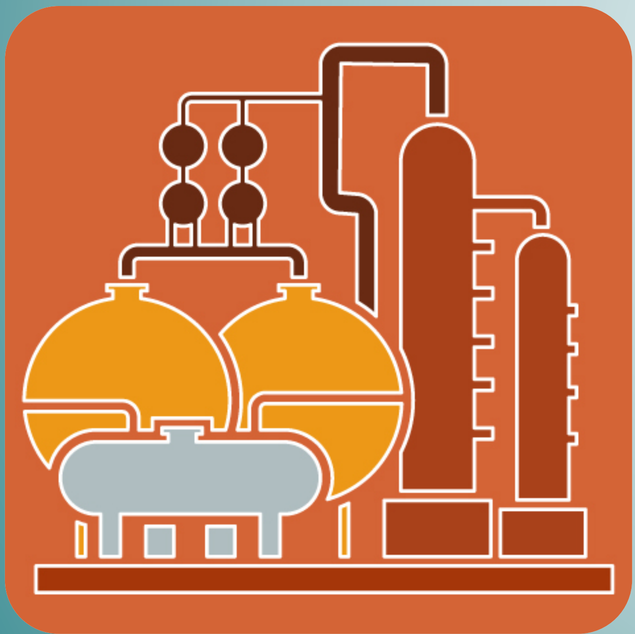
Chemical Process Design / Diseño de Procesos Químicos

Topic 3.2. Overview of process synthesis. Examples



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1.- Preliminary Process Synthesis

1.1.- Synthesis of Alternatives:

- **Electric Energy:**
  - From ……………………………………………………………..……
  - From ……………………………………………………………..……
- **Sodium carbonate Na_2CO_3:**
  - From: ………………………………………………………………...
  - From: ………………………………………………………………...
- **Depending on the chemical reaction route:**
  - Route 1: …………………………………………………………......
  - Route 2: …………………………………………………………......
- **Separations:**
  - Liquid/liquid: ……………………………………………………..
  - Solid/liquid: ………………………………………………………..

1.- Preliminary Process Synthesis

1.1.- Synthesis of Alternatives:

- Electric Energy:

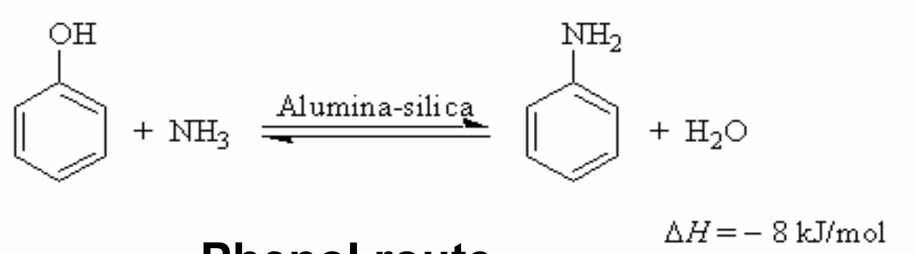
- **From renewable sources (wind, solar, sea, geothermic. Biomass).**
- **From non-renewable sources (coal, gas, oil).**

- Sodium carbonate Na_2CO_3:

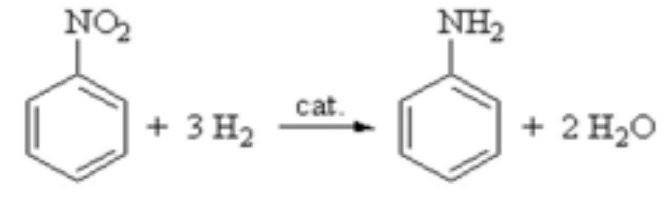
- **From: Solvay Process / Natural Deposits of Natron** ($Na_2CO_3 \cdot 10H_2O$) or **Trona** ($Na_3(HCO_3)(CO_3) \cdot H_2O$) → Q → Na_2CO_3

- Depending on the chemical reaction route:

- ***ANILINE:*** aromatic amine. Intermediate for isocyanates, dyes and pigments, agricultural or pharmaceutical chemicals. Additives for rubber.



Phenol route



Nitrobenzene route

1.- Preliminary Process Synthesis

1.1.- Synthesis of Alternatives:

- **Separations:**
  - **Liquid/Liquid:** Distillation / Liquid-Liquid Extraction / Pervaporation / Molecular Sieve (Adsorption) / Chromatography.
  - **Solid/Liquid:** Decantation (Settling) / Filtration / Centrifugation.

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.

