Innovative & Sustainable Chemical-Process Analysis, Design & Synthesis: Introduction

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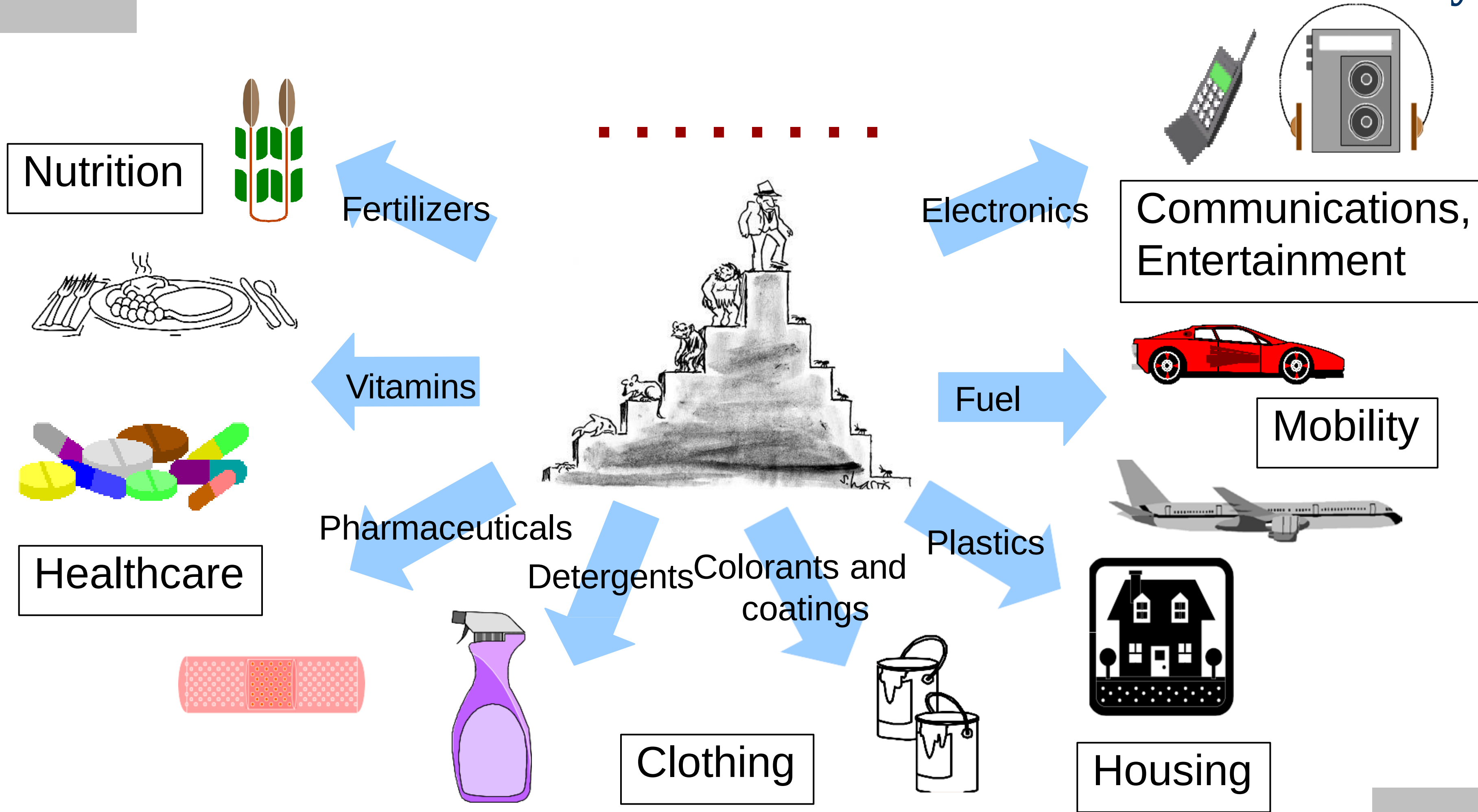
Sustainable Product-process Engineering, Evaluation & Design

The big picture

Master of the planet earth – how did we get there?

Positive contributions to society



Our survival depends on the products we make from the resources we have

Is our future sustainable? - motivation

Convert resources to products

↓

Use energy, water, ….

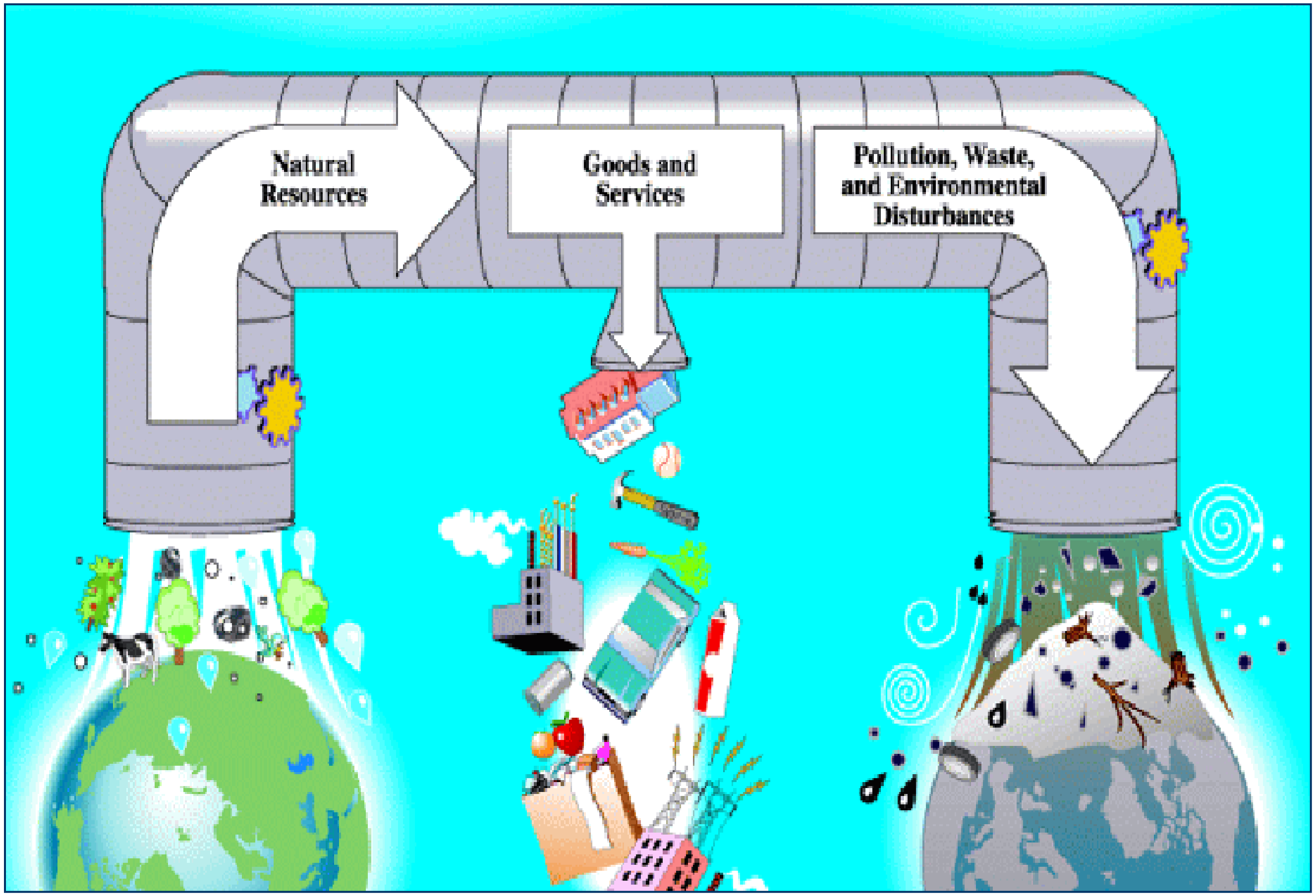
↓

Environmental Impacts (GWP, OD, HTTP, …)

↓

Produce waste

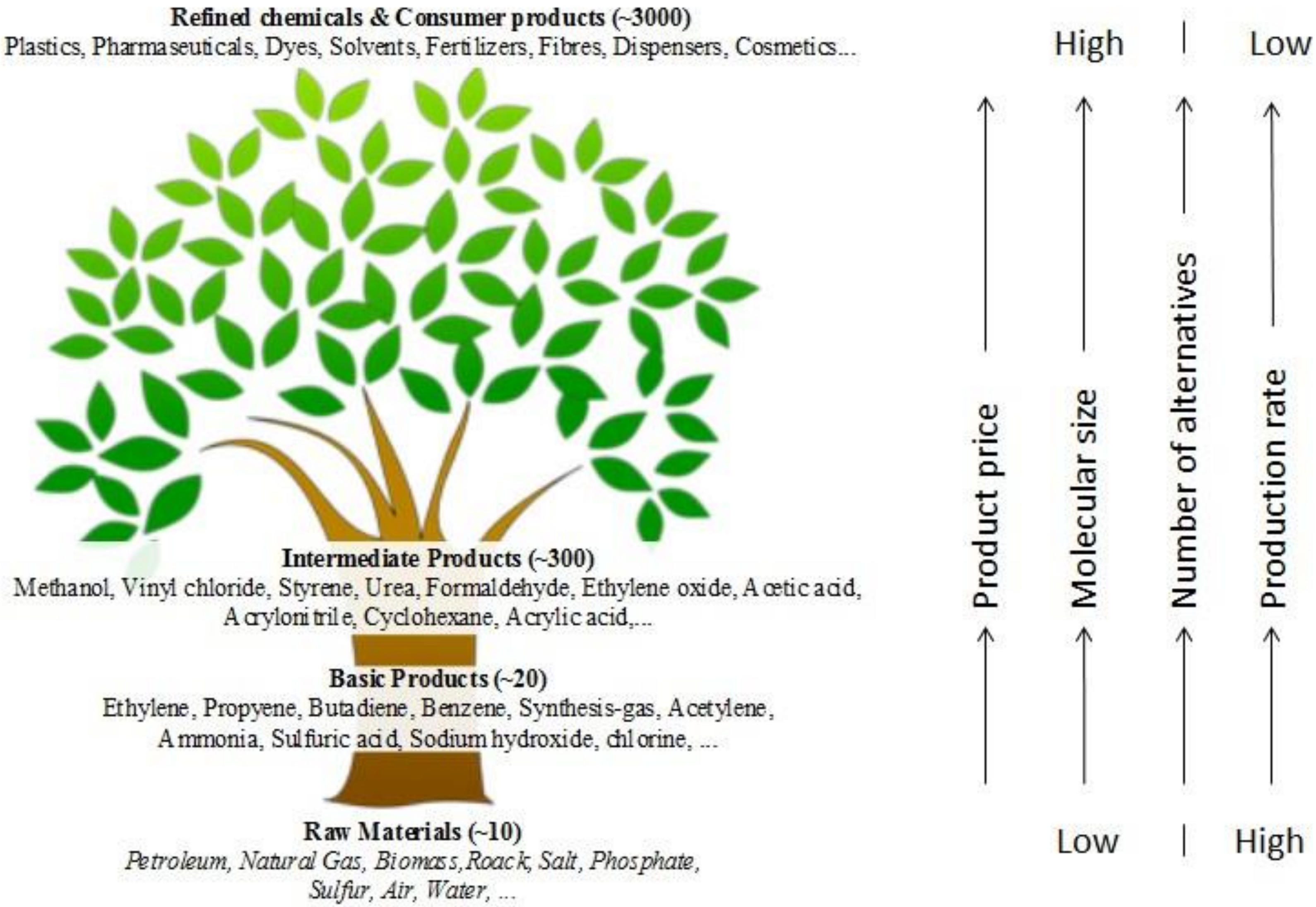
The challenges facing us



Only 25% converted; must be > 40% (Driolli 2007)

The chemical product tree

Question of what, why & when (how)?



