



## Sustainable Process Synthesis-Intensification

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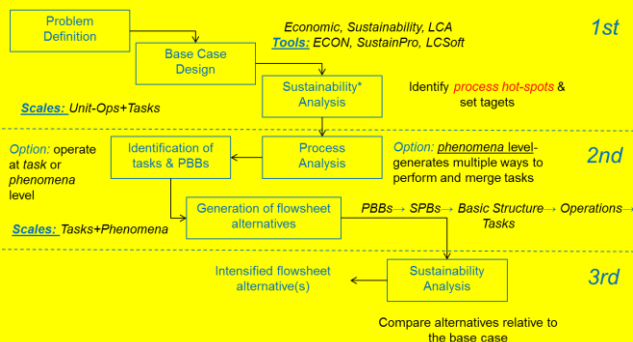
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## Introduction

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

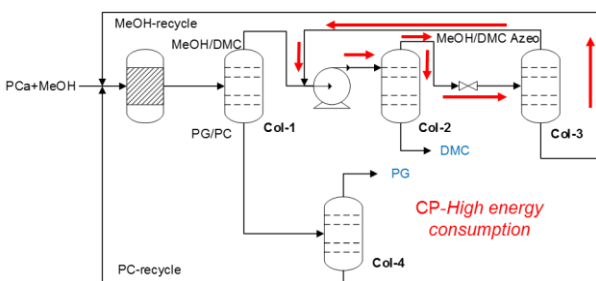


## 1st: Unit-Ops+Task scale

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

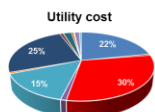
$$\text{Min } F_{obj} = \left( E_i C_{Ut,i} + \frac{C_{Equip}}{t_{proj}} \right) / m_{prod}$$

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



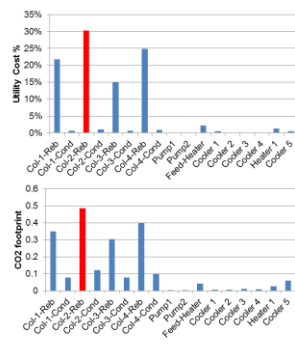
**Sustainability Analysis:** Consists of 5 unit operations: 1 reactor and 4 distillation columns.

Process hot-spots & targets



Economic, Sustainability, LCA:

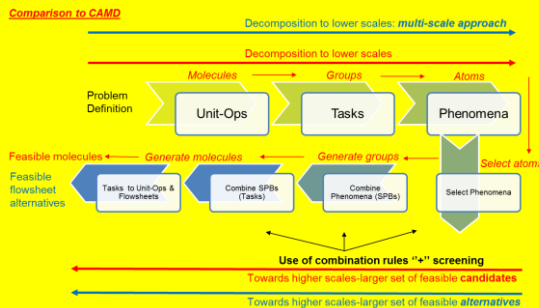
- ↑ Utility cost ↑ Energy Demand
- ↑ Energy Demand ↑ EWC in CP
- ↑ Energy Demand ↑ CO2 footprint



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**

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	

**Identification of PBBs**

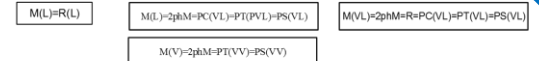
Task	Component	PBBs
R-Task	PCa+MeOH	M,R,C
S-Task-1	PG <sub>LK</sub> +PCa <sub>HK</sub>	M,2phM,H,C,PC,PT,PS by VL
S-Task-2	MeOH <sub>LK</sub> +PG <sub>HK</sub>	M,2phM,H,C,PC,PT,PS by VL
S-Task-3	MeOH <sub>LK</sub> +DMC <sub>HK</sub>	M,2phM,H,C,PC,PT,PS by VL

LK-Light key  
HK-Heavy key

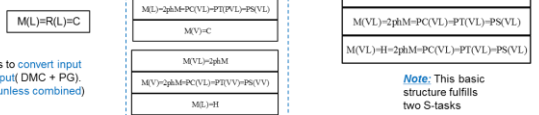
Tb-normal boiling point  
RG-radius of gyration  
SolPar-Solubility parameter  
VM-molar volume

Hints separation based on molecular size possible

**SPBs**



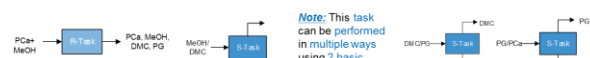
**Basic Structures**



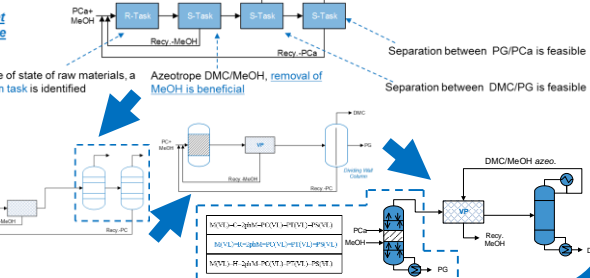
Note: The objective is to convert input (PCa + MeOH) to output (DMC + PG). One basic structure (unless combined) will not achieve this

Note: This basic structure fulfills two S-tasks

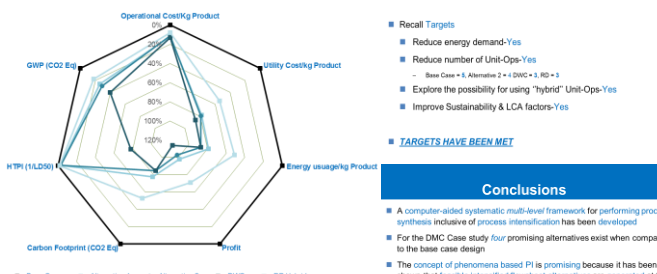
**Task fulfilled**



**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