Computer Aided Methods and Tools for Innovative Chemical Product and Process Design

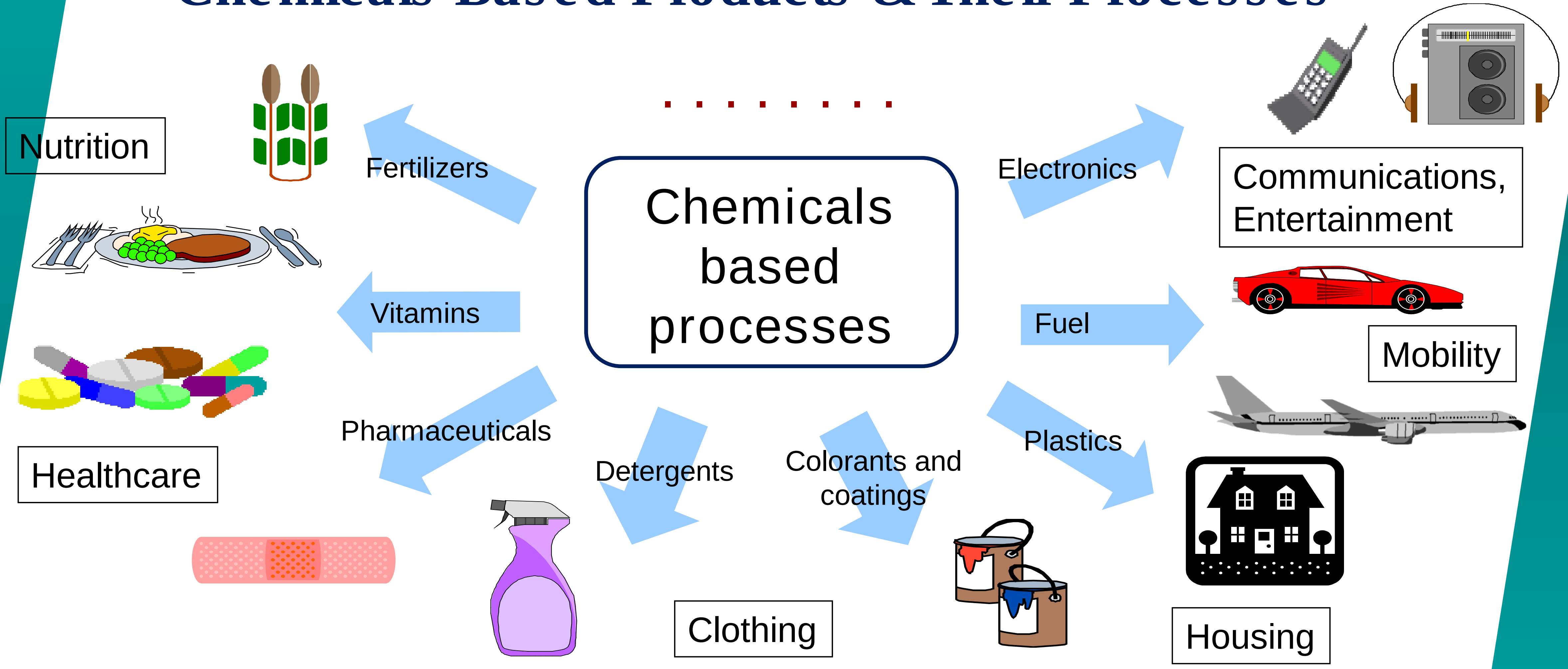
Rafiqul Gani

PSE for SPEED, Skyttemosen 6, DK3450 Allerod, Denmark
(Head office: Bangkok, Thailand)

