Chemical Process Design / Diseño de Procesos Químicos

Topic 3.1. Overview of process synthesis

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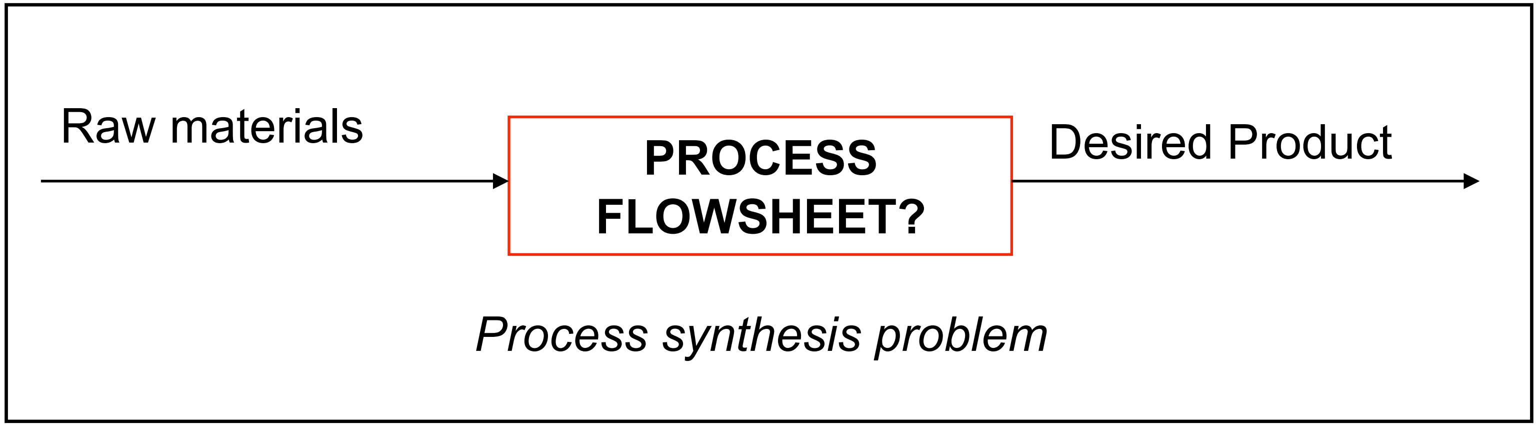
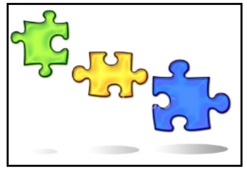
1.- Preliminary Process Synthesis

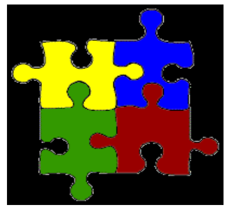


Process synthesis problem

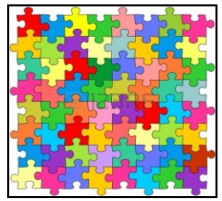
Steps in process synthesis: Process operations → unit Processes → Global Flowsheets.



- **Material Chemical State: Raw material and product. specifications *(Mass, composition, phase, form of solid phase, T, P, well-defined properties such as m, MW or color)*.**



- **Process Operations: Basic operations, connected + *task integration,* where operations are combined in *Unit Processes.***



- **Unit Processes: that connected create the *global Flowsheet.***

2.- Basic Steps in flowsheet synthesis

2.1.- Gathering Information and Database creation:

- **Basic thermo-physical properties for all chemicals considered.**
- **Information about reaction and conditions.**
- **Yield.**
- **Product purity.**
- **Raw materials.**
- **Process bounding (restrictions).**
- **Utilities.**
- **Environmental Impact and toxicity of components.**
- **Cost of equipment, utilities and subproducts. Chemical prices.**

Reactor Performance

Production of desired product

- Conversion
- Selectivity
- Yield

These terms quantify the amount of reactants reacted to form desired products. For a fixed reactor Volume (V), these parameters are functions of the T, P, space time, reactor and heat transfer configuration.

$$X_{\text{single-pass conversion}} = \frac{\text{reactant consumed in reactor}}{\text{reactant fed to reactor}}$$