Which problem to solve?

Stages in the life of a process

1. **Board of Directors' Design Problem**
2. **Discovery of possible new projects**
3. **Feedback & customer reaction**
4. **Planning & organizational design**
5. **Preliminary (conceptual) process design**
6. **Layout & three dimensional modelling**
7. **Construction**
8. **Startup & commissioning**
9. **Plant Operation**
10. **Debottelnecking**
11. **Decommissioning**

Interested to solve the conceptual process design problem*

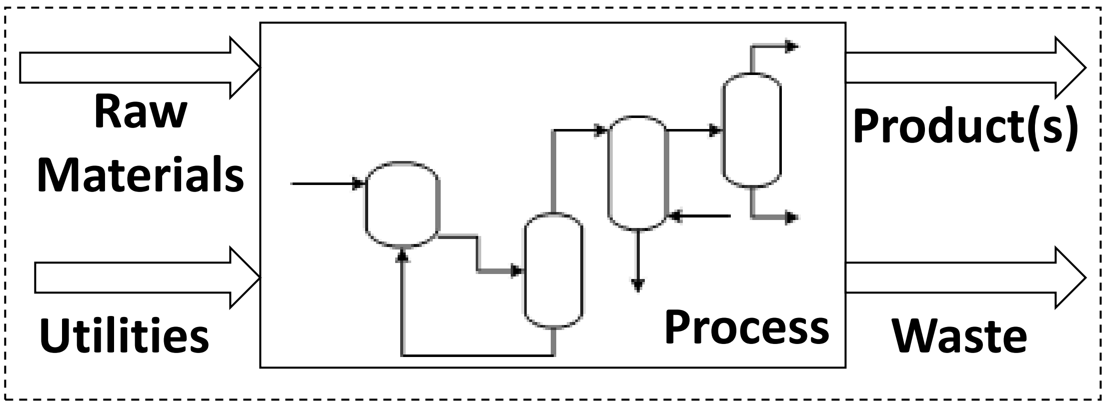
**** Considering issues 1-4 and 6-11***

New definition of process design problem

Chemical and bio-based industry faces enormous challenges to achieve and/or respond to:

Establish sustainable production

Adopt to changing markets



Survive global competition

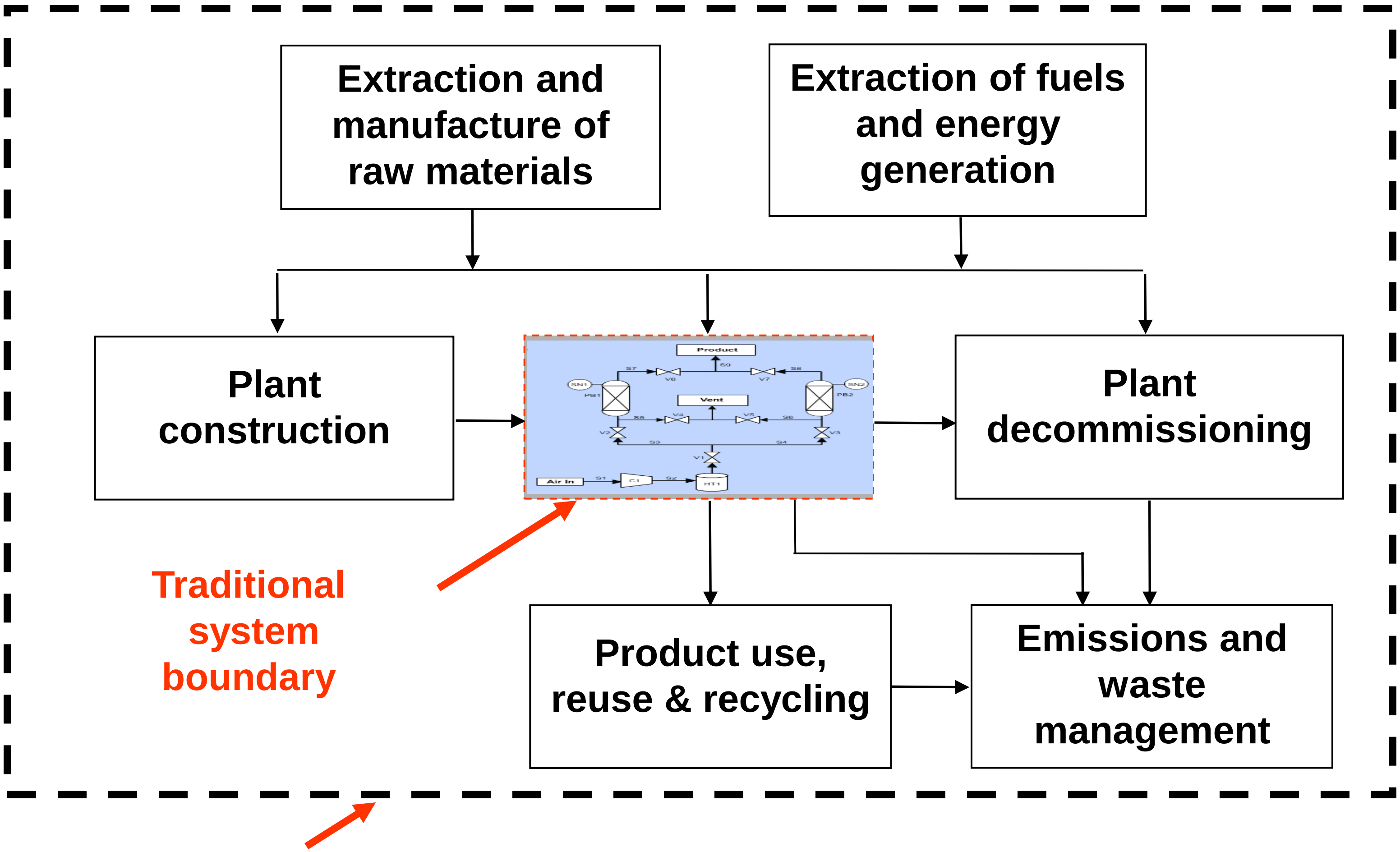
Demands for innovative products

<u>Processes need to be:</u>

Sustainable (Economically feasible; Reduced waste; Utility efficient; Environmentally acceptable); Safe; Operable; …….

New system boundary definition

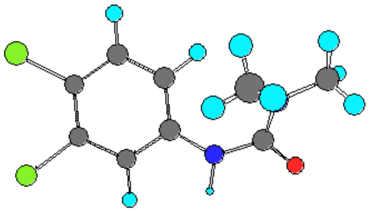
SYSTEM (from ‘cradle to grave’)



New system boundary

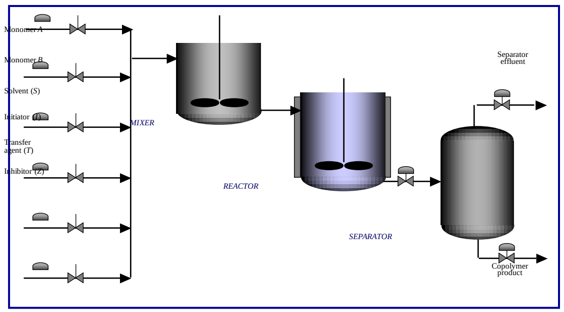
Background Information

Knowledge-data-models



Property models

$$Log\ P_i = A_i + [B_i/(C_i + T)]$$



Process models

$$\frac{dm_i}{dt} = f_{in,i} - f_{out,i} - r(m,T,P)V; i = 1, NC$$

Models for environmental impact

Operation models

Process models

Property-kinetics models

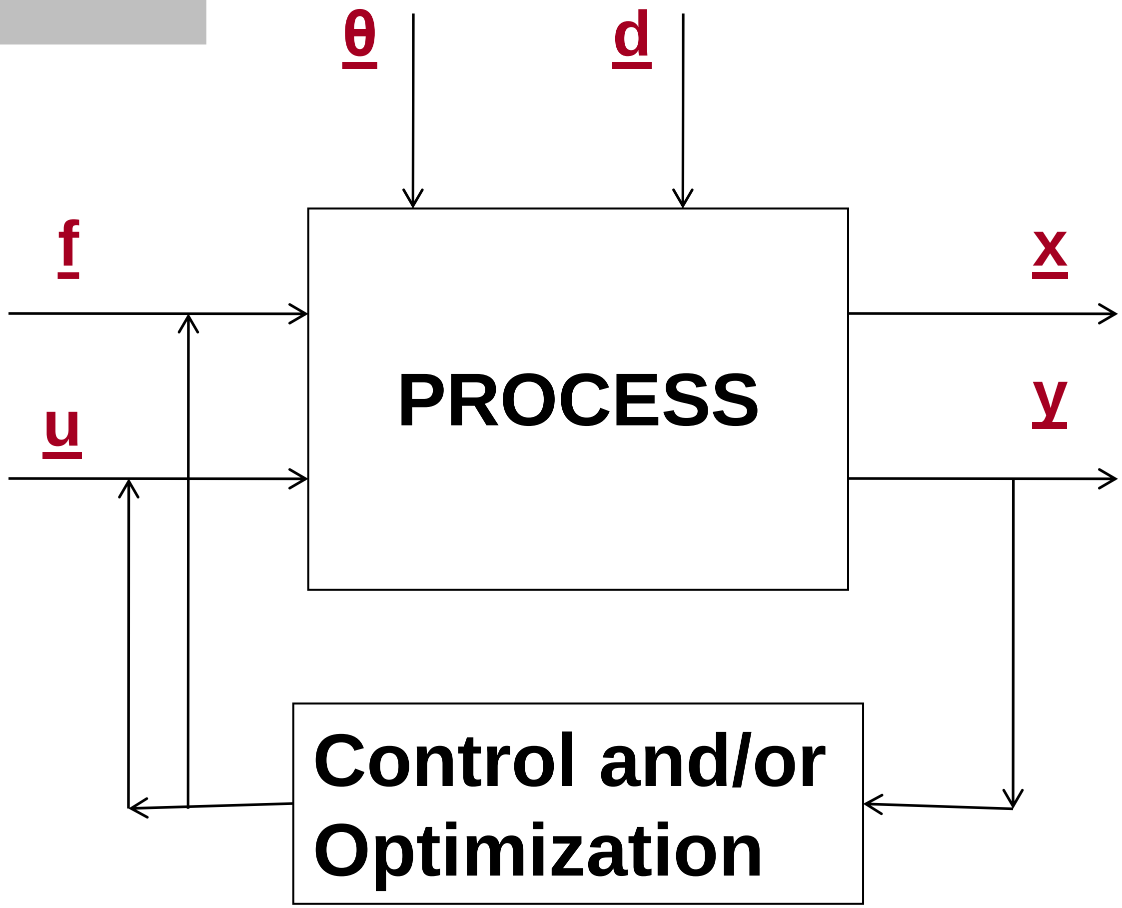
Cost models

Models for sustainability metrics

Formulation process model

Product evaluation model

Models and relationships



Models:

Process/property

$$\frac{d\underline{x}}{dt} = f(\underline{f}, \underline{u}, \underline{d}, \underline{\theta}, \underline{x})$$

$$\underline{y} = g(\underline{x})$$

$$\underline{\beta} = \beta(\underline{C}, \underline{f}, \underline{x})$$

Sustainability Metrics

$$\underline{S_e} = S_e(\underline{f}, \underline{u}, \underline{x}, \underline{y}, \underline{d}, \underline{\theta})$$

$$\underline{S_i} = S_i(\underline{C}, \underline{f}, \underline{x}, \underline{y}, \underline{\theta})$$

$$\underline{S_s} = S_s(\text{size, profit, ?})$$

Safety & Hazards

$$\underline{H_c} = Hc(\underline{C}, \underline{f}, \underline{x}, \underline{y}, \underline{d}, \underline{\theta})$$

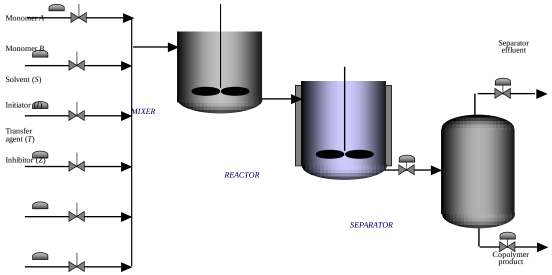
$$\underline{Hp} = H_p(\underline{u}, \underline{f}, \underline{x}, \underline{d}, \underline{\theta})$$

Mathematical model derivation

$$Fobj = \min \{C^T\underline{Y} + f(\underline{x}, \underline{y}, \underline{u}, \underline{d}, \underline{\theta}) + S_e + S_i + S_s + H_c + H_p\}$$

Process-product model

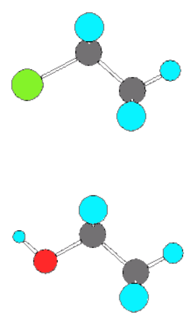
$$P = P(\underline{f}, \underline{x}, \underline{y}, \underline{d}, \underline{u}, \underline{\theta})$$

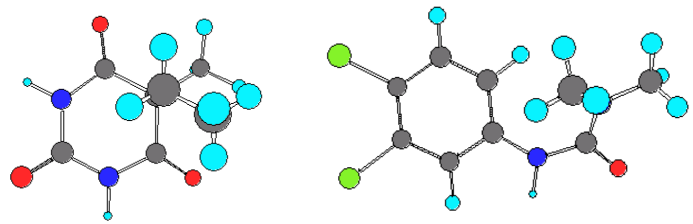


Process-product

$$0 = h_1(\underline{x}, \underline{y})$$

Equipment-material

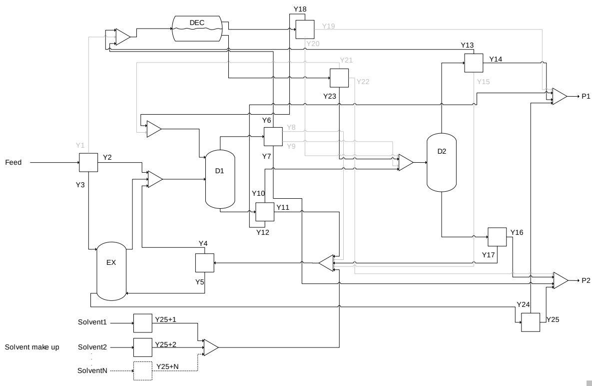




$$0 \geq g_1(\underline{x}, \underline{u}, \underline{d})$$

$$0 \geq g_2(\underline{x}, \underline{y})$$

Flowhseet-chemical alternatives



$$B\,\underline{x} + C^T\underline{Y} \geq D$$

Generic problem formulation

$$Fobj = \min \{C^T\underline{y} + f(\underline{x}, \underline{y}, \underline{u}, \underline{d}, \underline{\theta}) + S_e + S_i + S_s + H_c + H_p\} \quad (1)$$

$$0 = h_1(\underline{x}, \underline{y})$$ process constraints (Eq. 2)

$$0 = P(\underline{f}, \underline{x}, \underline{y}, \underline{d}, \underline{u}, \underline{\theta})$$ process model (Eq. 3)

$$\underline{\theta} = \underline{\theta}(\underline{f}, \underline{x}, \underline{y})$$ property model (Eq. 4)

$$l_1 \leq g_1(\underline{x}, \underline{u}, \underline{d}) \leq u_1$$ process variable constraints (Eq. 5)

$$l_2 \leq g_2(\underline{x}, \underline{y}) \leq u_2$$ molecular structure constraints (Eq. 6)

$$B\,\underline{x} + C^T\underline{y} \geq D$$ process networks (Eq.7)

$\underline{x}$: real-process variables; $\underline{y}$ integer-decision variables;
u: process design variables; d: process input variables;
θ: property; B, C, D coefficient matrices

Generic problem formulation & solution

Fobj = min {$C^T\underline{y}$ + f($\underline{x}$, $\underline{y}$, $\underline{u}$, $\underline{d}$, $\underline{\theta}$) + S_e + S_i + S_s + H_c + H_p} (1)

$0 = h_1(\underline{x}, \underline{y})$ (Eq. 2)

$0 = P(\underline{f}, \underline{x}, \underline{y}, \underline{d}, \underline{u}, \underline{\theta})$ (Eq. 3)

$\underline{\theta} = \underline{\theta}(\underline{f}, \underline{x}, \underline{y})$ (Eq. 4)

$l_1 \le g_1(\underline{x}, \underline{u}, \underline{d}) \le u_1$ (Eq. 5)

$l_2 \le g_2(\underline{x}, \underline{y}) \le u_2$ (Eq. 6)

$B\,\underline{x} + C^T\underline{y} \ge D$ (Eq.7)

Problems:
LP, NLP, MILP, MINLP,
process simulation, ...

Solution strategies:
Direct,
Decomposition based

$\underline{x}$: real-process variables; $\underline{y}$ integer-decision variables;
u: process design variables; d: process input variables;
θ: property; B, C, D coefficient matrices

The concepts

What is sustainability?

How do we go from here…

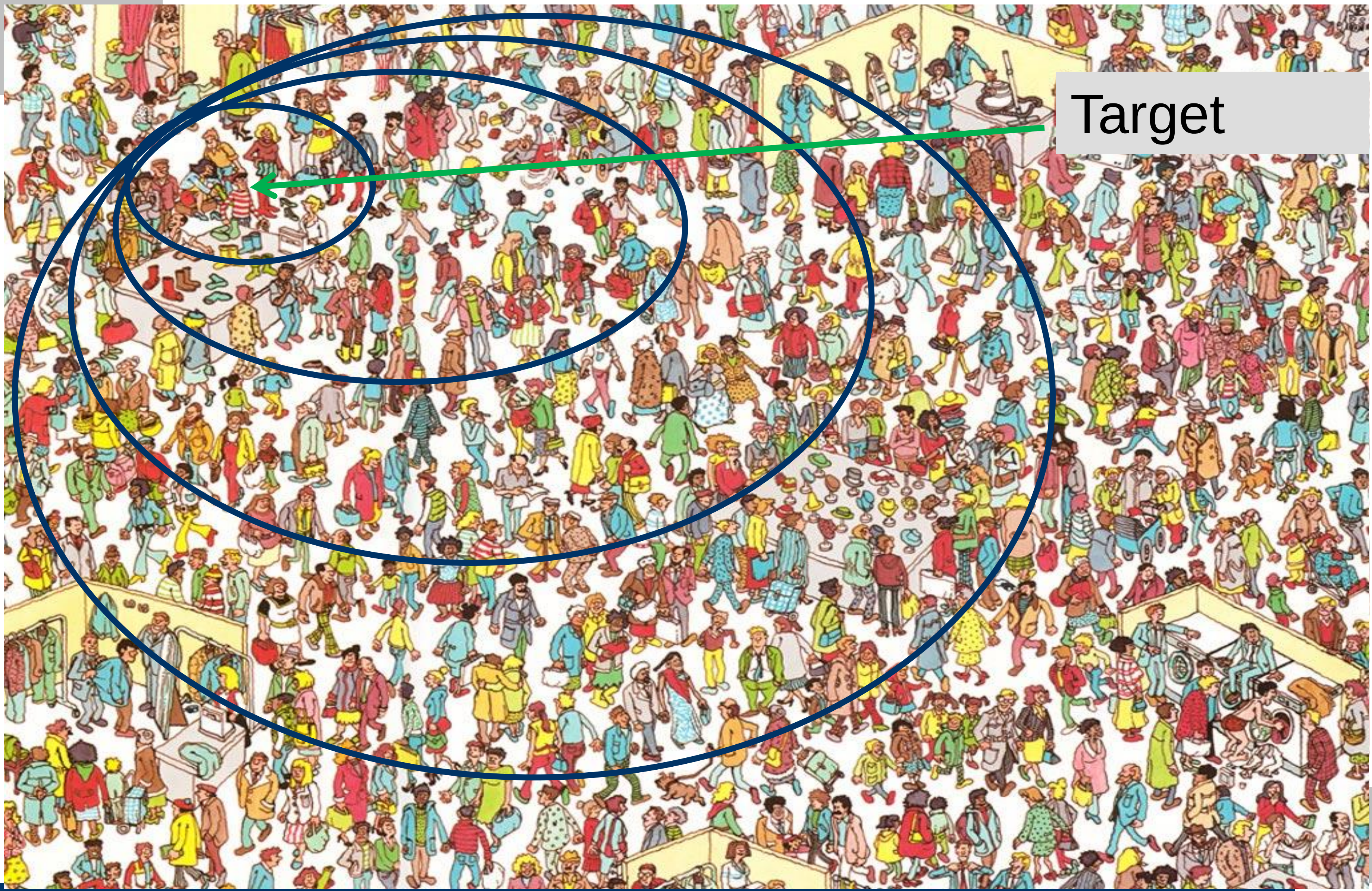
Azapagic 2013

What is sustainability?