rganі2018@gmail.com
http://www.pseforspeed.com/

1. Introduction

Chemicals Based Products & Their Processes



Survival of our modern society depends on the products from ChE

Motivation to Find New & Improved Solutions

Convert resources to products

↕

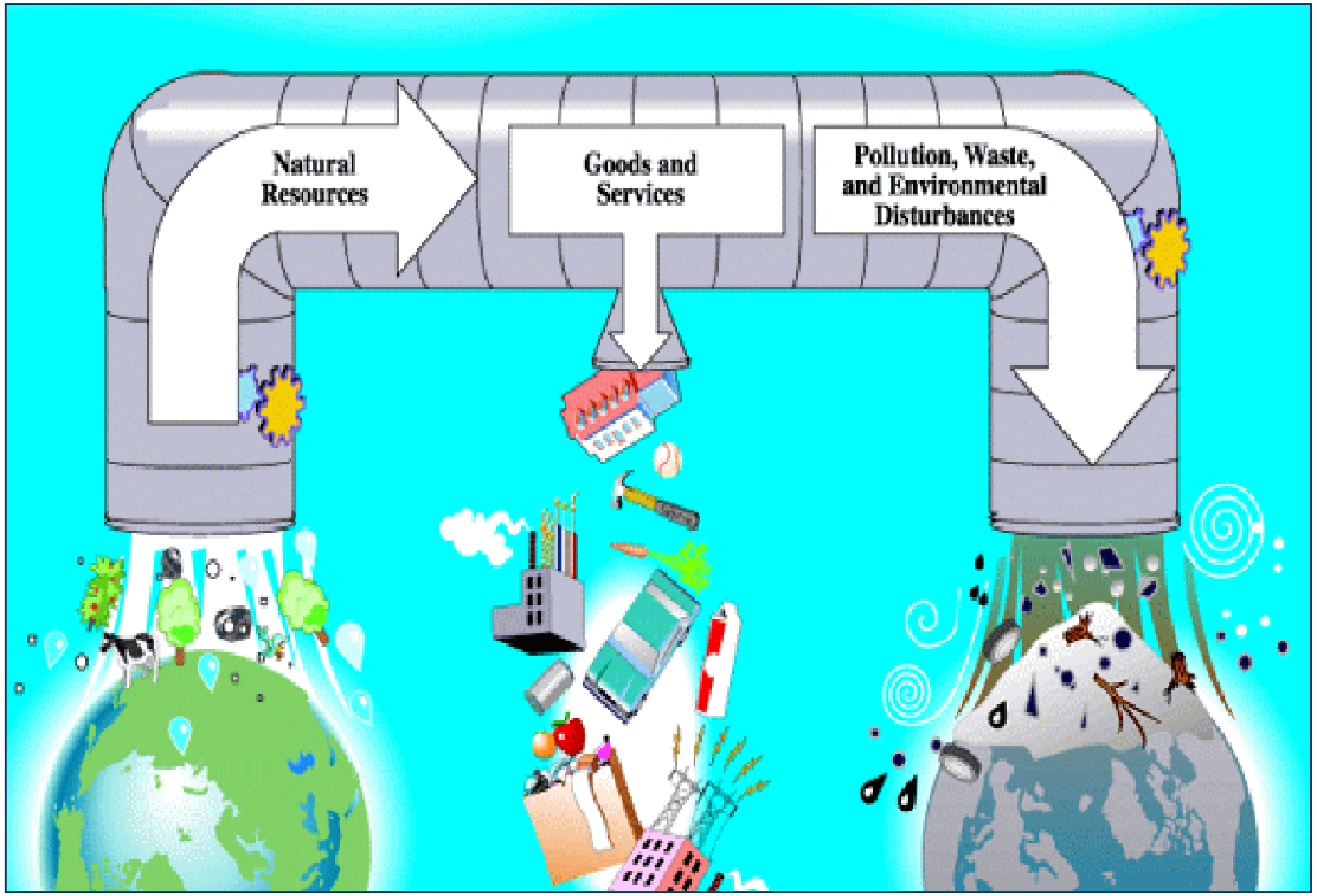
Use energy, **water, ….**

↕

Environmental Impacts (GWP, **OD, HTTP, …)**

↕

Produce waste



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

Process Systems Engineering: Main Topics

How?	Topic	Why?
Numerical analysis =>	Simulation	=> Behavior of process-product
Mathematical Programming =>	Optimization	=> Synthesis/design
Systems and Control Theory =>	Process Control	=> Manufacture
Computer Science =>	Advanced Info./Computing	=> Efficient problem solving
Management Science =>	Operations/Business	=> Supply chain

Models of various types, forms & application range play important roles in all of the above!