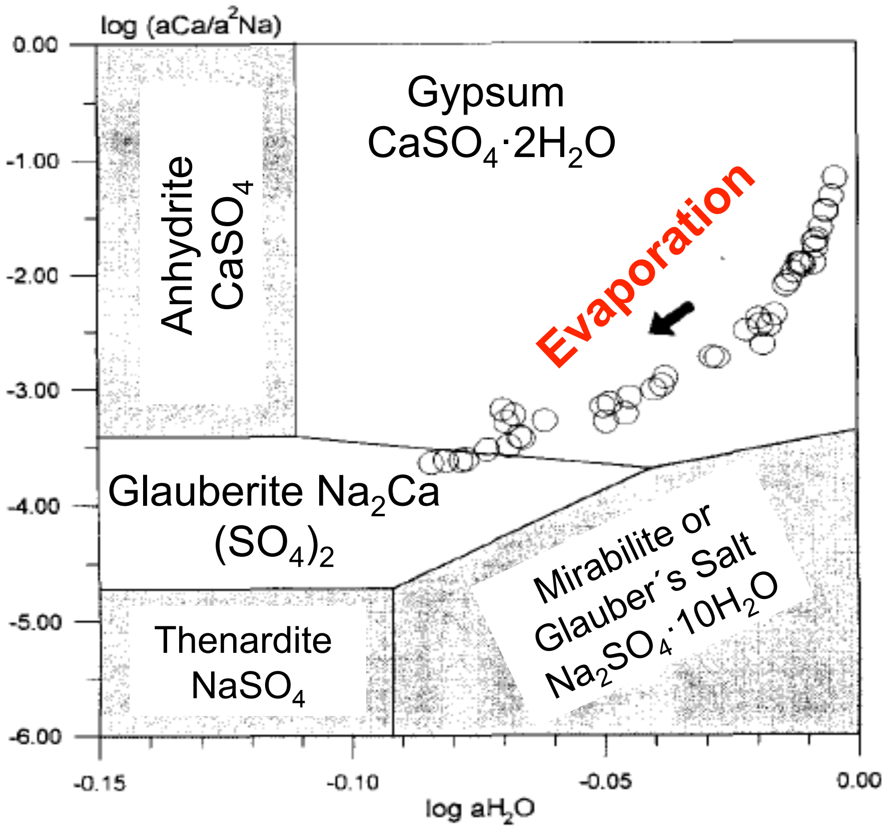
- **COMPLETE FLOWSHEET:** Equipment and inter-connection:
  - Block Flow Diagram (BFD). Process Flow Diagram (PFD). Flowsheet → Unit operations.
  - Task Diagram (Change of P, T, Comp.) → Batch Processes where all the tasks are developed in the same equipment but at different times.

- **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).

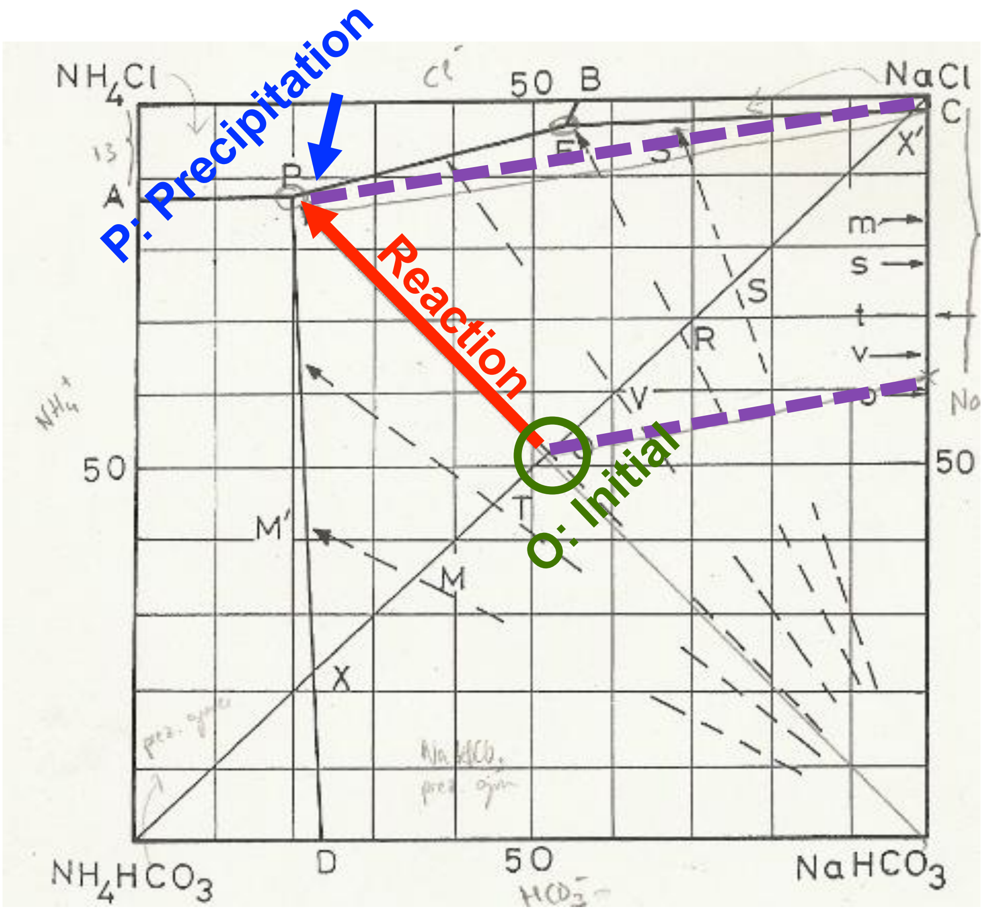
- **REPRESENTATION OF THE PROCESS TRANSITIONS IN THE SPACE OF CHEMICAL COMPOSITION:** Useful to synthesis of reactor networks and non-ideal separation processes.

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

2.- Basic Steps in flowsheet synthesis



Na–Ca–SO_4–H_2O Phase diagram.
López *(et al.)* (1996).
Estudios Geol., 52. Pp. 197-209.



Solvay Process: Quaternary diagram.

$$NaCl + Ca\ CO_3 \leftrightarrow Na_2CO_3 + CaCl_2$$

2.- Basic Steps in flowsheet synthesis: Example

- Criteria for Assessing preliminary design: Pareto Optimal Frontiers (POF); F1(Costs, NPV), F2(EI99, GWP100, RCO2).

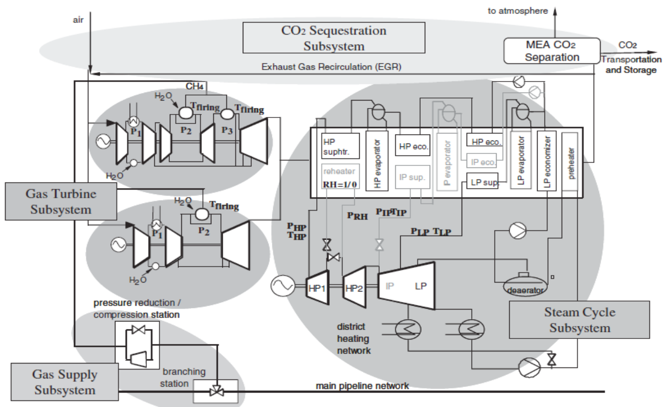


Fig. 1. Superstructure of an advanced NGCC with MEA and EGR option.

