



Sustainable Process Synthesis-Intensification

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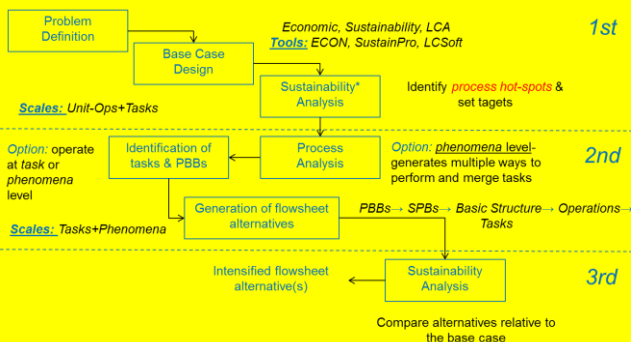
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Introduction

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

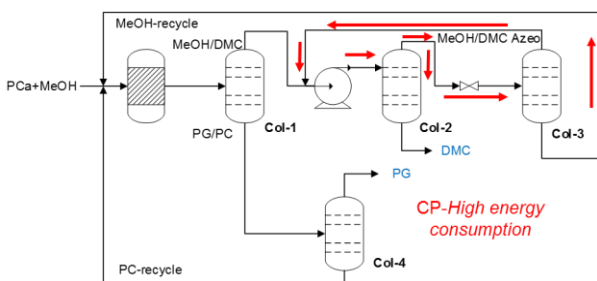


1st: Unit-Ops+Task scale

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

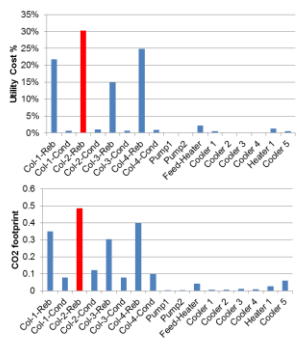
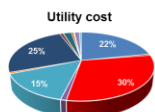
$$\text{Min } F_{obj} = \left(E_i C_{Ut,i} + \frac{C_{Equip}}{t_{proj}} \right) / m_{prod}$$

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



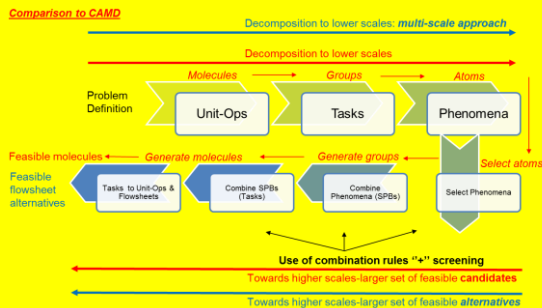
Targets (e.g.):

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

Economic, Sustainability, LCA:

1. ↑ Utility cost ↑ Energy Demand
2. ↑ Energy Demand ↑ EWC in CP
3. ↑ Energy Demand ↑ CO2 footprint

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,2pH,M,H,C,PC,PT,PS by VL
S-Task-2	MeOH _{LK} +PG _{HK}	M,2pH,M,H,C,PC,PT,PS by VL
S-Task-3	MeOH _{LK} +DMC _{HK}	M,2pH,M,H,C,PC,PT,PS by VL

LK-Light key
 HK-Heavy key

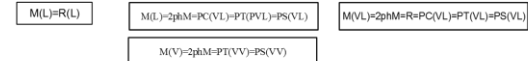
Excerpt of properties used for the generation of the binary ratio matrix

	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	

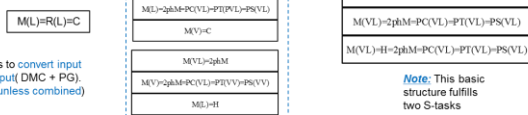
Tb-normal boiling point
 RG-radius of gyration
 SolPar-Solubility parameter
 VM-molar volume

Hints separation based on molecular size possible

SPBs



Basic Structures



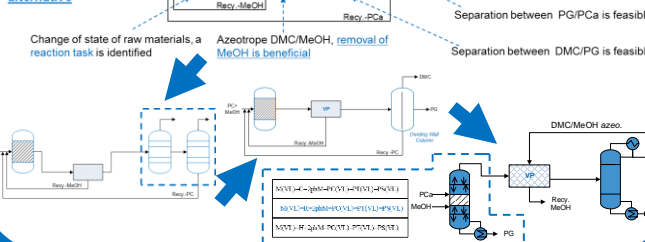
Note: The objective is to convert input (PCa + MeOH) to output (DMC + PG). One basic structure (unless combined) will not achieve this

Note: This basic structure fulfills two S-tasks

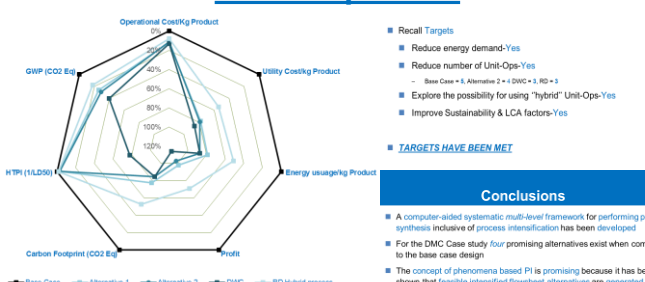
Task fulfilled



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