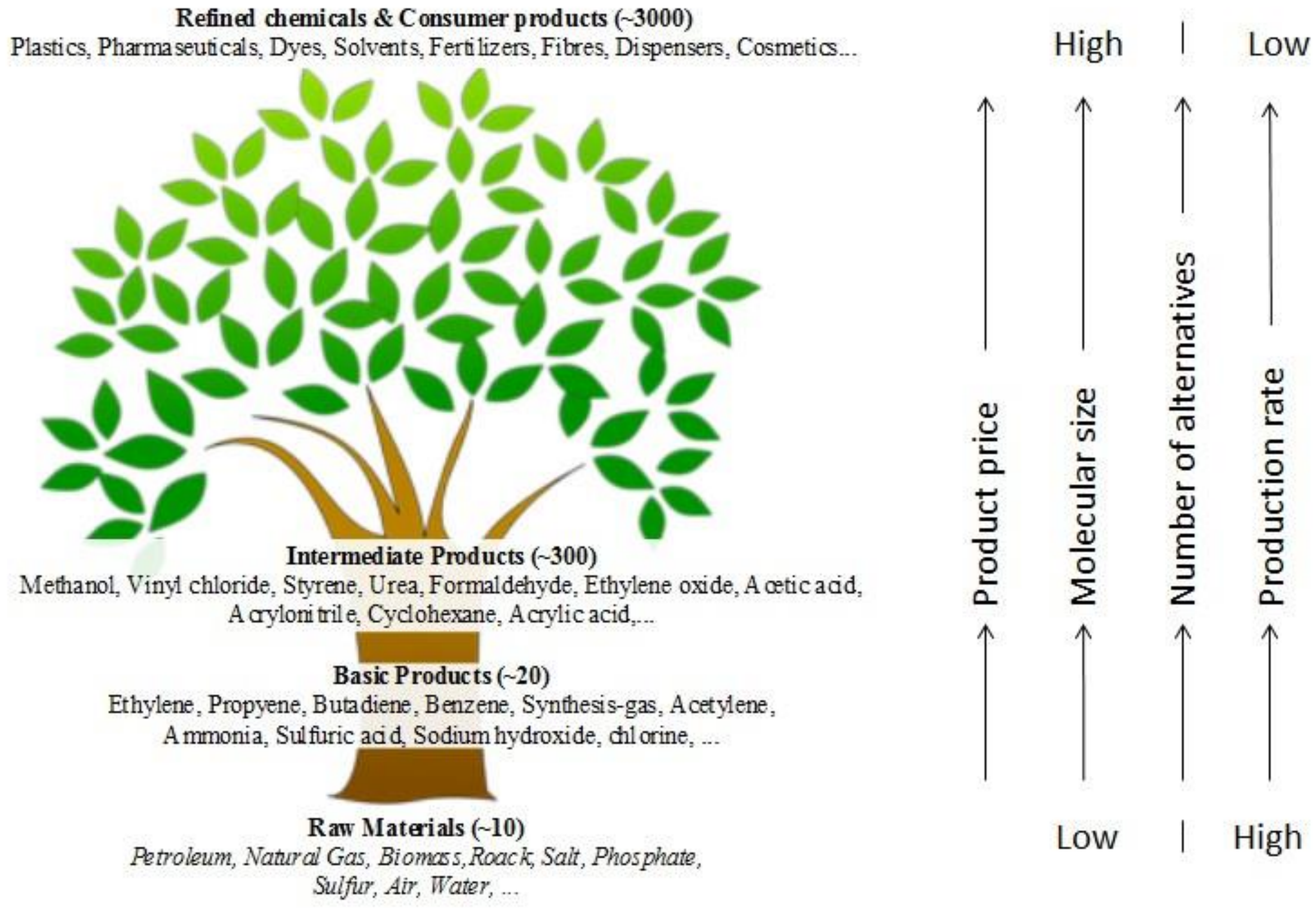
2. Problem Definition

Which product to make (selection, design, …)?

How to make it (process synthesis, design, **sustainability, ….)?**

Other questions (When? Why?)