……. Somewhere here?

Azapagic 2013

Mathematical problem solution - concept



Solution strategy : Decomposition method (example)

Objective function	$\min 2x_1 + 3x_2 + 1.5y_1 + 2y_2 - 0.5y_3$	IV	(1)
	$s.t.$		
Process model	$x_1^2 + y_1 = 1.25$	II	(2)
	$x_2^{1.5} + 1.5y_2 = 3.0$		(3)
Process constraints	$x_1 + y_1 \le 1.60$	III	(4)
	$1.333x_2 + y_2 \le 3.00$		(5)
Flowsheet constraints	$-y_1 - y_2 + y_3 \le 0$	I	(6)
	$y_1 y_2 = 1$		(7)
Variable bounds	$x_1, x_2 \ge 0$		(8)
	$y_1, y_2, y_3 = \{0,1\}$		(9)

***Solution strategy*:**

Solve I: Y1 = 1, Y2 = 1, Y3 =0; Y1= 1, Y2= 1, Y3 = 1 (only two feasible sets)

Solve II: X1 = 0.5; X2 = 0.544 (for both sets of Y)

Solve III: Eq. 4 & Eq. 5 are satisfied for both sets of Y and the calculated values of X

Solve IV: Eq 1 = 6.132 for set 1; = 5.632 for set 2

Global optimal solution: set 2 (X1=0.5, X2=0.544, Y1=1, Y2=1, Y3=1)

Concept of 3-stages synthesis-design approach

Decompose the problem into stages to manage the complexity

Given: set of feedstock & products
Find: processing route

Given: feasible design (base case)
Find: alternative more sustainable design

Define problem

↓

Generate superstructure

↓

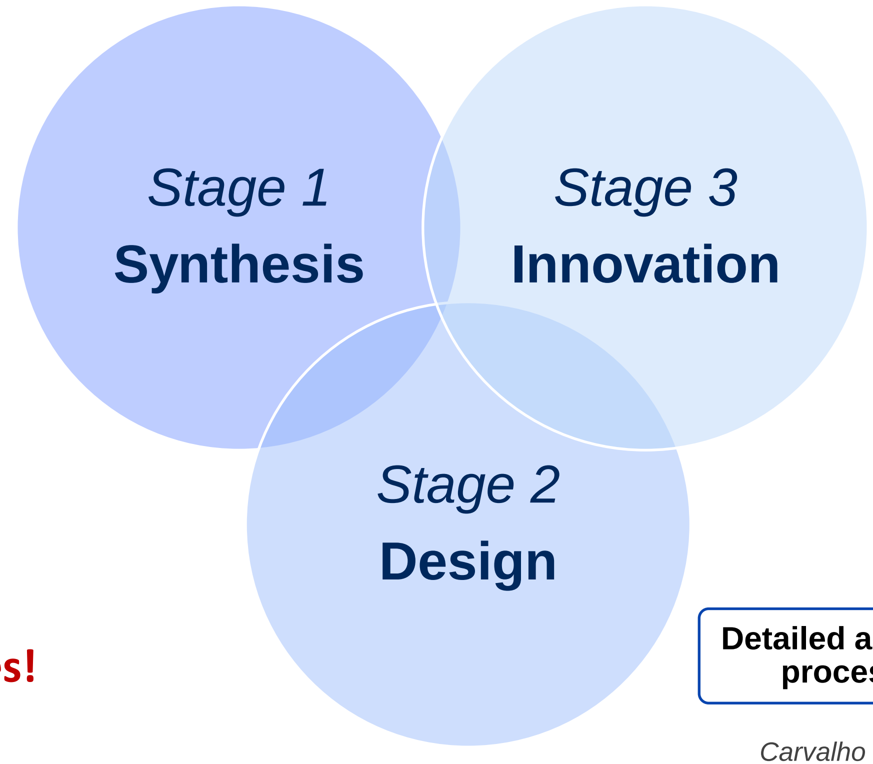
Mathematical formulation

↓

Solve optimization problem

Quaglia et al. (2012)

Generate alternatives!



Generate sustainable intensified alternatives

Babi et al. (2015)

Improve & innovate!

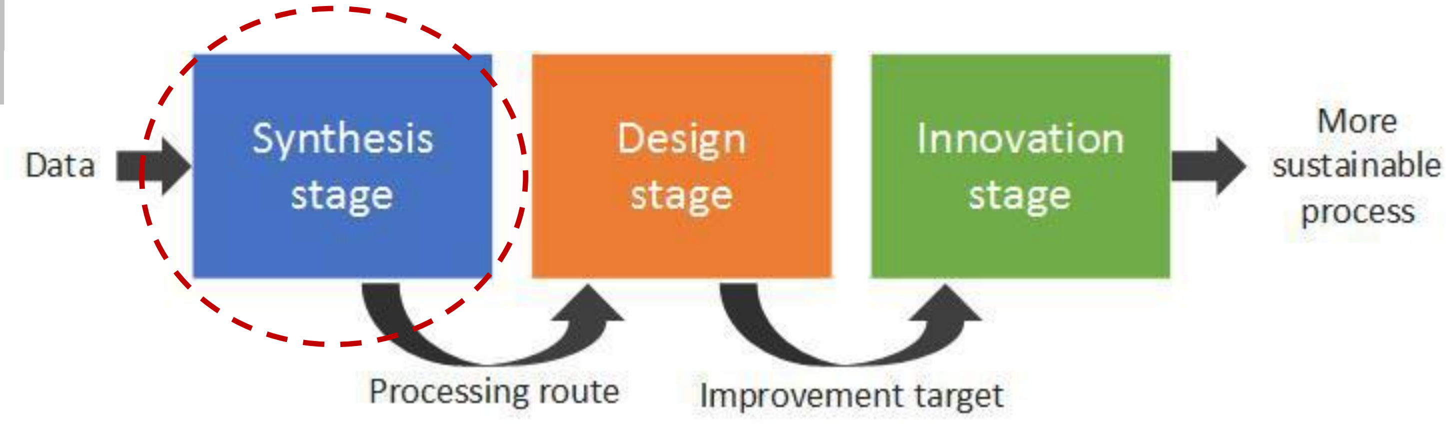
Detailed analyses to identify process bottlenecks

Carvalho et al. (2013)

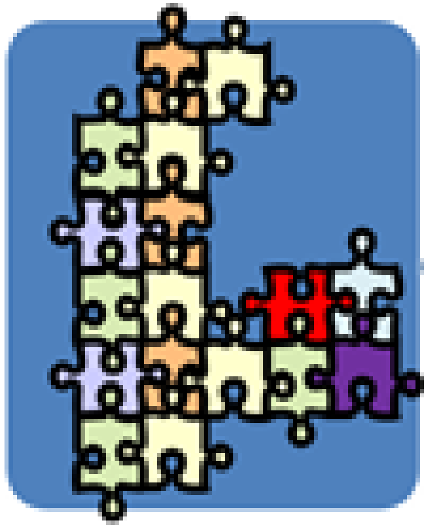
Given: processing route
Find: feasible design

Calculate & analyze!

Sustainable Product-Process Development

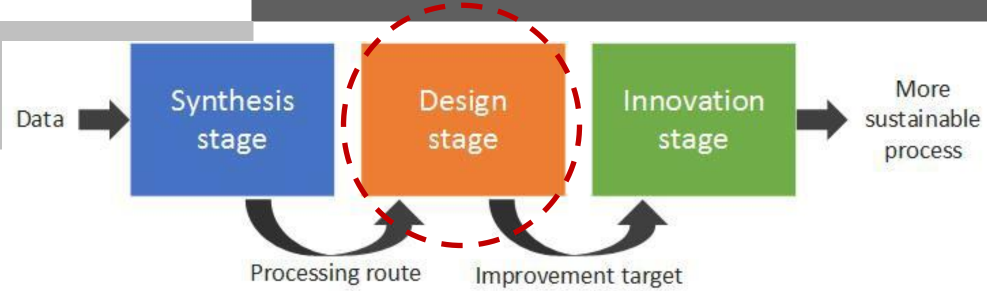


From the available information and supplied specification, determine one or more processing routes to convert identified raw materials to desired products

