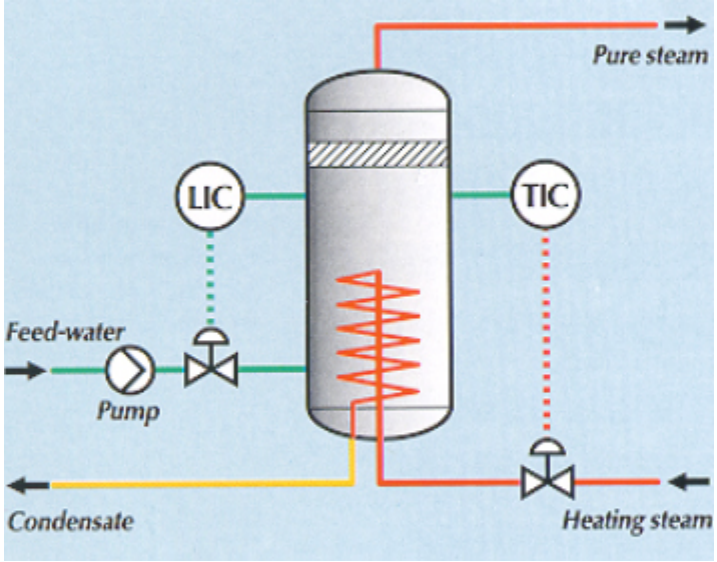
Distillation Column



Pressure Filter

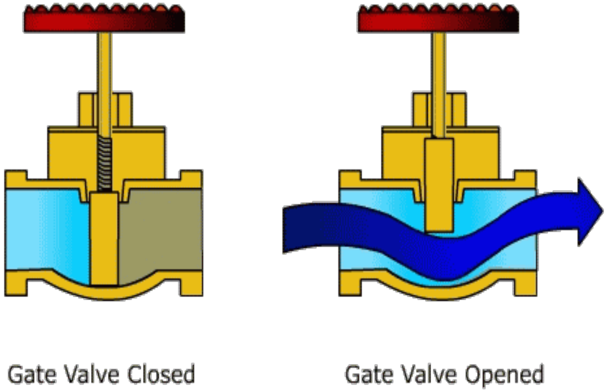
Equipment
(main & surrounding)



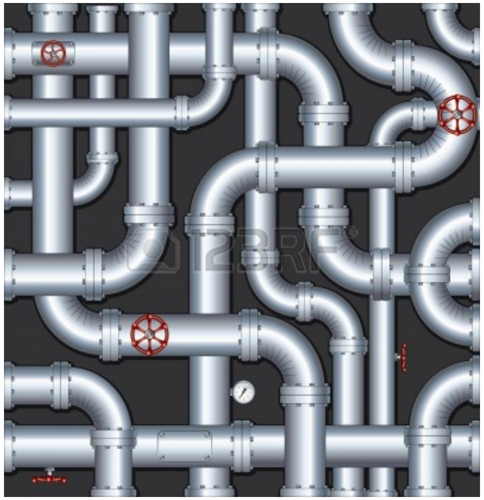


Energy generators (vapor, *etc*.)

Heat exchanger


Gate Valve Closed

Gate Valve Opened



Pumps, compressors, valves, pipes, *etc*.

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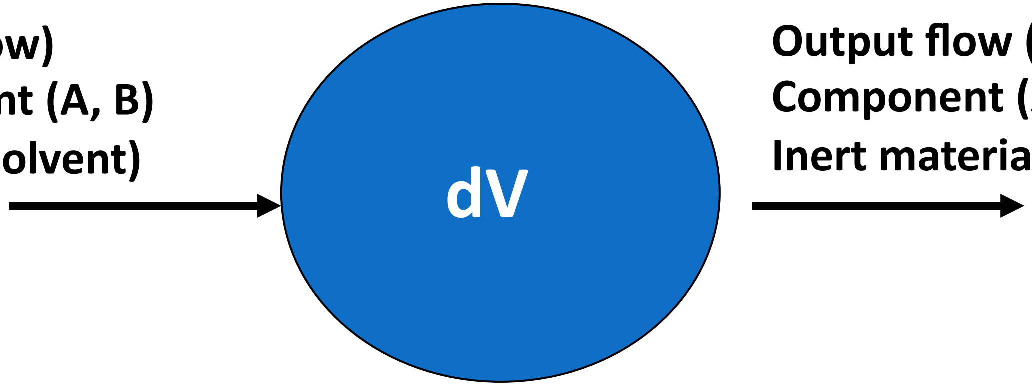
Mass Balance