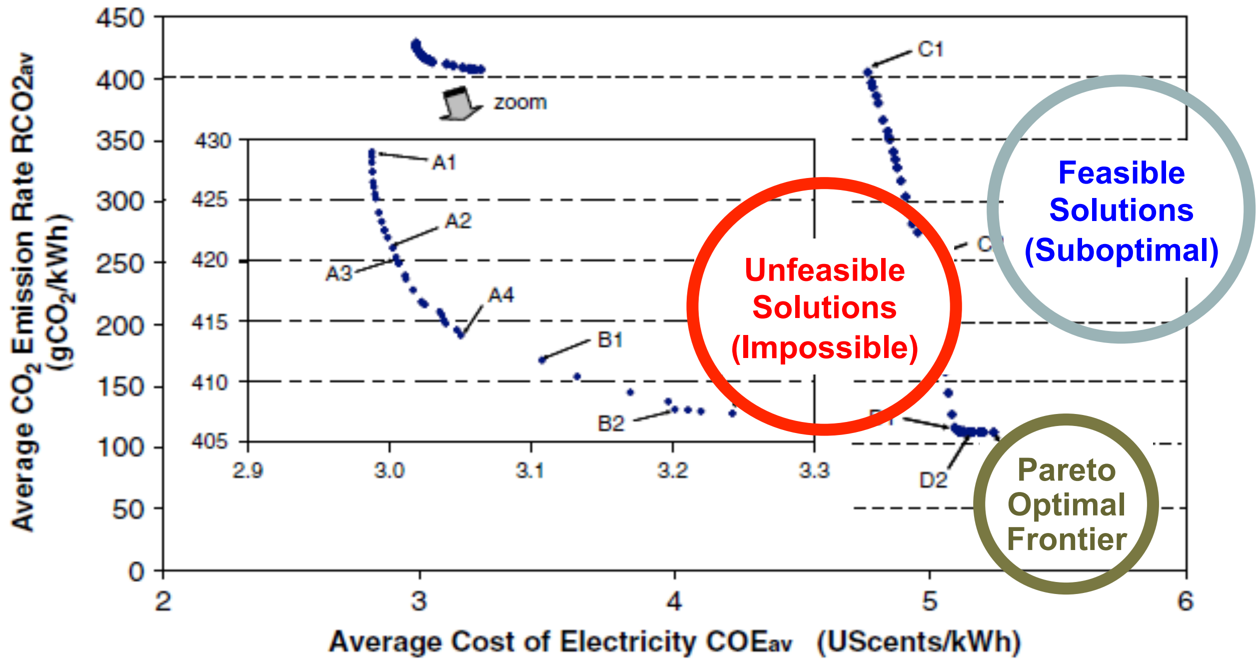
In order to:

1. Maximize NPV.
2. Minimize the environmental impact for a given probability level.

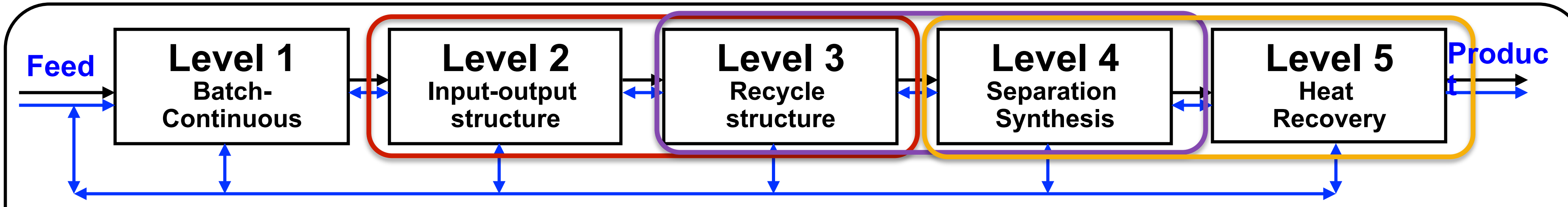
POF approaches:

- Power Plants: Li *(et al.),* 2006; Bernier *(et al.),* 2010; Pelster *(et al.),* 2001; Yokohama and Ito, 1995.
- Process systems: Mele *(et al.),* 2011; Gerber *(et al.),* 2011; Gillen-Gosalbez & Grossmann, 2010, 2009.

Fuente: Li, H.; Marechal, F.; Burer, M. & Favrat, D. (2006): *«Multi-objective optimization of an advanced combined cycle power plant including CO2 separation options».* Energy, 31. Pp. 3117-3134.