Low values mean high recycle

$$X_{\text{overall conversion}} = \frac{\text{reactant consumed in process}}{\text{reactant fed to process}}$$

For expensive reactant that is recycled, this will (hopefully) be close to 100%.

$$S_{\text{selectivity}} = \frac{\text{rate of production of desired product}}{\text{rate of production of undesired product(s)}}$$

High value is desirable but may occur at v.low s-p c

$$\eta_{\text{yield}} = \frac{\text{moles of reactant reacted to produce desired product}}{\text{moles of limiting reactant reacted}}$$

Process efficiency

2.- Basic Steps in flowsheet synthesis

2.2.- Representing Alternatives:

- **AGREGATION IN A SINGLE OBJECT.**

- **EQUIPMENT AGREGATION REPRESENTING A FUNCTION OF HIGHER LEVEL** like: Feed preparation, reaction, recovery, separation.

- **COMPLETE FLOWSHEET:** Equipment and inter-connection:
  - Block Flow Diagram (BFD). Process Flow Diagram (PFD). Flowsheet → Unit operations.
  - Task Diagram (Change of P, T, Comp.) → Batch Processes where all the tasks are developed in the same equipment but at different times.

- **MORE SPECIALISED REPRESENTATIONS:** (Process Subsystems): T *vs.* Transferred Heat amount. Allow to obtain alternatives to the heat exchange between streams, minimum heat and cool utilities, etc., in the HEN (Heat Exchange Networks).

- **REPRESENTATION OF THE PROCESS TRANSITIONS IN THE SPACE OF CHEMICAL COMPOSITION:** Useful to synthesis of reactor networks and non-ideal separation processes.

- **OTHER REPRESENTATIONS:** Useful to think about the design problem. Describe design alternatives.

2.- Basic Steps in flowsheet synthesis

2.3.- Criteria for Assessing preliminary design:

- **EQUIPMENT AGREGATION REPRESENTING A FUNCTION OF HIGHER LEVEL**:
  Need → Equipment and utilities Cost. Mass and heat balances solved.

- **ENVIRONMENTAL CONCERNS:**
  Need → Satisfy regulations / EIA / LCA / CF.

- **SAFETY ANALYSIS:**
  Determine whether any reasonable combination of events leads to unsafe situations. HAZOP Analysis.

- **FLEXIBILITY:**
  Requires → manufacture of specified products in spite of variations in the feeds it handles ($, supply), T cooling water, heat transfer coefficient.

  Oil Refinery: Earnings = F (capacity of process different oils at different time + scheduling).

- **CONTROLLABILITY:**
  Ability of operate the process satisfactorily while undergoing dynamic changes in operation conditions, or while recovering from disturbances.

3.- Generation of flowsheets: How are flowsheets generated?

Exhaustive enumeration → may involve $10^3 – 10^6$ flowsheets

→ Methods to reject non-viable alternatives easy and quickly:

- **Hierarchical Decomposition:**
  - **Order or levels of decisions:**
    - **+ Much simpler.**
    - **+ Obtaining flowsheets to apply optimization.**
    - **– Successive Refinement.**
    - **– Ignore some strong interactions between the levels.**

- **Superstructure optimization:**
  - **Optimize superflowsheet that contains all alternatives:**
    - **+ Interactions between levels can be considered systematically (with more powerful strategies).**
    - **– Much more complicated.**

3.- Generation of flowsheets: How are flowsheets generated?

3.1.- Hierarchical Decomposition:

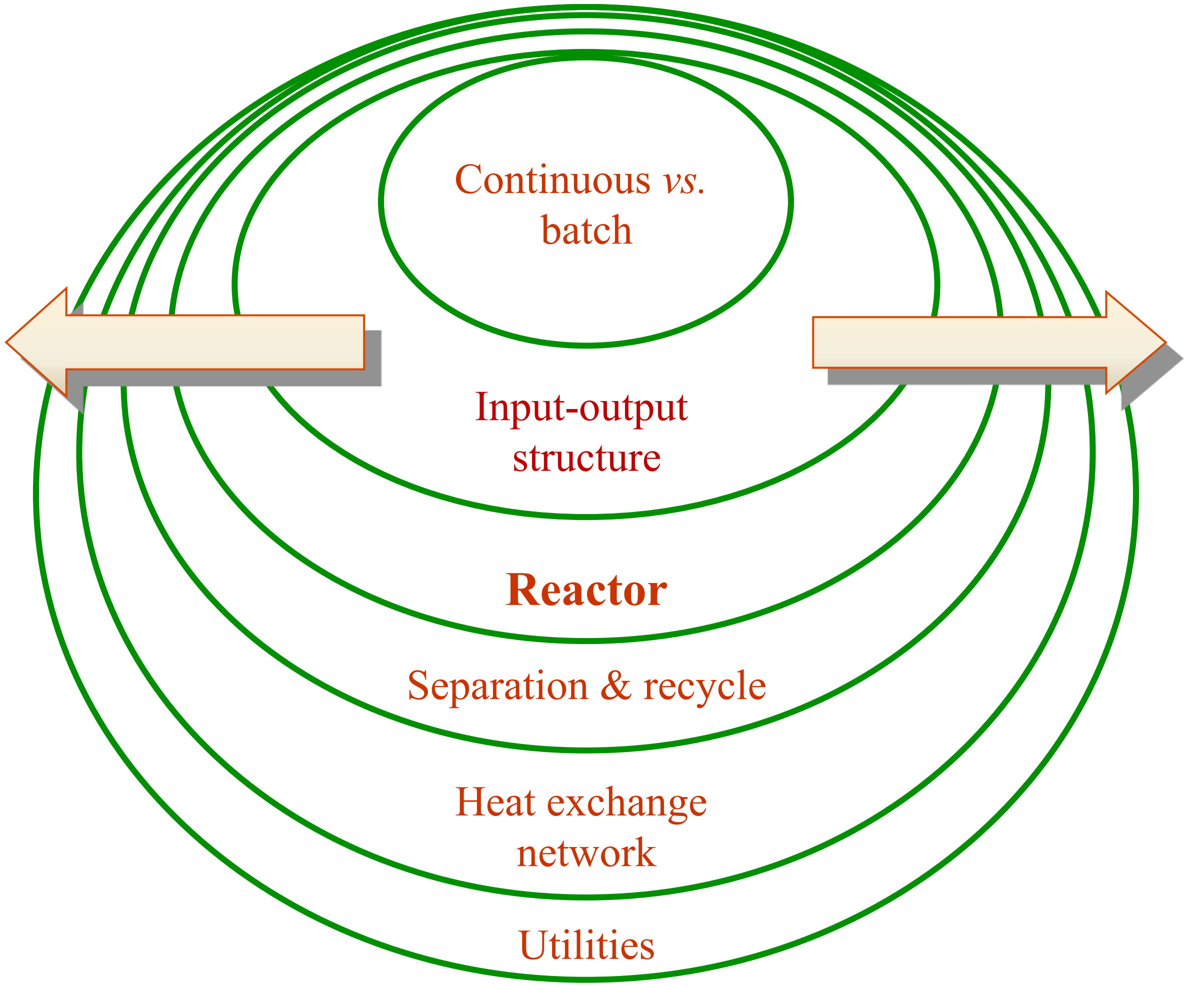
1.- Consider several levels of decisions:

- **Level 1. Batch vs. Continuous.**
- **Level 2. Input-output structure (Economic Potential).**
- **Level 3. Recycle structure → main decision is the Reactor.**
- **Level 4. Separation Synthesis:**
  - **a) Vapor recovery.**
  - **b) Liquid recovery.**
- **Level 5. Heat Recovery.**

3.- Generation of flowsheets: How are flowsheets generated?