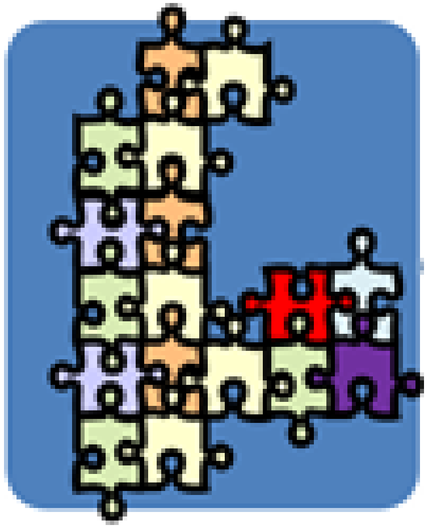


Lectures 1-3

Sustainable Product-Process Development



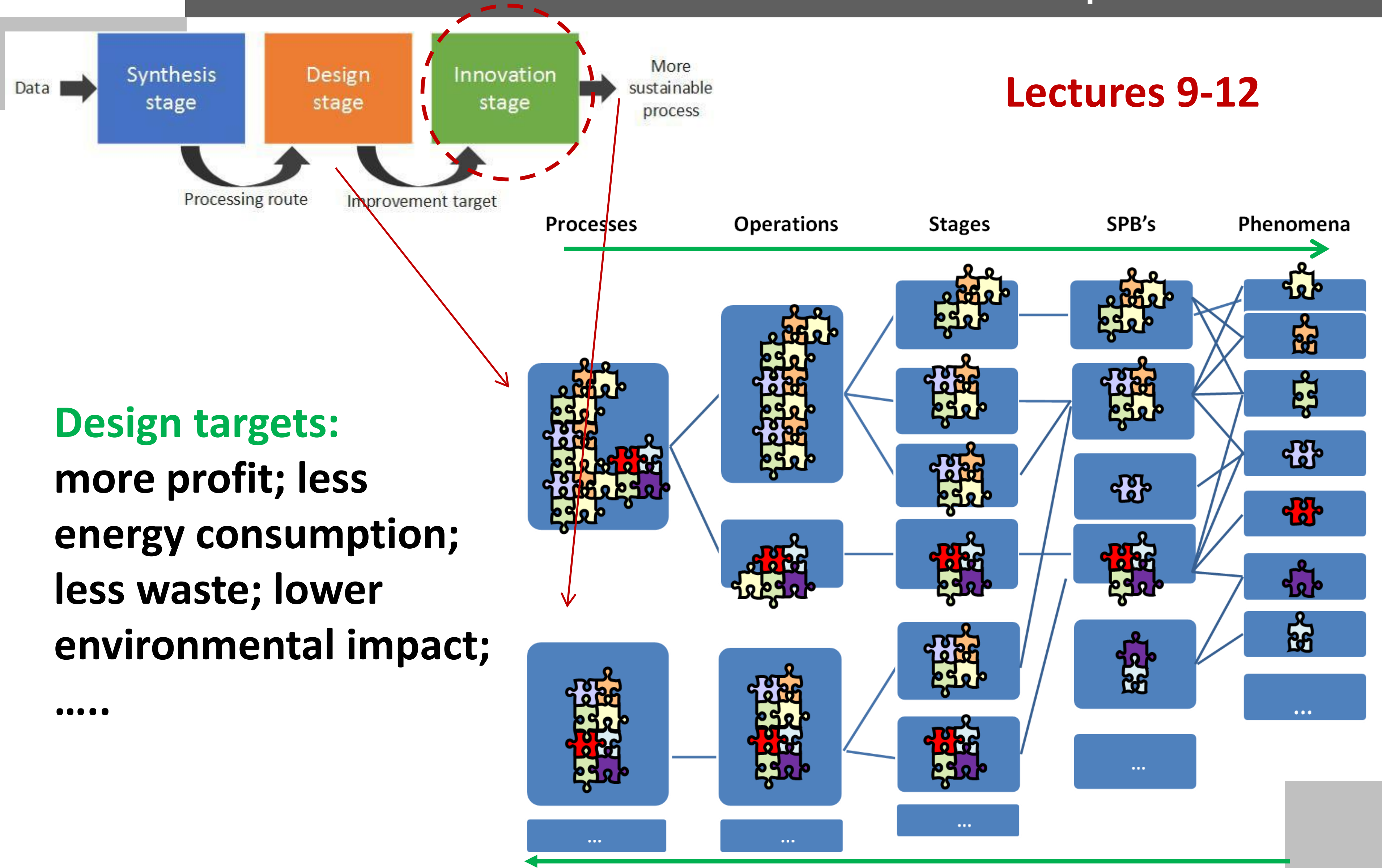
Lectures 4-9



- **Represent processing route as a process flowsheet**
- **Determine the designs of each unit operation to match the process specifications**
- **Perform process simulaton to verify and analyze the design**
- **Determine design targets for process improvement**

Design targets: more profit; less energy consumption; less waste; lower environmental impact; …..

Sustainable Product-Process Development



Lectures 9-12

Design targets:
more profit; less energy consumption; less waste; lower environmental impact; …..

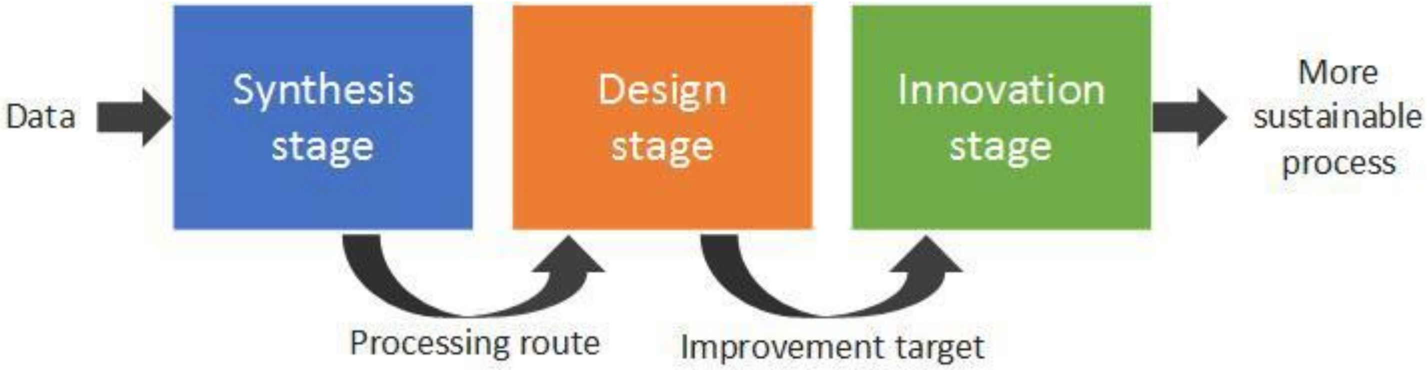
Solution Approach

Solution approach: Multi stage-task approach

Many ways to solve the generic sustainable process synthesis-design-analysis problem. The multi stage-task approach:

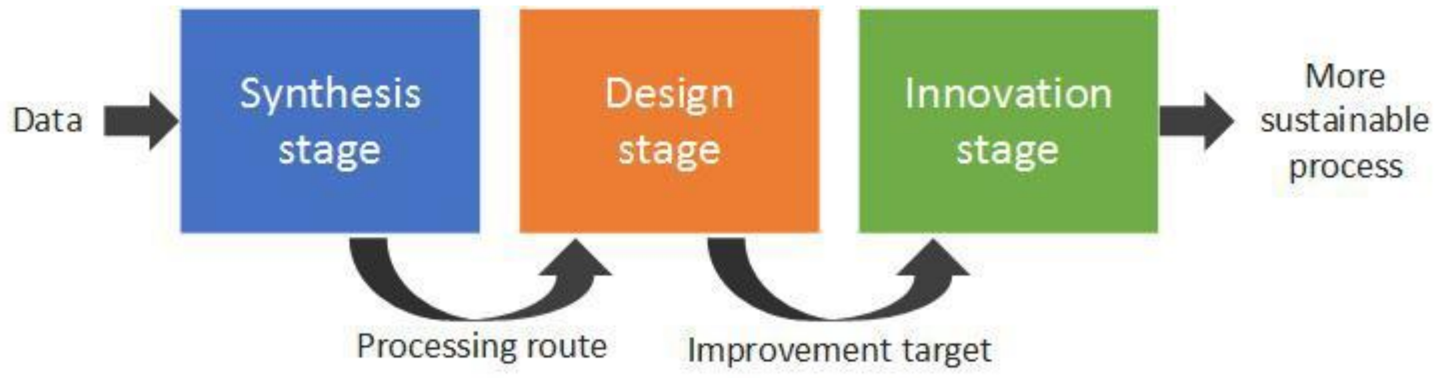
- **Decomposes the problem into 3-stages where a set of 12 tasks (work-flow) are performed**
- **Arranges the tasks in a specific sequence**
  - **Within each task, a set of decisions need to be made**
  - **Calculations are made to verify the decisions**
  - **Data generated in one task is used in the subsequent tasks**

Tasks for synthesis stage



- **Task 1**: Collect information on the product
- **Task 2**: Collect information on the process; alternative paths to convert other raw materials to the desired product
- **Task 3**: Generate (and/or select) preliminary process flowsheet
- **Task 4**: Decide process conditions (such as reaction conversion, separation factor, purge, etc.) and perform a simple mass balance on the selected flowsheet

Tasks for design stage



•***Task 4****: Decide process conditions (such as reaction conversion, separation factor, purge, etc.) and perform a simple mass balance on the selected flowsheet*

• **Task 5**: Based on the results from above, set temperatures and pressures on the process flowsheet

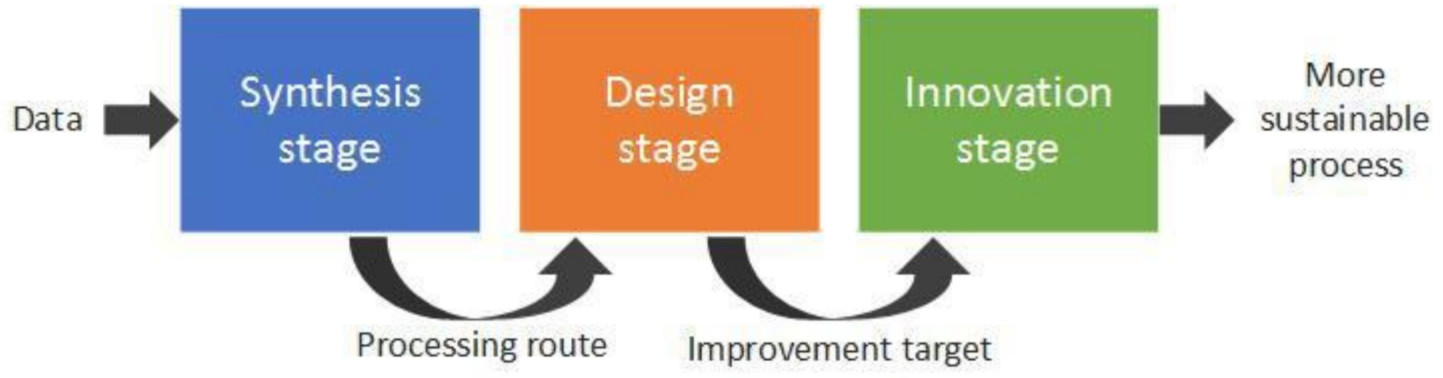
• **Task 6**: Based on the results from above, perform a simple mass & energy balance

•**Task 7**: Perform detailed process simulation – convert each of the simple models with the more rigorous option, one at a time, until all simple models have been converted.

• **Task 8**: Based on the simulation results from task 7, perform equipment sizing and costing calculations

• **Task 9**: Based on the results from tasks 1-8, perform an economic evaluation, using the current design as the "base case"

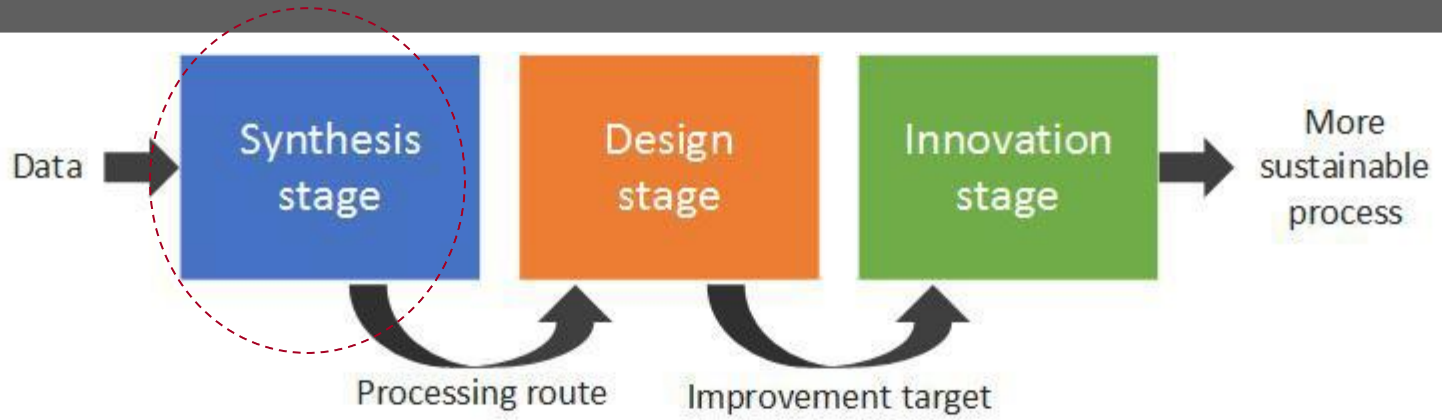
Tasks for innovation stage



- ***Task 9**: Based on the results from tasks 1-8, perform an economic evaluation, using the current design as the "base case"*
- **Task 10**: Investigate if opportunities for heat and mass transfer exist. If yes, apply them and check by how much the cost of operation can be further reduced?
- **Task 11**: Perform environmental impact analysis
- **Task 12**: Generate innovative alternatives with PI approach