3.- Generation of flowsheets: Integrated Chemical Processes

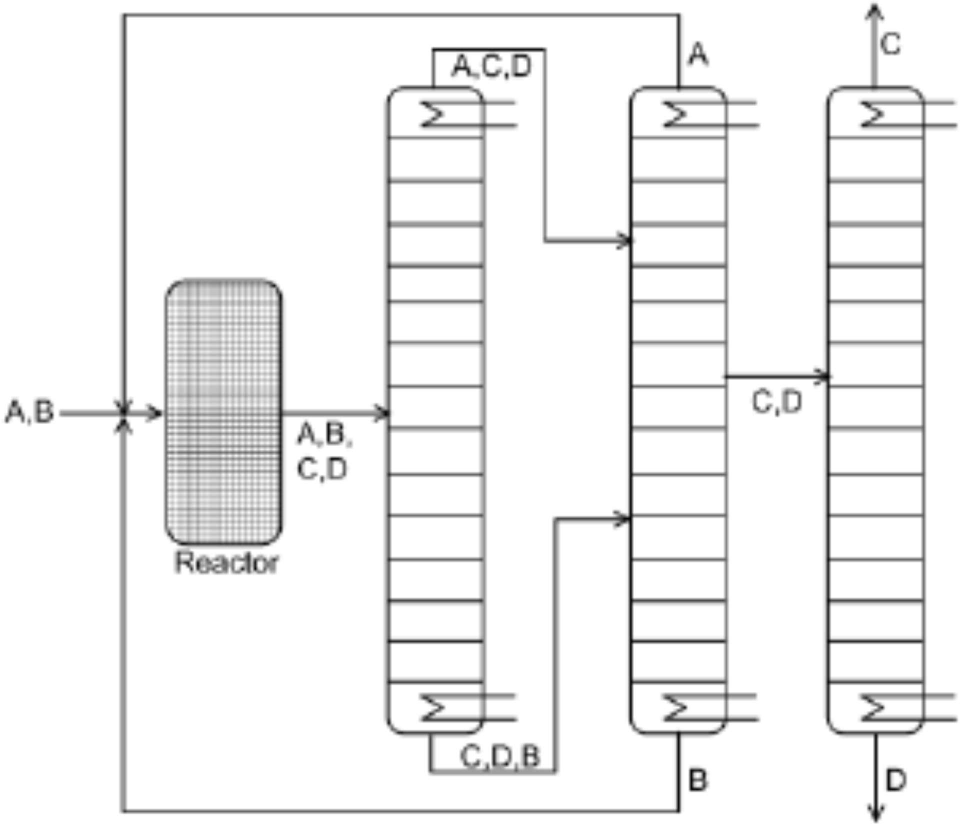


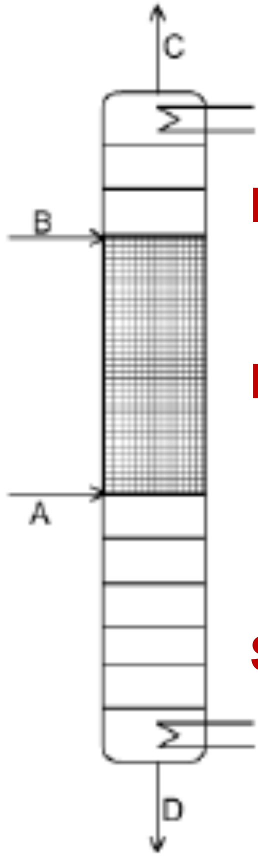
DESIGN: Hierarchical decomposition approach; Integrated approach.

- Process Integration Examples:

- Heat and Power Integration.
- Heat Transfer + Chemical reactions (fuel cell with internal reforming).
- Separation Process + Chemical reactions (reactive distillation).
- Mechanical Unit Operations + Chemical reactions (reactive extrusion).

$$\mathrm{A} + \mathrm{B} \rightleftharpoons \mathrm{C} + \mathrm{D}$$





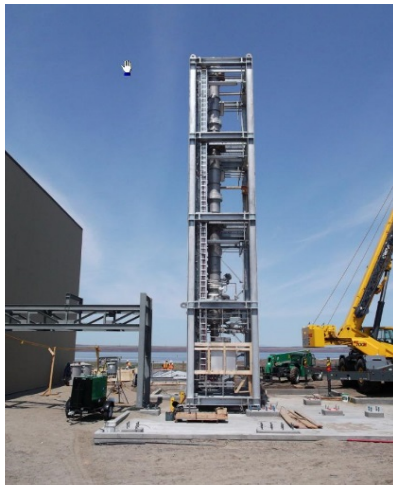
Rectification

Reaction

Stripping

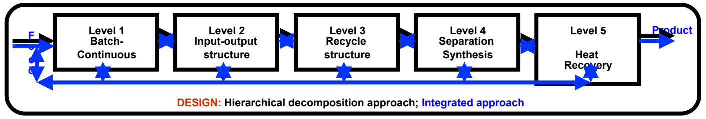
$$\alpha_C > \alpha_A > \alpha_B > \alpha_D$$

Reactive distillation is a continuous process where the chemical reaction and distillation take place in the same device.



https://www.sulzer.com

3.- Generation of flowsheets: Process Intensification



- Process Integration Examples:

- **Equipment:** heat exchanger in the form of the printed circuit/diffusion bonded unit; microchannel heat exchangers; structured packed columns; heat exchange reactor; supersonic gas liquid reactor.

- **Methodologies:** reactive distillation, reactive extraction, membrane separations, oscillating flows in reactors, membrane reactions, fuel cells. Use of ultrasound, microwave, centrifugal fields, supercritical fluids.

- **Industrial applications:** small intensely stirred reactors and microchannel reactors in Organic Nitration (nitroglycerine); isothermal reactor crystallizer in Phosphoric acid; a single device for latex coagulation, washing, extrusion, dewatering and drying in styrene-butadiene rubber. Methyl isocyanate (MIC-Bhopal accident) generated and immediately converted to final pesticide in process with a total inventory <10 kg MIC.

Microchannel REACTOR

Microchannel REACTOR
applied to a fine-chemical
process at DSM.