3.1.- Hierarchical Decomposition:

The "Onion diagram"

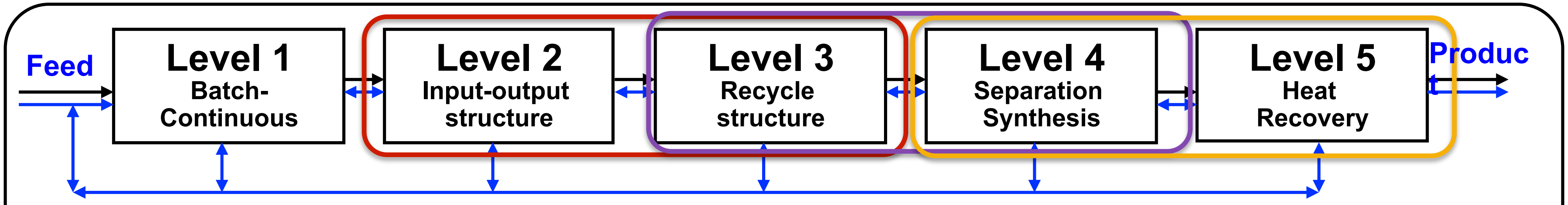


2.- Develop alternatives: starting from the highest level.

- It's economic potential at any level < 0 → STOP.
- Otherwise continue until finding feasible base case.
- Evaluate using short-cut techniques.

3.- Generation of flowsheets: How are flowsheets generated?

3.2.- Generation of flowsheets: Integrated Chemical Processes:



DESIGN: Hierarchical decomposition approach; Integrated approach.

- **Integration** of unit operations → to design multifunctional integrated chemical manufacturing systems.

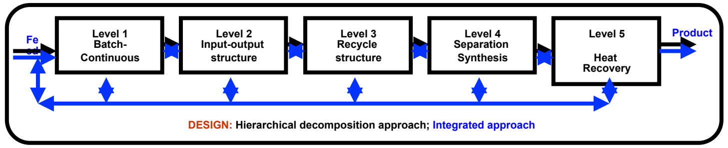
- **Advantages/Challenges of process integration:**

  - Higher productivity.
  - Higher selectivity.
  - Reduced energy consumption.
  - Improved operational safety.
  - Improved ecological harmlessness by avoidance of auxiliary agents and chemical waste.

* Due to the **interaction of several process steps in one apparatus** (system), the steady-state and the dynamic operating behavior of an integrated process unit (system) is **much more complex** than the behavior of single, non-integrated units (systems).

3.- Generation of flowsheets: How are flowsheets generated?

3.2.- Generation of flowsheets: Integrated Chemical Processes



- The **aim** of **Process Intensification** is to optimize capital, energy, environmental and safety benefits by radical reduction in the physical size of the plant.

- **Development** of novel apparatuses and techniques, as compared to the present state-of-art, to bring about *dramatic* improvements in manufacturing and processing, substantially decreasing equipment size/production-capacity ratio, energy consumption, or waste production.

- **Advantages of process intensification:**
  - 99% reduction in impurity levels → **Better product quality** → more valuable.
  - Just-in-time manufacture becomes feasible with **ultra-short residence times**.
  - **Distributed** (rather than centralized) manufacture →more economic. 60% **capital cost** reductions.
  - 70% reduction in **energy** usage and hence substantial reduction in **operating costs.**
  - Lower **waste** levels reduce downstream purification costs.
  - 99.8% reduction in **reactor volume** for a potentially hazardous process, leading to an inherently safe operation. **Smaller inventories** lead to improved intrinsic **safety**.
  - Better **control of process** irreversibility's can lead to lower energy use.

3.- Generation of flowsheets: How are flowsheets generated?

3.3.- Superstructure Optimization

- Representation that contains all the alternatives to be considered for a design.
- Useful with a high number of alternatives.

State-Task Network (STN)
2 kinds of Nodes: State and Task. 1 Task in 1 Device.

State-Equipment Network (SEN)
2 kinds of Nodes: State and Equipment. Several Tasks in 1 Device.

- *Example 1: Heat exchange of H1 with C1, C2, C3 and H1, H2 with C1, C2.*
- *Example 2: Wastewater treatment network.*
- *Example 3: Synthesis of ammonia plant*

Practical Chapter !!

4.- Further Reading and References

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RELEVANT TO LEARNING

- **Design problem vs. yield problem.**
- **Meaning of FLEXIBILITY as criteria for assessing preliminary design.**
- **What is process Integration? And process Intensification? Examples?**
- **Meaning, use and kind of Superstructures.**
- **Examples of hierarchical decomposition.**
- **Why is it useful to determine the maximum potential benefits when analyzing a process at the input-output structure level?**