Methods & Tools

Synthesis stage: Methods & tools



Methods

- **Task 1**: Collect information on the product
- **Task 2**: Collect information on the process; alternative paths to convert other raw materials to the desired product

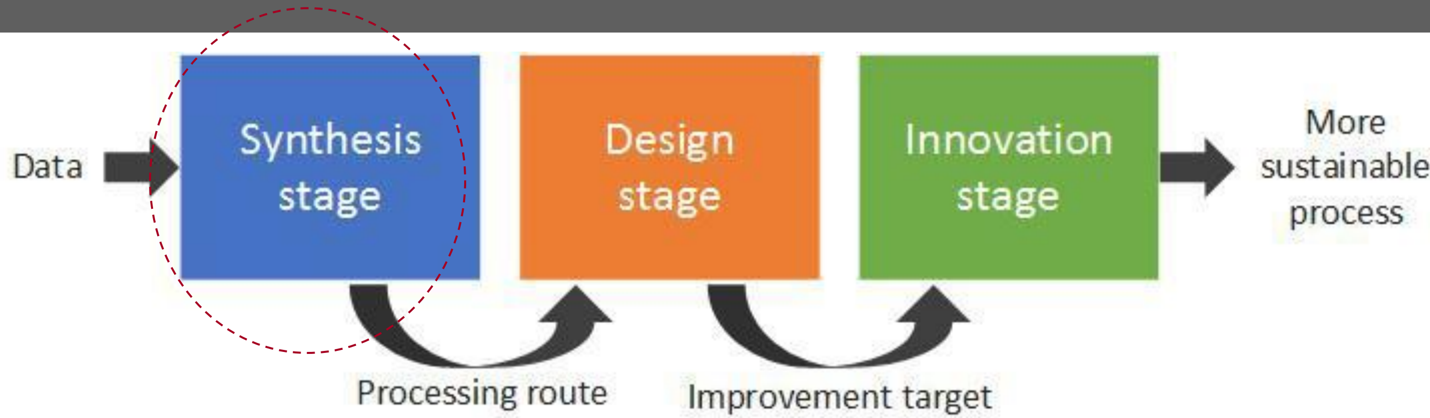
Data collection & analysis

Data generation & analysis

- **Task 3**: Generate (and/or select) preliminary process flowsheet
- **Task 4**: Decide process conditions (such as reaction conversion, separation factor, purge, etc.) and perform a simple mass balance on the selected flowsheet

- **Existing process**
- **Heuristic (Douglas method)**
- **Generate & test**
- **Mathematical programming**
- **Hybrid**

Synthesis stage: Methods & tools



- **Task 1**: Collect information on the product
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- **Task 4**: Decide process conditions (such as reaction conversion, separation factor, purge, etc.) and perform a simple mass balance on the selected flowsheet

Methods

Data collection & analysis

Data generation & analysis

Existing process
Heuristic (Douglas method)
Generate & test
Mathematical programming
Hybrid

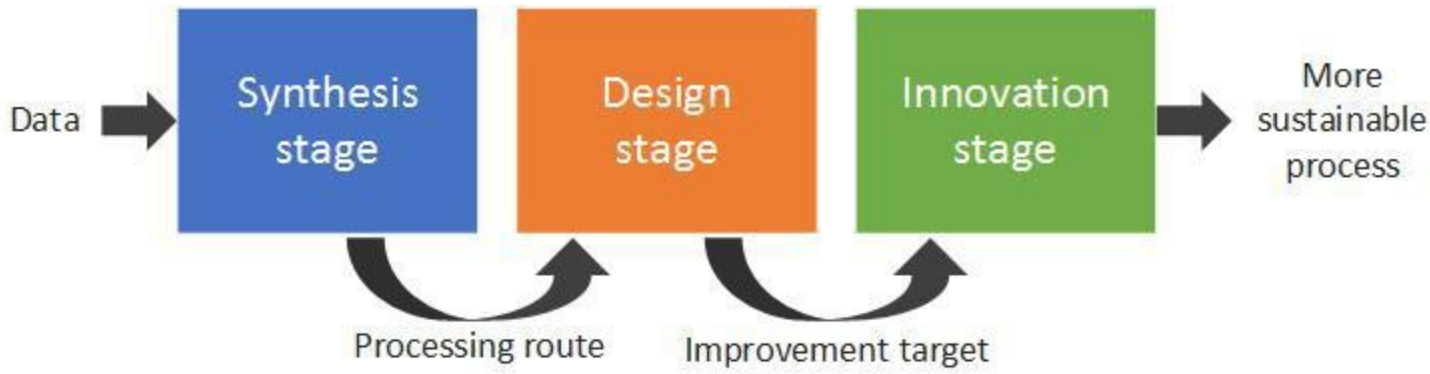
Tools

Databases

Utility tools

Process synthesis tools (ProCAFD; Super-O)

Design-analysis stage: Methods & tools



- ***Task 4***: *Decide process conditions (such as reaction conversion, separation factor, purge, etc.) and perform a simple mass balance on the selected flowsheet*
- **Task 5**: Based on the results from above, set temperatures and pressures on the process flowsheet
- **Task 6**: Based on the results from above, perform a simple mass & energy balance

→ Design methods based on simple models for mass balance; Use of thermodynamics to set temperatures, pressures and to calculate enthalpies

- **Task 7**: Perform detailed process simulation – convert each of the simple models with the more rigorous option, one at a time, until all simple models have been converted.

→ Rigorous model based process simulation

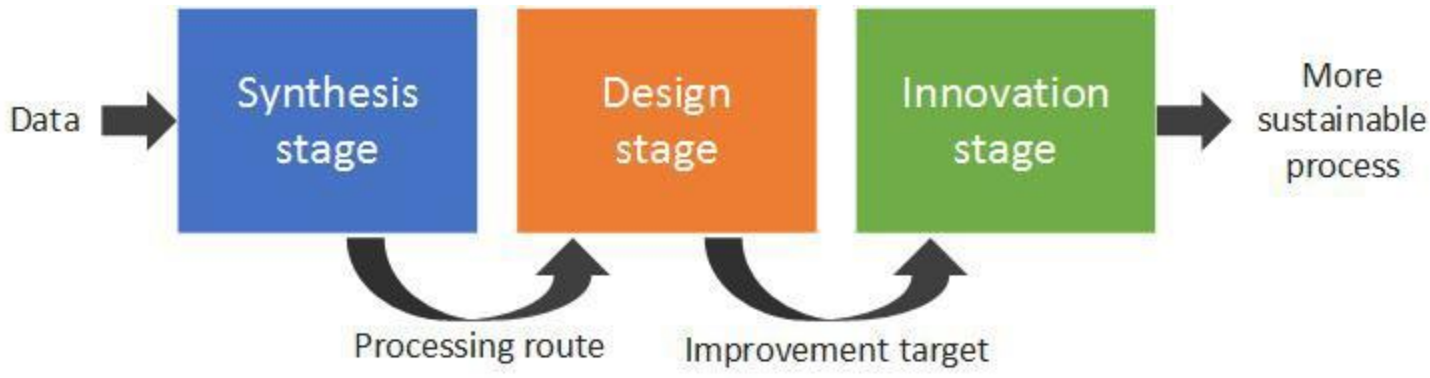
- **Task 8**: Based on the simulation results from task 7, perform equipment sizing and costing calculations

→ Equipment sizing and costing methods

- **Task 9**: Based on the results from tasks 1-8, perform process analysis on the current design as the "base case" & define targets for improvement

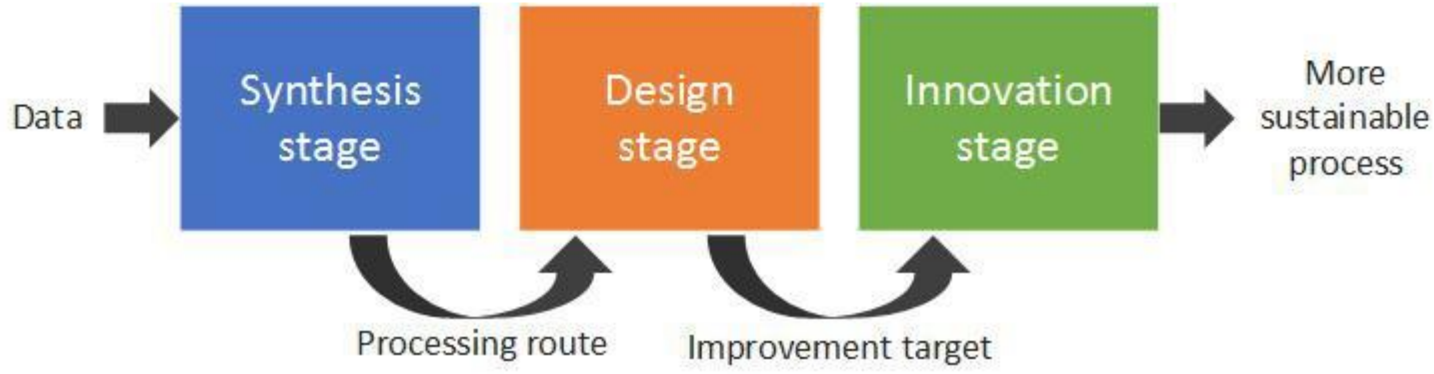
→ Economic analysis; LCA; sustainability analysis…

Design-analysis stage: Methods & tools



Tasks	Methods	Tools
•*Task 4*: •Task 5: •Task 6:	Design methods based on simple models for mass balance; Use of thermodynamics to set temperatures, pressures and to calculate enthalpies	ProCAFD (ICAS; PROII; ASPEN) ProPred (properties package; database)
•Task 7:	Rigorous model based process simulation	ProII; ASPEN; ICAS; ….
•Task 8:	Equipment sizing and costing methods	Sizing (PROII; ASPEN); Costing (ECON)
•Task 9:	Economic analysis; LCA; sustainability analysis…	LCSoft (ECON; SustainPro)

Innovation stage: Methods & tools



- ***Task 9**: Based on the results from tasks 1-8, perform process analysis on the current design as the "base case" & define targets for improvement*
- **Task 10**: Investigate if opportunities for heat and mass transfer exist. If yes, apply them and check by how much the cost of operation can be further reduced?
- **Task 11**: Investigate how the current design can be further improved; formulate process optimization problems
- **Task 12**: Generate innovative alternatives with PI approach