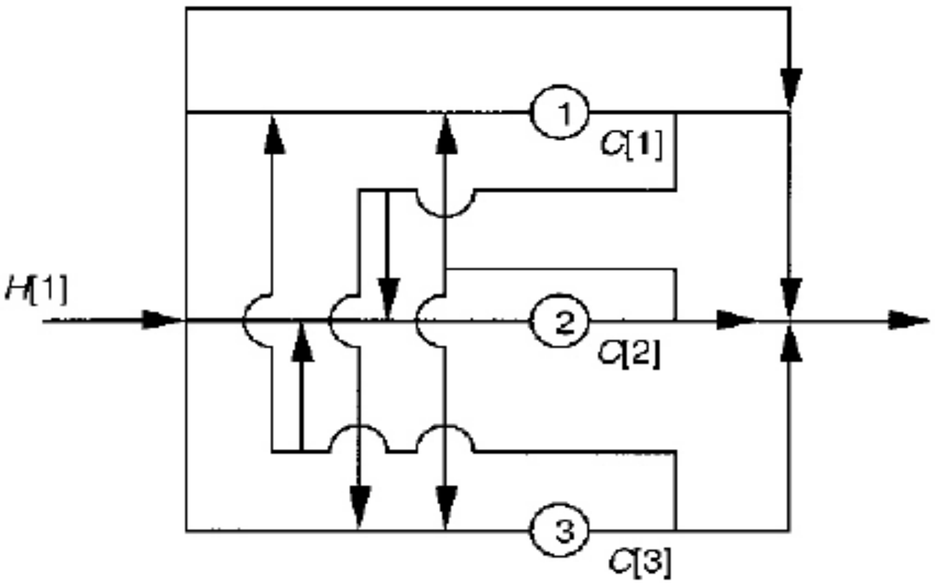
Amaya Arteche & Enrique Ipiñazar.
Área de Biorrefinería y Valorización de Recursos.
«Intensificación de Procesos para una Industria Química más sostenible».

Tecnalia Research & Innovation, 2014.

http://www.suschem-es.org/docum/pb/asambleas/Asamblea%2014/08.Intensificaci%C3%B3n_de_Procesos_para_una_Industria_Qu%C3%ADmica_m%C3%A1s_sostenible.pdf

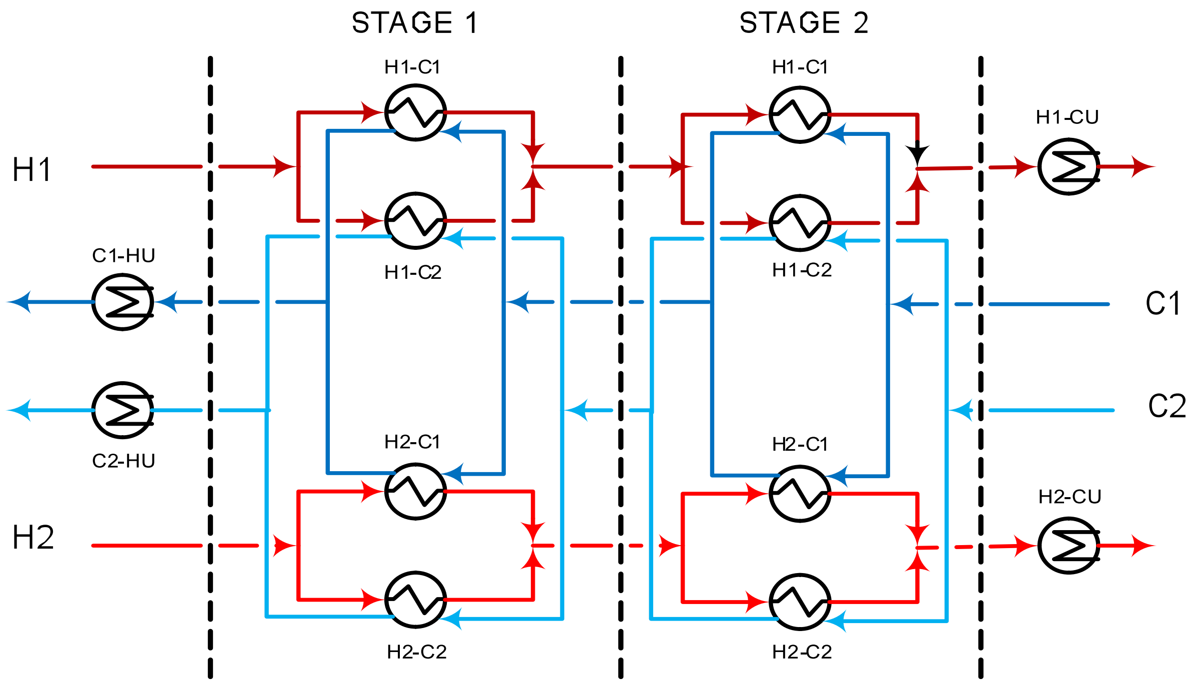
Example 1.

Heat exchange of H1 with C1, C2, C3 and H1, H2 with C1, C2



Superstructure

(Floudas *(et al.)*, 1986).