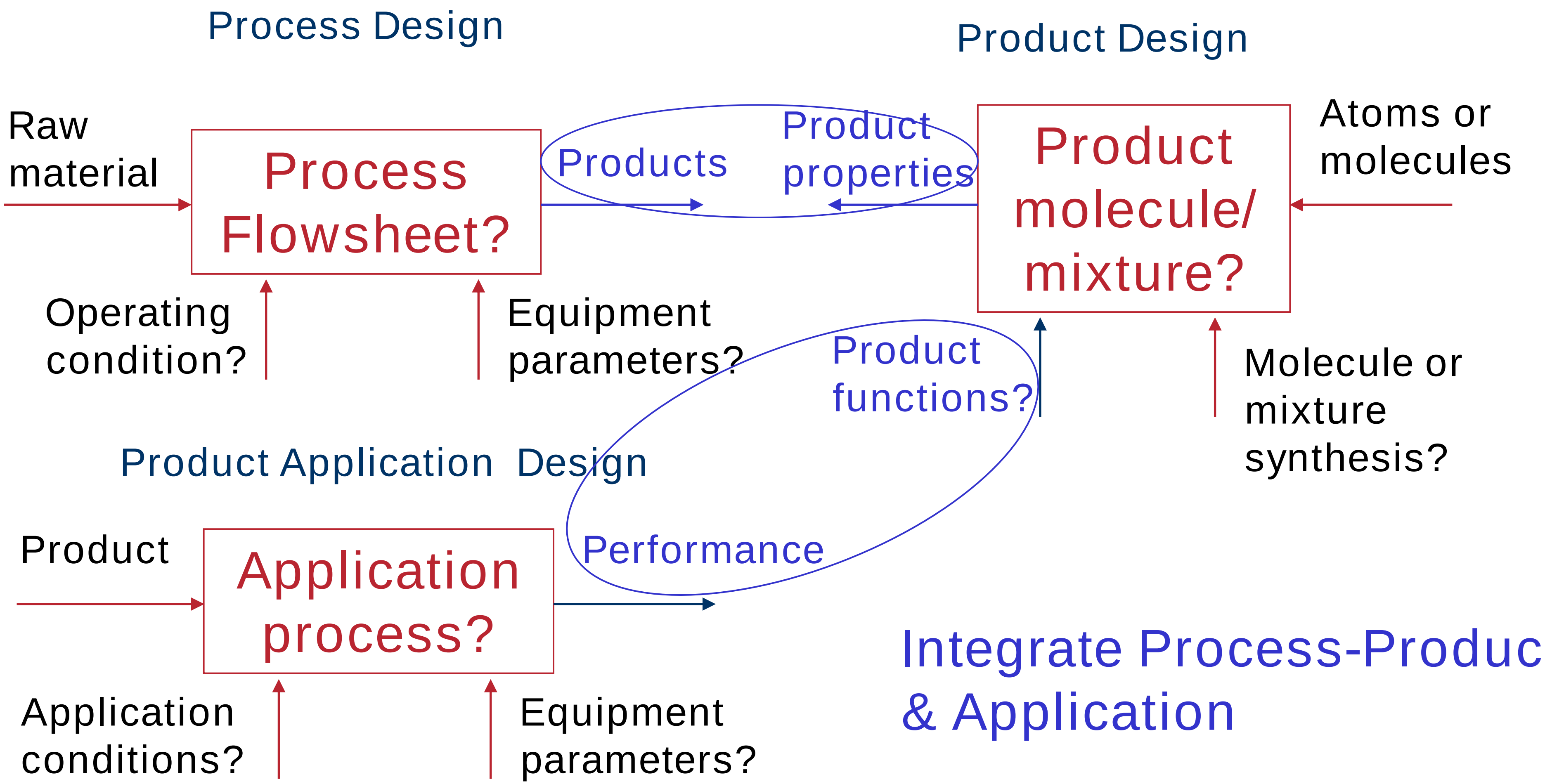
The Chemical Product Tree



Questions: what, why & when (how)?