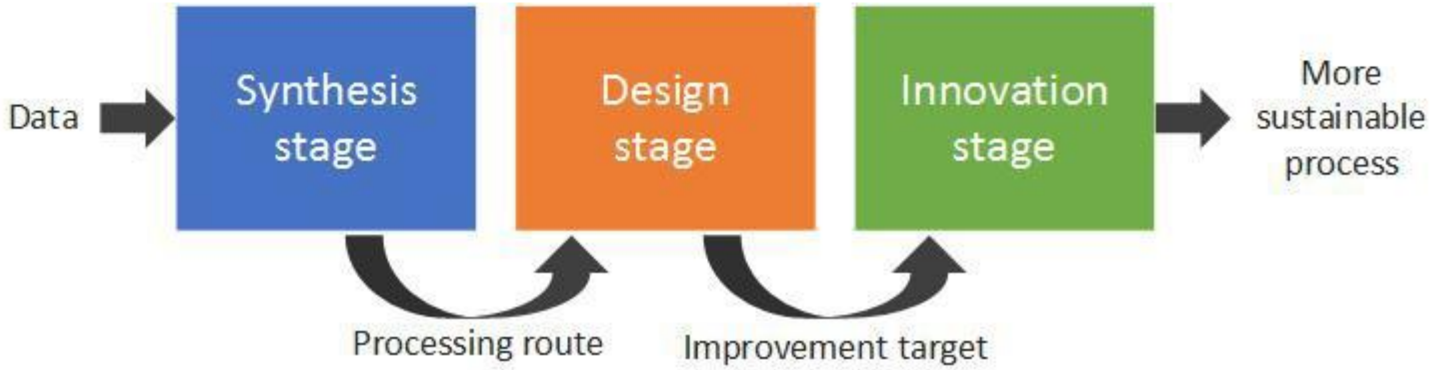
Identify process "hot-spots"; variables involved and targets for improvement

Methods for heat-mass integration

Process optimization – sequential & simultaneous

Phenomena based PI method to generate innovative & new designs

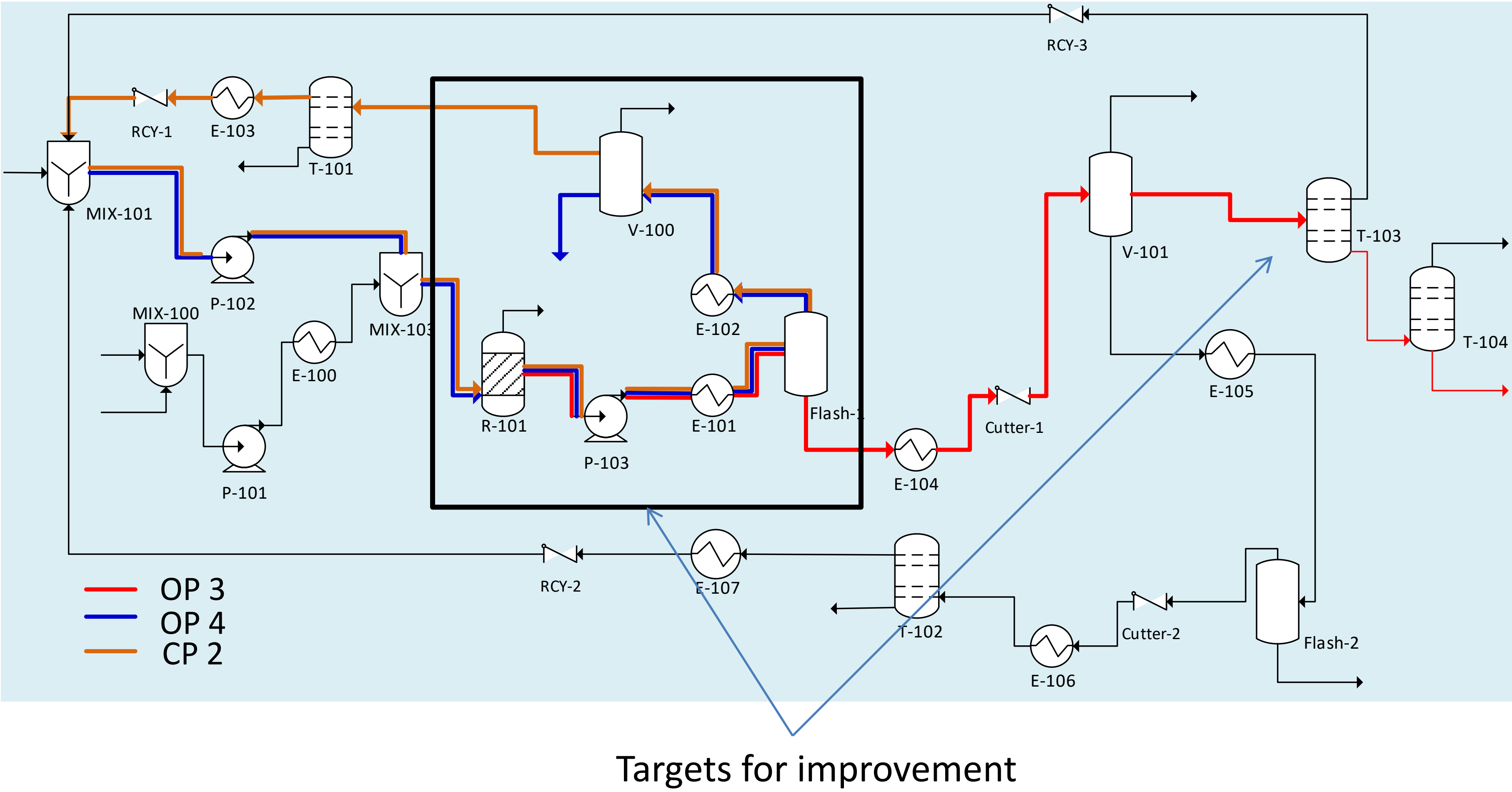
Innovation stage: Methods & tools



• ***Task 9***:	Identify process ”hot-spots”; variables involved and targets for improvement	Analysis of results from LCSoft
•**Task 10**:	Methods for heat-mass integration	ProCAFD; ICAS; PROII; ASPEN
•**Task 11**:	Process optimization – sequential & simultaneous	PROII; ASPEN; ICAS
•**Task 12**:	Phenomena based PI method to generate innovative & new designs	Algorithm based framework (provides work-flow)

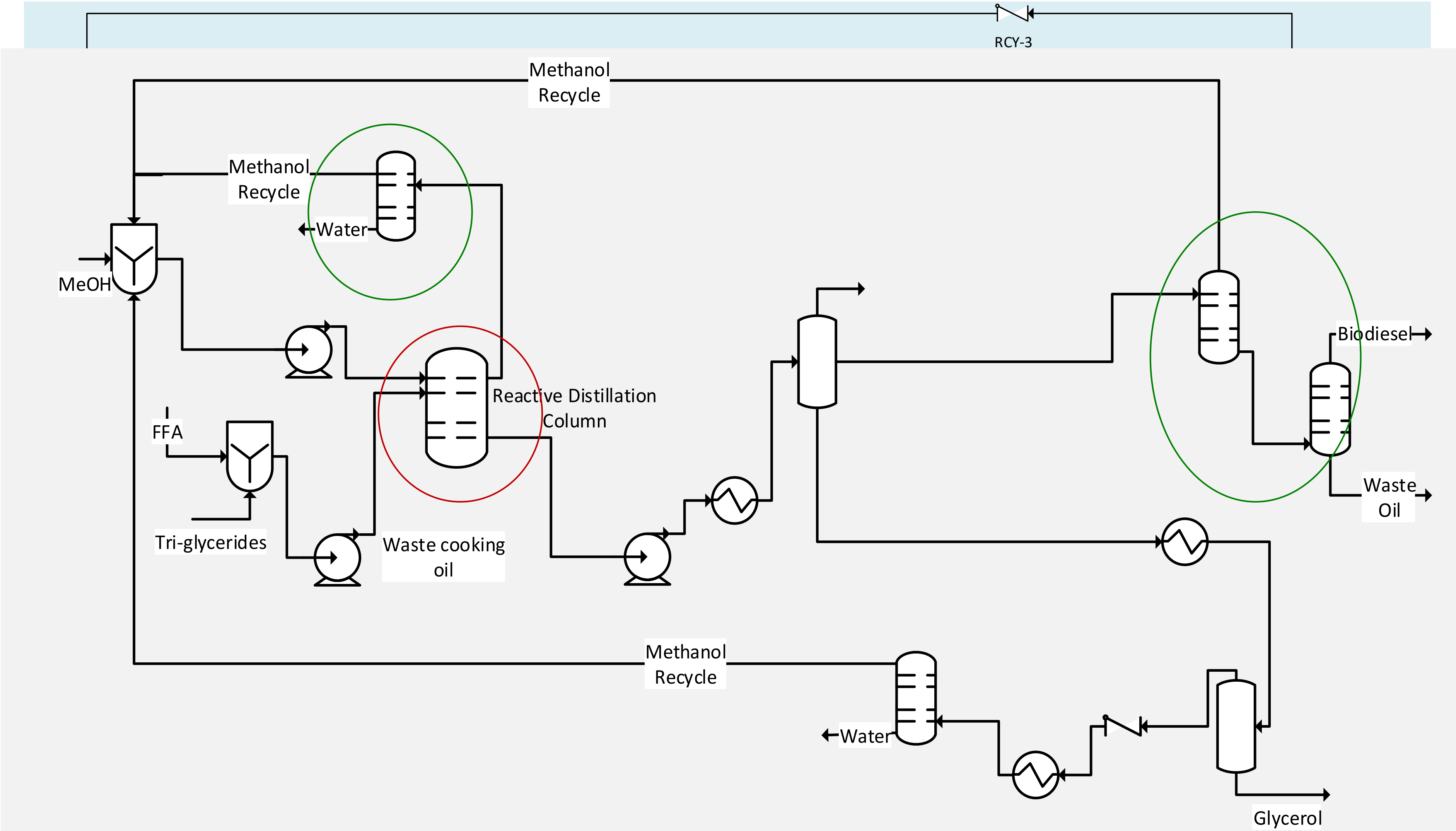
More sustainable design (visualization)