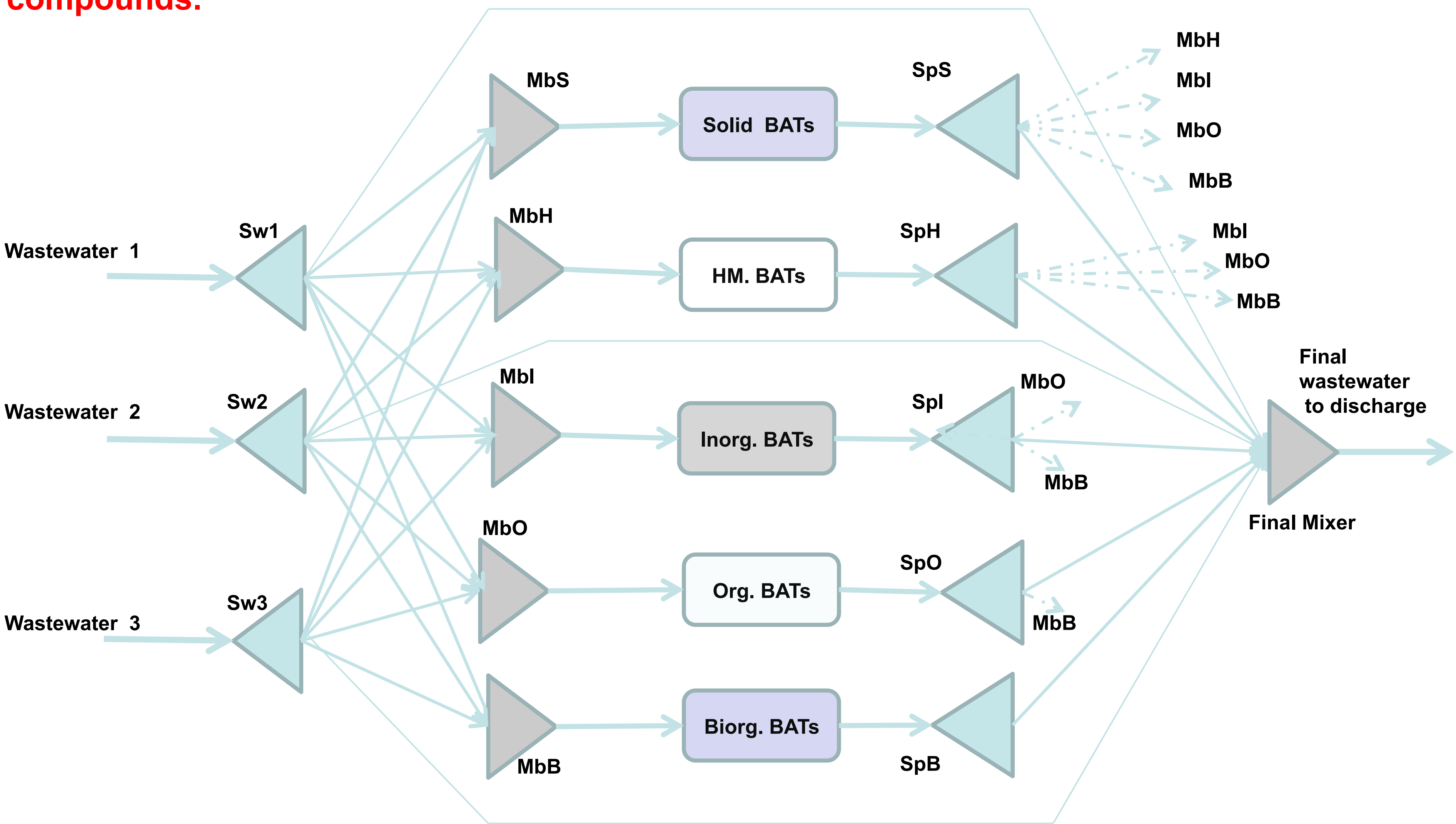
Superstructure

(Yee and Grossmann, 1990)

Example 2.

Wastewater treatment network

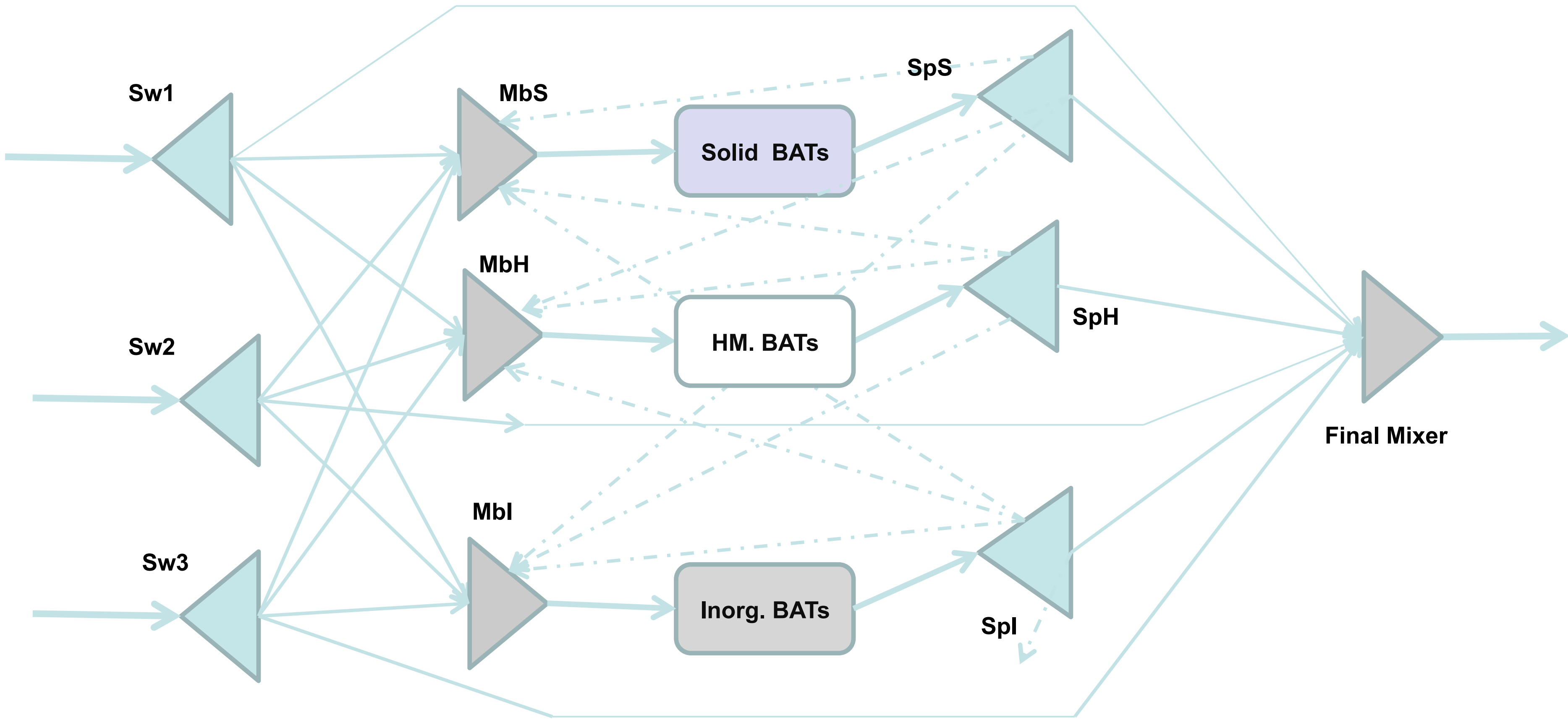
Super-structure for industrial wastewater treatment, eliminating suspended solids, heavy metals, inorganic salts, organic compounds unsuitable for biological treatment, bioorganic compounds.