1- To define an elementary volume dV

- ↳ **To define the boundaries**
  - ↳ **To write the boundary conditions**



Input flow (feed flow)
Reactive Component (A, B)
Inert component (solvent)

Output flow (withdrawal flow)
Component (A, B, P)
Inert materials (solvent)

2 –To know the involved (bio-)chemical kinetics

e.g. A is converted at a volumetric rate $r_A\ (kg \cdot m^{-3} \cdot s^{-1})$

3 – To establish the mass balance between t → t + dt

- **On the whole flow**
- **For each (bio-)chemical component**

4 – To integrate the mass balance from t = 0 → t = end

Mass Balance

element of volume dV; time interval dt;

A: chemical species / substance / component / material

(rate of material A flowing into dV during dt) + **(Rate of material A Produced in dV during dt)** =

[IN] **[P]**

(rate of material A flowing out of dV during dt) + **(Rate of reactant A consumed / converted in dV during dt)** + **(Rate of accumulation of reactant A in dV during dt)**

[OUT] **[C]** **[Acc] = [Final] – [Initial]**

INPUT [IN] + Production [P] = OUTPUT [OUT] + Conversion [C]+ Accumulation [Acc]

$\geqslant 0$ $\geqslant 0$ $\geqslant 0$ $\geqslant 0$ $\geqslant 0$ or $\leqslant 0$

[Acc] = ([IN] - [OUT]) + ([P] - [C])

Mass Balance

element of volume dV; time interval dt;

A: chemical species / substance / component / material

INPUT [IN] + Production [P] = OUTPUT [OUT] + Conversion [C]+ Accumulation [Acc]
⩾0 ⩾0 ⩾0 ⩾0 ⩾0 or ⩽0

[Acc] = ([OUT] - [IN]) + ([P] - [C])

<u>Several situations:</u>

- ❖ A = Reactant → no production of A , only conversion → [P] = 0 and [C] > 0
- ❖ A = Product or by-product → no conversion, only production → [C] = 0 and [P] > 0
- ❖ A = Inert → no conversion, no production → [C] = [P] = 0

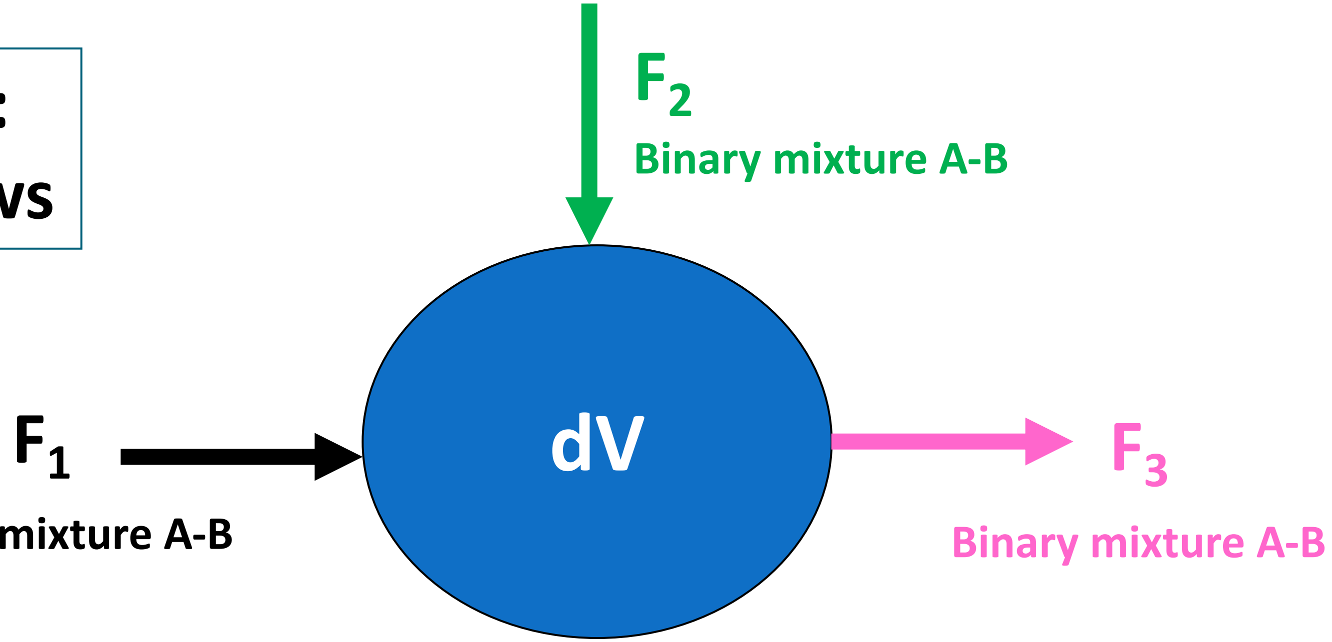
- ➢ Close system (Batch) → [OUT] = [IN] = 0
- ➢ Semi Open system (Fed Batch) → [IN] > 0 and [OUT] = 0 (no withdrawal)
- ➢ Open system (Continuous) → [IN] > 0 and [OUT] > 0