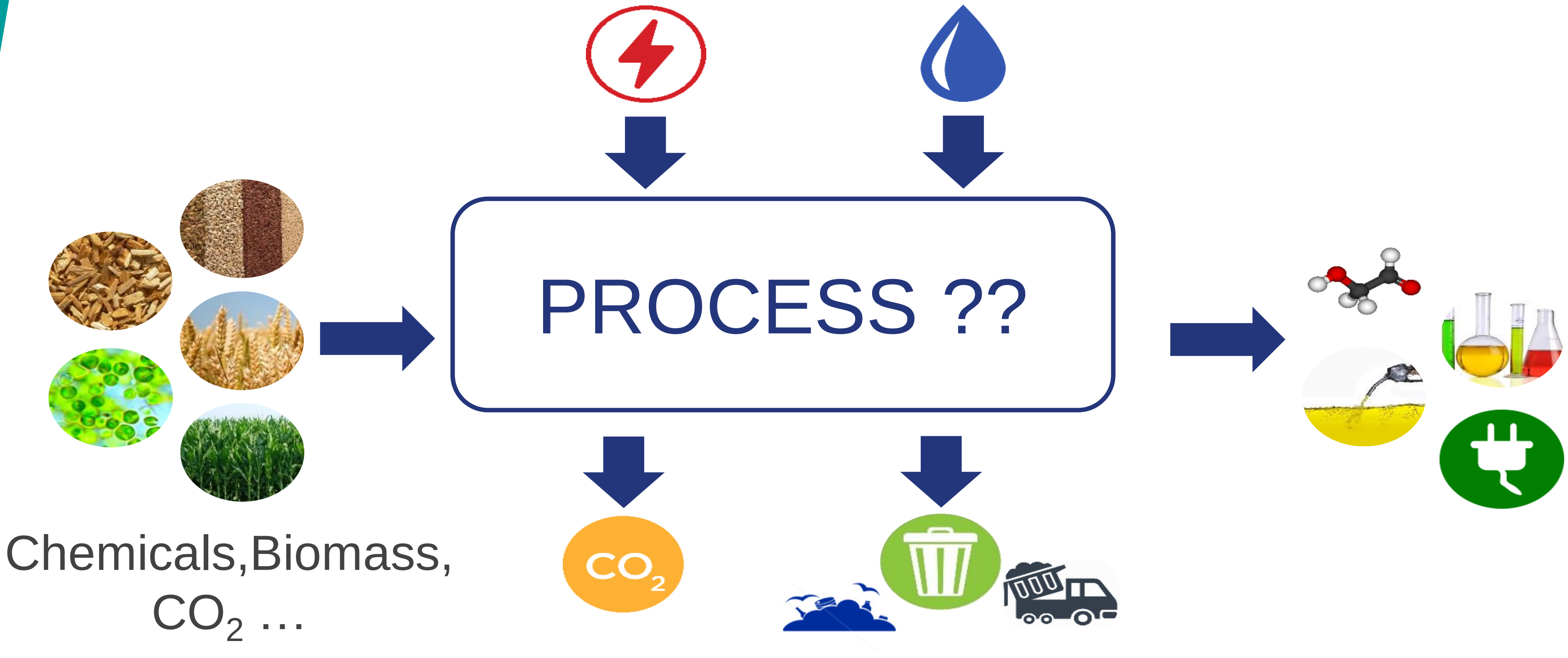
related to process

Chemical Product-Process Design & Application



Integrate Process-Product & Application

Chemical Process Synthesis-Design



- New process design objectives and constraints
- Discovery of new technologies (catalysts, solvents, etc.)
- Switch to renewable raw materials (biomass, CO_2)
- ……..

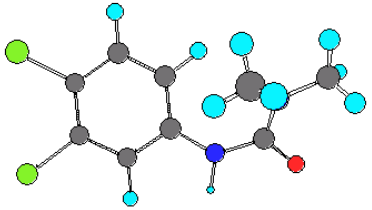
3. Mathematical Problem Formulation

Need & role of models

Generic formulation

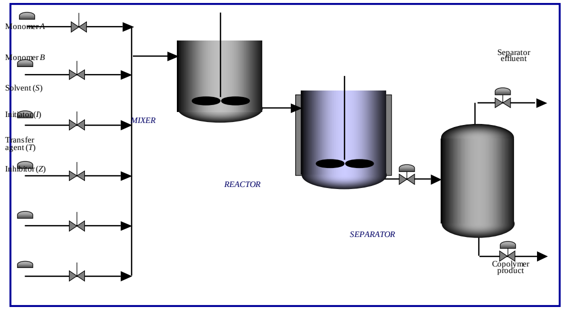
Various problem formulations

Model Types & Their Role (Verification-Test)