Example 2.

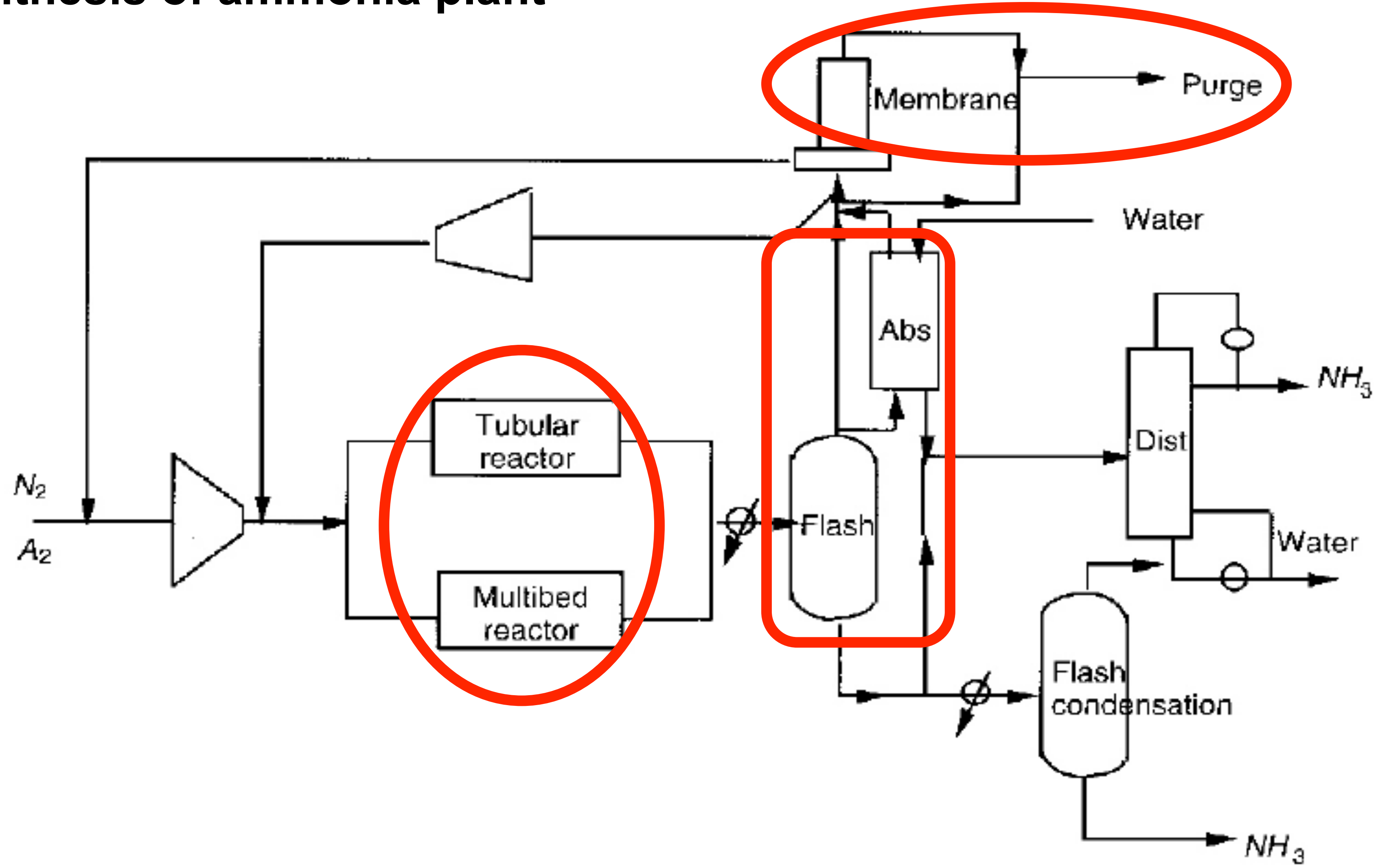
Wastewater treatment network

Super-structure for industrial wastewater treatment, eliminating suspended solids, heavy metals and inorganic salts (Galan & Grossmann, 1998, 2011).



Example 2.

Synthesis of ammonia plant



Superstructure
(Biegler *(et al.),* 1997).

Example 4.

Distillation

Make the possible superstructures for the separation of a mixture of components A, B and C (ordered by volatility) by distillation.

