



Sustainable Process Synthesis-Intensification

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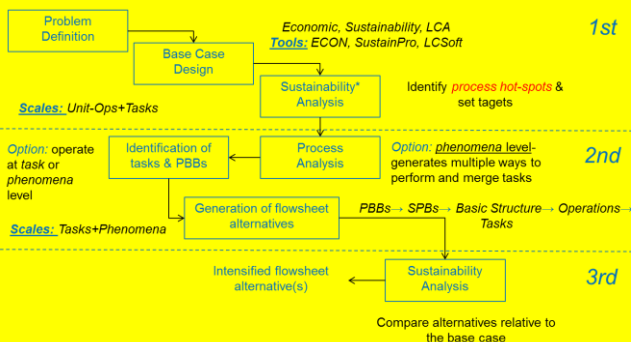
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Introduction

Industry **needs improvements** related to:

- The use of sustainable technologies/processes
↓ **Capital/Operation cost**
- The efficient use of raw materials
↓ **Waster generation**
- The environmental and life cycle issues
↓ **Energy consumption**

Multi-level Framework

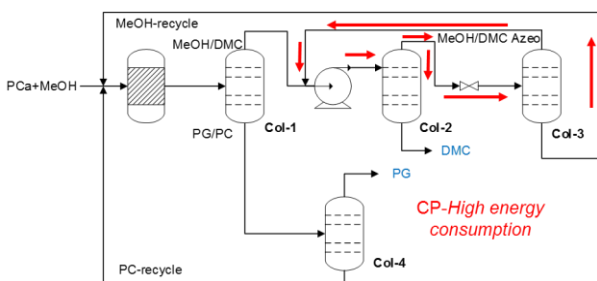


1st: Unit-Ops+Task scale

Problem Definition: Find intensified process design options for the production of DMC by minimizing the objective function:

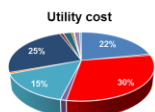
$$\text{Min } F_{obj} = \left(E_i C_{Ut,i} + \frac{C_{Equip}}{t_{proj}} \right) / m_{prod}$$

Base Case Design: Consists of 5 unit operations: 1 reactor and 4 distillation columns.



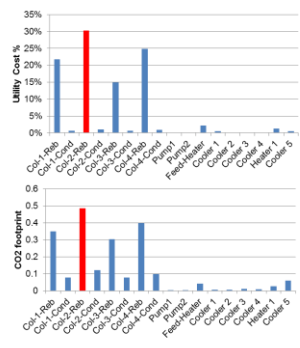
Sustainability Analysis: Consists of 5 unit operations: 1 reactor and 4 distillation columns.

Process hot-spots & targets



Economic, Sustainability, LCA:

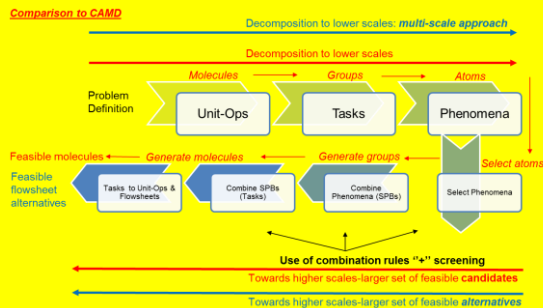
- ↑ Utility cost ↑ Energy Demand
- ↑ Energy Demand ↑ EWC in CP
- ↑ Energy Demand ↑ CO2 footprint



Targets (e.g.):

1. Reduce energy demand
2. Reduce number of Unit-Ops
3. Explore the possibility for using "hybrid" Unit-Ops
4. Improve Sustainability & LCA factors

Concepts



2nd : Tasks+Phenomena Scale

Process Analysis (e.g.):

Thermodynamic insights

Identification of PBBs

| Task | Component | PBBs |
|----------|---------------------------------------|---------------------------|
| R-Task | PCa+MeOH | M,R,C |
| S-Task-1 | PG _{LK} +PCa _{HK} | M,2phM,H,C,PC,PT,PS by VL |
| S-Task-2 | MeOH _{LK} +PG _{HK} | M,2phM,H,C,PC,PT,PS by VL |
| S-Task-3 | MeOH _{LK} +DMC _{HK} | M,2phM,H,C,PC,PT,PS by VL |

LK-Light key
HK-Heavy key

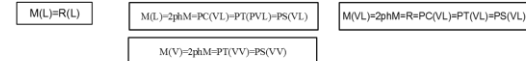
Excerpt of properties used for the generation of the binary ratio matrix

| | f_i | Tb | RG | SolPar | VM |
|----------|-------|------|------|--------|----|
| MeOH/PC | 1.52 | 2.2 | 1.13 | 2.1 | |
| MeOH/DMC | 1.08 | 2.09 | 1.46 | 2.09 | |
| MeOH/PG | 1.36 | 2.03 | 1.1 | 1.82 | |
| PC/DMC | 1.42 | 1.05 | 1.3 | 1.01 | |
| PC/PG | 1.12 | 1.08 | 1.12 | 1.16 | |
| DMC/PG | 1.27 | 1.03 | 1.46 | 1.15 | |

Tb-normal boiling point
RG-radius of gyration
SolPar-Solubility parameter
VM-molar volume

Hints separation based on molecular size possible

SPBs



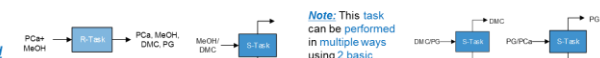
Basic Structures



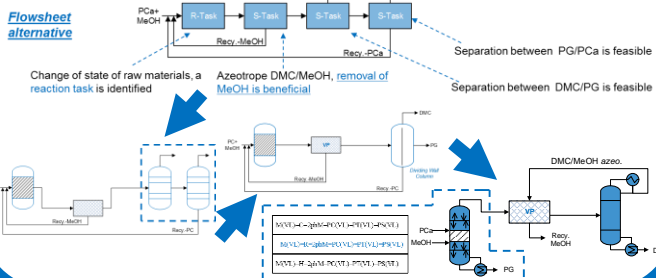
Note: The objective is to convert input (PCa + MeOH) to output (DMC + PG). One basic structure (unless combined) will not achieve this

Note: This basic structure fulfills two S-tasks

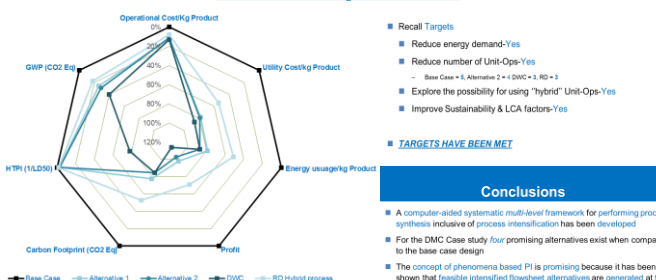
Task fulfilled



Flowsheet alternative



3rd: Comparison



- Recall Targets
 - Reduce energy demand-Yes
 - Reduce number of Unit-Ops-Yes
 - Explore the possibility for using "hybrid" Unit-Ops-Yes
 - Improve Sustainability & LCA factors-Yes
- TARGETS HAVE BEEN MET

Conclusions

- A computer-aided systematic multi-level framework for performing process synthesis inclusive of process intensification has been developed
- For the DMC Case study four promising alternatives exist when compared to the base case design
- The concept of phenomena based PI is promising because it has been shown that feasible intensified flowsheet alternatives are generated at this lower scale