Identify more sustainable (1): Base case



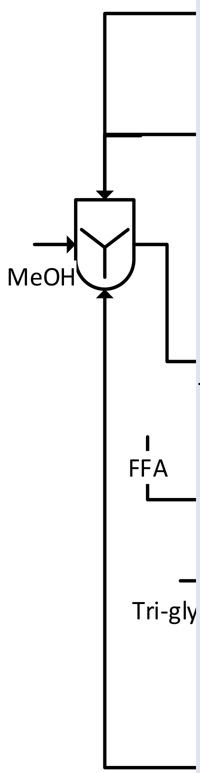
Mansouri et al. 2013

Identify more sustainable (2) : PI solution



Mansouri et al. 2013

Compare more sustainable (PI) alternatives



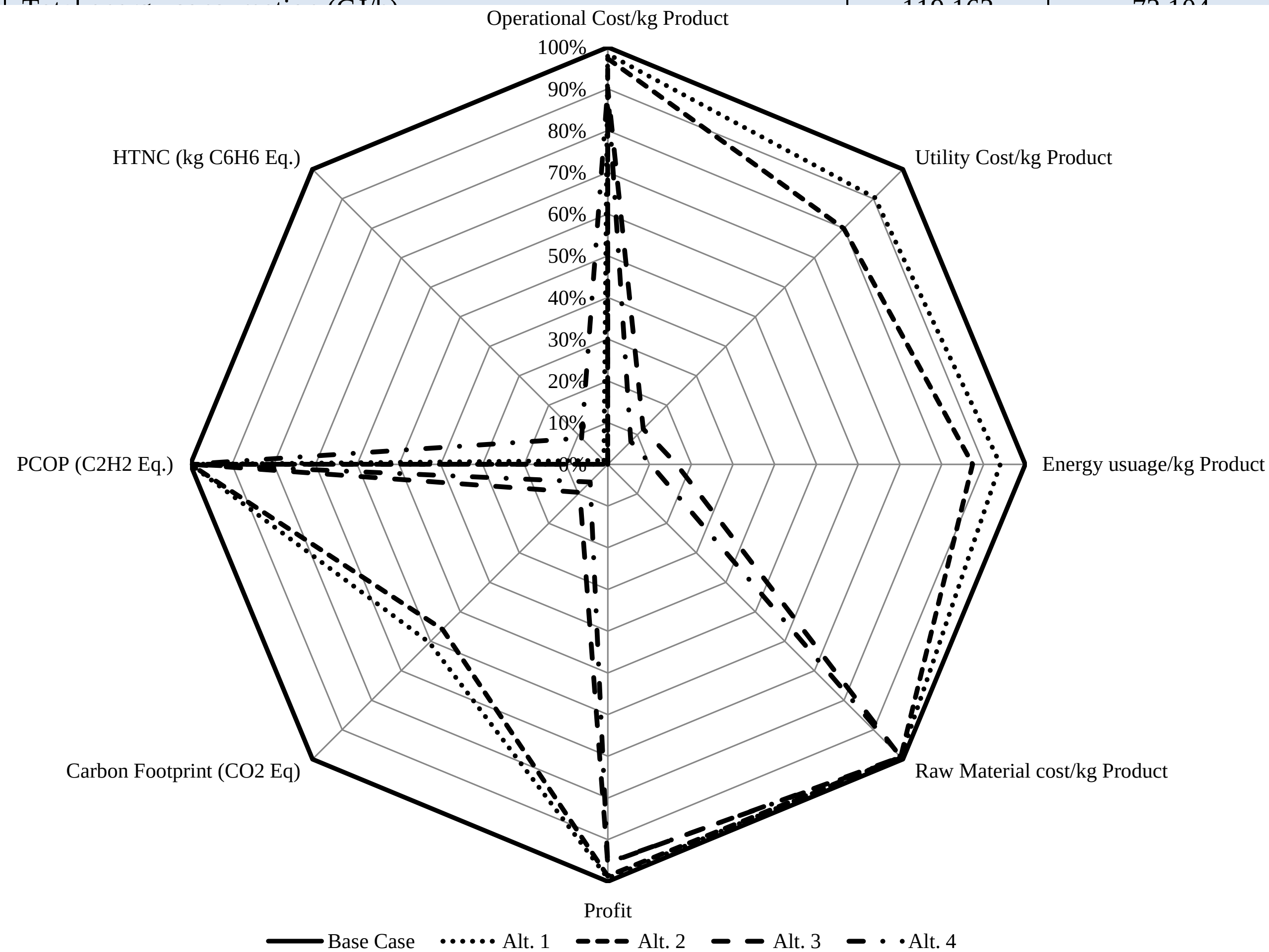
	Sustainability Metrics	Base case design	Intensified alternative	%Improvement
Performance metrics	Total utility cost ($/year)	7,790,000	4,660,000	40.2
	Total energy consumption (GJ/h)	119.163	73.104	38.6
	product/raw material (kg/kg)	0.94	0.94	0
	Energy/ products (GJ/kg)	0.0025	0.0017	32
	Net water added to the system (m^3)	0	0	0
	Water for cooling/product (m^3/kg)	0.017	0.017	0
	Waste/raw material (kg/kg)	0.032	0.026	18.8
	Waste/products (kg/kg)	0.034	0.028	17.6
	Hazardous raw material/product (kg/kg)	0	0	0
	Number of unit operations	9	7	22
LCA	Total carbon footprint (kg CO_2 eq.)	0.183	0.143	21.8
	HTPI - Human Toxicity Potential by Ingestion ($1/LD_{50}$)	0.51811	0.51111	0
	HTPE - Human Toxicity Potential by Exposure ($mg_{emiaaion}/m^3$)	0.03558	0.03564	0
	GWP - Global Warming Potential (CO_2 eq.)	0.55214	0.55241	0
	ODP - Ozone Depletion Potential (CFC-11 eq.)	5.18E–09	5.18E–09	0
	PCOP - Photochemical Oxidation Potential (C_2H_2 eq.)	0.04968	0.04976	0
	AP - Acidification Potential (H^+ eq.)	0.00010	0.00010	0
	ATP - Aquatic Toxicity Potential ($1/LC_{50}$)	0.00366	0.00366	0
	TTP - Terrestrial Toxicity Potential ($1/LD_{50}$)	0.51811	0.51111	0
	HTC (Benzene eq.) - human toxicity (carcinogenic impacts)	2062.7	1794.5	13
	HTNC (Toluene eq.) - human toxicity (non-carcinogenic impacts)	1.3301	1.1795	11.3
	ET (2, 4-D eq.) - Fresh water ecotoxicity	0.00525	0.00490	6.7

LC_{50} is lethal concentration ($mg_{emission}/kg_{fathead\ minnow}$)
LD_{50} is one kg body weight of rat administered in milligrams of toxic chemical by mouth ($mg_{emission}/kg_{rat}$)

Mansouri e

Compare more sustainable (PI) alternatives

	Sustainability Metrics	Base case design	Intensified alternative	%Improvement
	Total utility cost ($/year)	7,790,000	4,660,000	40.2



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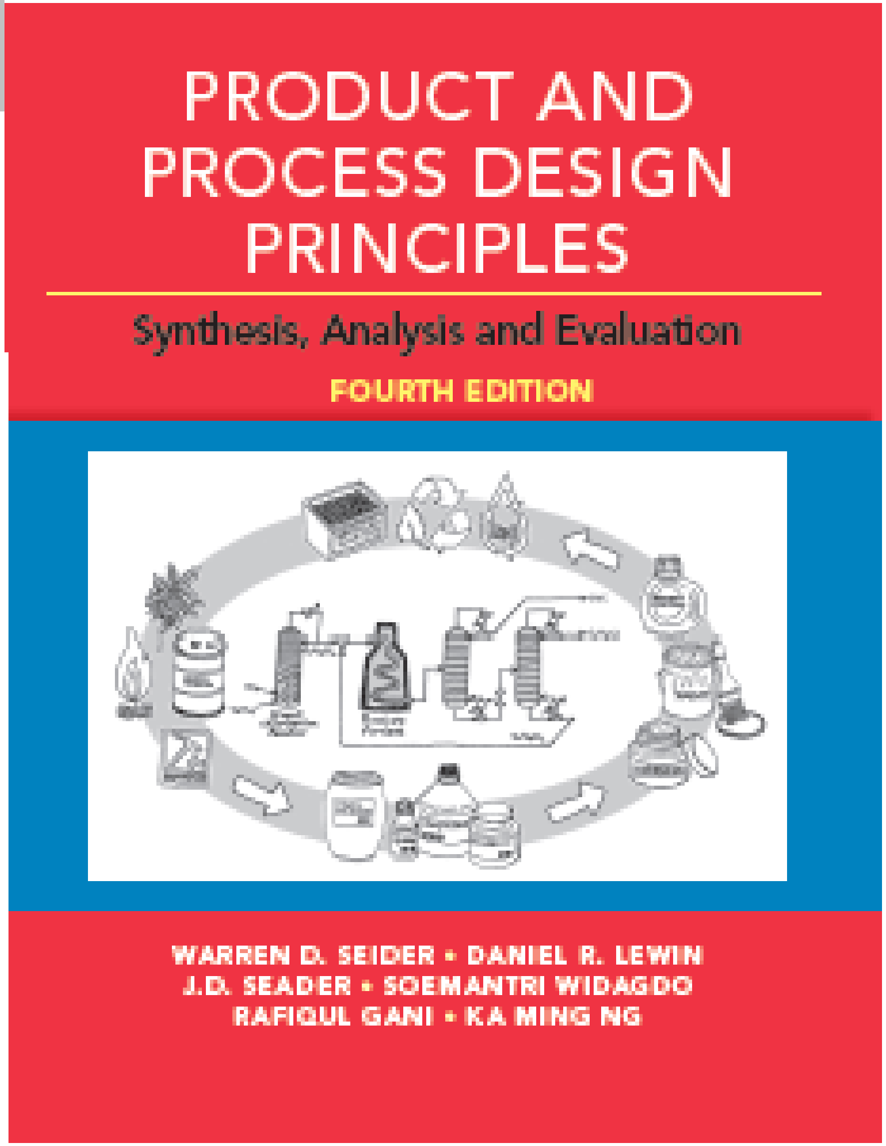
Workshop plan

- **Day 1**: Introduction & Stage-1 (methods-tools for Tasks 1-3); data collection, generation & analysis
- **Day 2**: Stage-1 (methods-tools for Task 3) & Stage-2 (methods-tools for Tasks 4-6); Super-O & ProCAFD
- **Day 3**: Stage-2 (methods-tools for Tasks 7-8); Process simulation with PROII/ASPEN); LCSoft (ECON)
- **Day 4**: Stag-2 (LCSoft – LCA, sustainability, etc.) & Stage-3 (heat integration with ProCAFD-ICAS; PROII-user module)
- **Day 5**: Stage-3 (simultaneous heat integration & optimization with PROII-user modules) and phenomena-based process intensfication (theory, method & application examples)

Summary

- Sustainable process synthesis, design and analysis in 12 sequential steps
  - Guaranteed improved design compared to base-base
  - Non-tradeoff optimal solution
  - Important to first establish a base-case
  - Analyze the base-case to identify opportunities for improvement
  - Define targets for improvement
  - Apply PI-synthesis methods to find alternative designs that match the targets
- Introduction to ProCAFD software tool
- Integration of methods-tools needed to solve these problems



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Suitable for BSc, MSc level teaching of

- **Product design**
- **Process design**
- **Integrated product-process design**