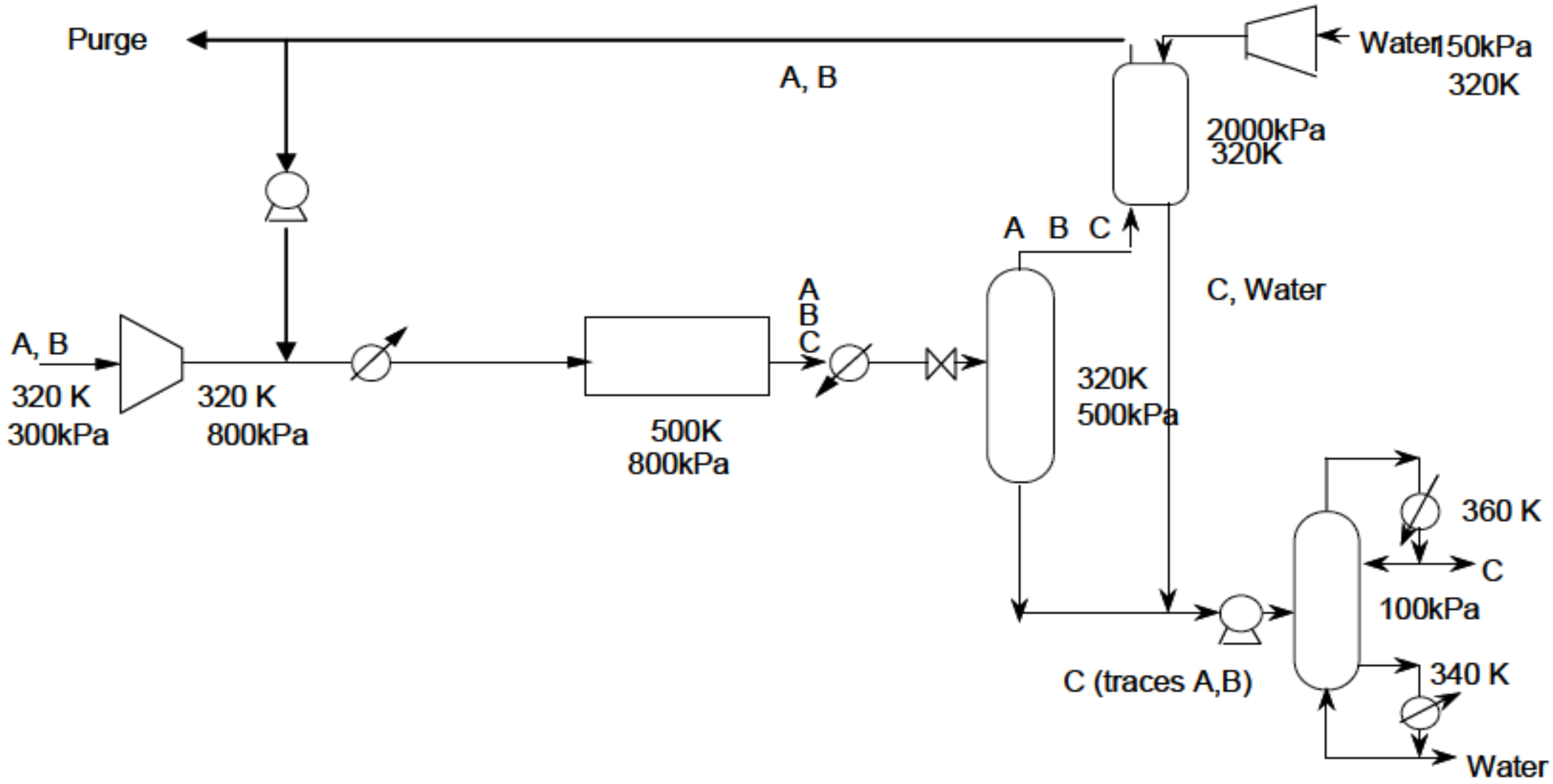
Example PFD.

The Figure in the next slide shows a process for making C from A. The feed, consisting of reagent A and an inert B, is preheated and enters the reactor operating at 800 kPa and 500 K. The reactor effluent is cooled to 320 K and is sent to a flash unit at 500 kPa where most of C separates from A and B. Since a significant amount of C is lost in the vapor stream, an absorber operating at 2000 kPa is used to recover this C from the vapor phase. The vapor outlet of the absorber is recycled to the reactor. Both the liquid flash product and the liquid stream from the absorber are mixed and sent to a distillation column operating at 100 kPa to separate C from the water used in the absorber.

Find the errors in the flowchart shown and list how they could be corrected.

Example PFD.

- Direction of flow arrows?
- State of currents (g, l, s)?
- Is the proper fluid movement equipment used?
- Are outputs consistent with the process equipment (or with the operation that is taking place)?



Example 5.

Take into consideration the following reaction system to obtain Acetic Anhydride (use for the conversion of cellulose to cellulose acetate, which is a component of photographic film and other coated materials, and is used in the manufacture of cigarette filters):

Acetone	→	Ketene + CH4	(700 ºC, 1 Atm)
Ketene	→	CO +1/2 C_2H_4	(700 ºC, 1 Atm)
Ketene + Acetic Acid	→	Acetic Anhydride	(80ºC, 1 Atm)

Ketene is an unstable intermediate reactive that totally converts. The economic value of the components involved is:

- $CO + CH_4 + C_2H_4$ = 4 €/10^6Btu.
- Acetone: 15.66 €/mol.
- Acetic Acid: 15 €/mol.
- Acetic Anhydride: 44.41 €/mol.

The Boling Points are in ºC:

- CO: –191.
- CH_4: –161.
- C_2H_4: –104.
- Ketene: –41.
- Acetone: 56.
- Acetic Acid: 118.
- Acetic Anhydride: 139.

Build the diagrams of the following structures, labeling the components in each stream:

a) Input-output.

b) Reaction-recycle.

c) Global separation system and d) detailed separation system using acetic acid as sorbent for the acetone.