- ❑ Continuous mode in steady state regime → [Acc] = 0 (no time dependency)

Mass Balance:

case 1: Continuous + Steady State Regime *without reaction*

F_1, F_2, F_3:
Mass flows



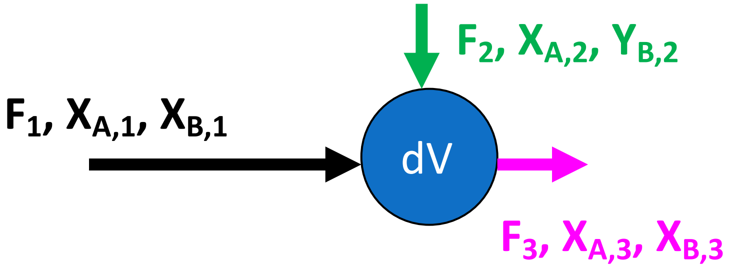
Mass fraction of A: X_A
Mass fraction of B: X_B

$$\begin{cases} X_A = \dfrac{Mass \quad A}{Total \quad mass} \\[2ex] X_B = \dfrac{Mass \quad B}{Total \quad mass} \end{cases}$$

$X_A + X_B = 1$

Mass Balance:

case 1: Continuous + Steady State Regime *without reaction*



$$\underset{>0}{[IN]} + \underset{=0}{[P]} = \underset{>0}{[OUT]} + \underset{=0}{[C]} + \underset{=0}{[Acc]}$$

$$\left(\begin{array}{c}\text{rate of reactant}\\ \text{A flowing into dV}\end{array}\right) = \left(\begin{array}{c}\text{rate of reactant A}\\ \text{flowing out of dV}\end{array}\right)$$

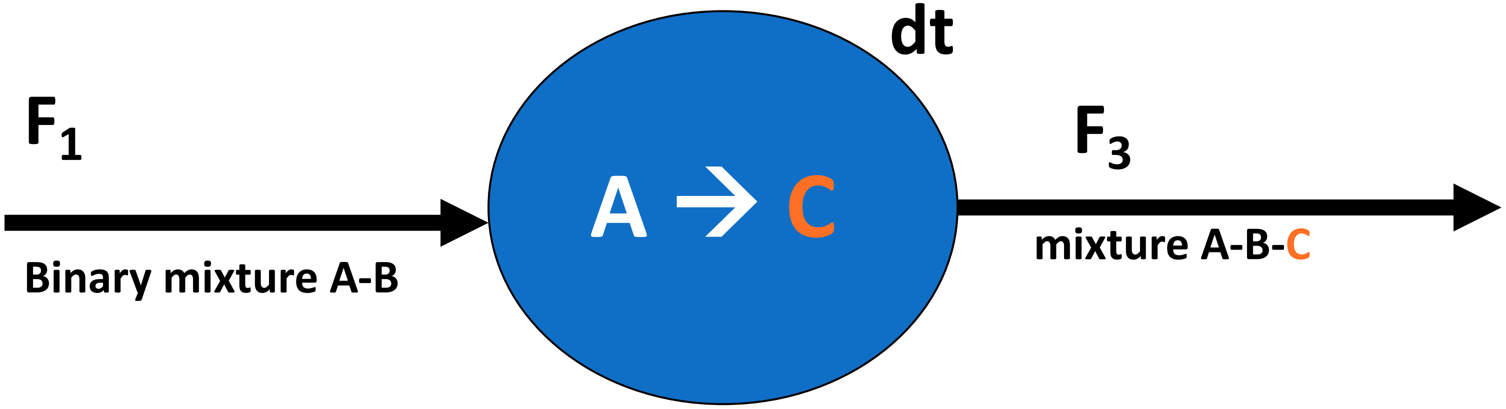
Balance on A (mass flow of A): $F_1 \cdot X_{A,1} + F_2 \cdot X_{A,2} = F_3 \cdot X_{A,3}$