Property models

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



Process models

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

Operation models

Models for environmental impact

Process models

Property-kinetics models

Models for sustainability metrics

Cost models

Formulation process model

Product evaluation model

Mathematical (Generic) Problem Formulation

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

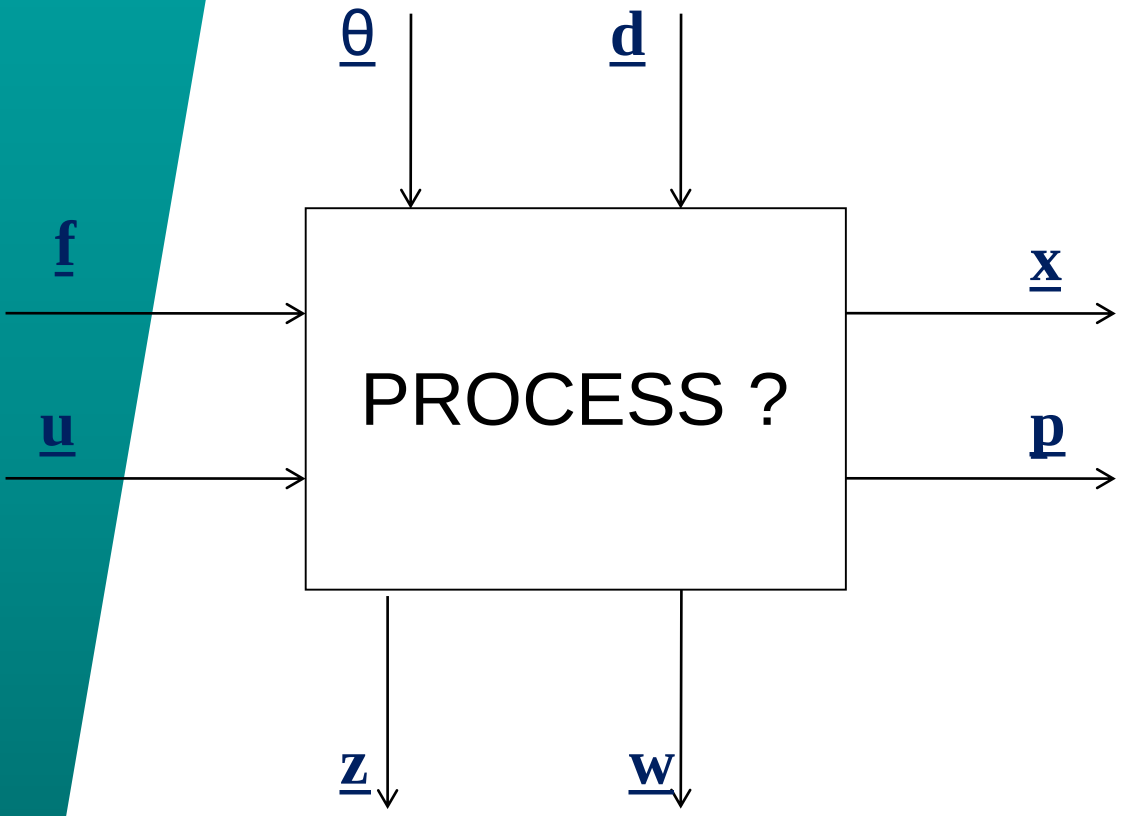
$l_2 \leq g_2(\underline{x}, \underline{y}) \leq u_2$ **molecular structure constraints (Eq. 6)**