Balance on B (mass flow of B): $F_1 \cdot X_{B,1} + F_2 \cdot X_{B,2} = F_3 \cdot X_{B,3}$

Overall balance A+B (overall mass flow): $F_1 + F_2 = F_3$

Mass Balance:

case 2: Continuous + Steady State Regime *<u>with</u> reaction*



dt

F_1

Binary mixture A-B

$A \rightarrow C$

F_3

mixture A-B-C

Element of volume dV

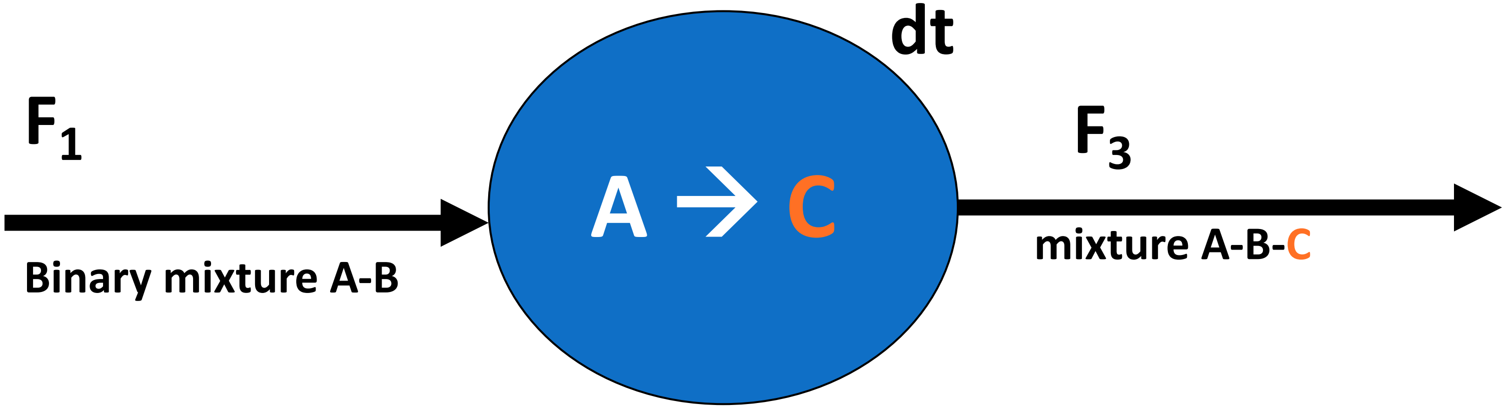
Mass Balance on reactant A in dV during dt:

(Rate of flow A into dV) + (Rate of reactant A Produced in dV) = (Rate of flow A out dV) + (Rate of reactant A consumed in dV) + (Rate of accumulation of reactant A in dV)

[IN]	+	[P]	=	[OUT]	+	[C]	+	[Acc]
>0		=0		>0		>0		=0

Mass Balance:

case 2: Continuous + Steady State Regime ***with*** *reaction*



Element of volume dV

Mass Balance on reactant A in dV during dt :

[IN]	+	[P]	=	[OUT]	+	[C]	+	[Acc]
>0		=0		>0		>0		=0
$F_1 \cdot X_{A,1}$	+	0	=	$F_3 \cdot X_{A,3}$	+	$dV \cdot (-dX_A/dt)$	+	0

with chemical conversion rate $r_A = -dX_A/dt > 0$ since $dX_A < 0$

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2. Processes in industry – Process engineer
3. Sustainable Development: main principles
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