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

Sustainable Product-Process Engineering, Evaluation & Design

Synthesis-Design Issues

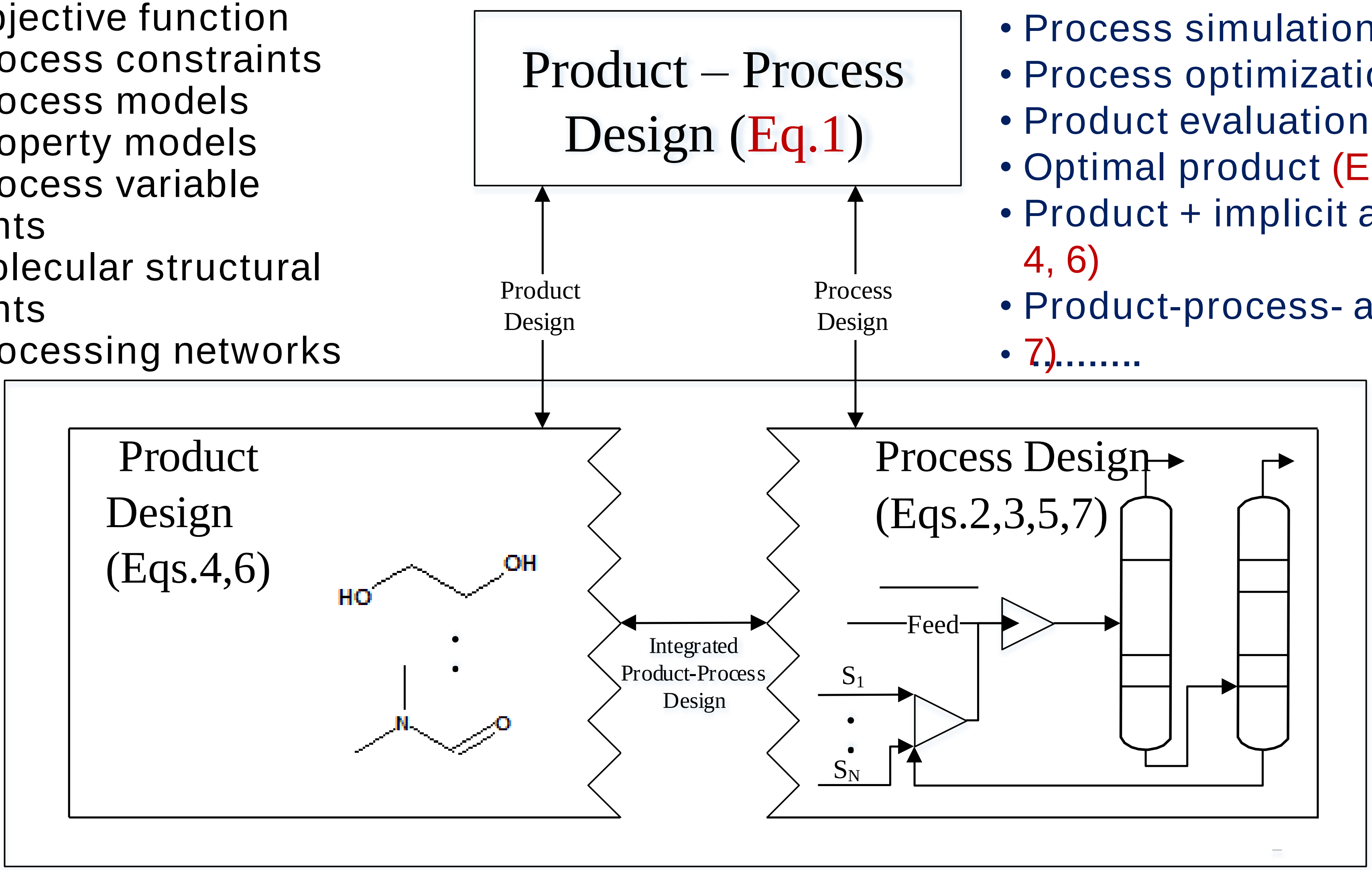


- Which raw materials to use (y, f)
- Which products to make (y, p)
- Which utilities (y, u)
- How many processing steps (y)
- For each processing step, how many alternatives (y)
- Values of process variables (x)
- Process design specifications (d)
- Model parameters (θ)
- How much waste (w)
- How un-utilized utilities (z)
- ……..

Y: decision variables;
Others: real variables

Different Problem Formulations

Eq. 1: Objective function
Eq. 2: Process constraints
Eq. 3: Process models
Eq. 4: Property models
Eq. 5: Process variable constraints
Eq. 6: Molecular structural constraints
Eq. 7: Processing networks



- Process simulation (Eq 3)
- Process optimization (Eq 1-3)
- Product evaluation (Eq 4, 6)
- Optimal product (Eq 1, 4, 6)
- Product + implicit application (Eq 3, 4, 6)
- Product-process- application (Eq. 1-7)
- ……….

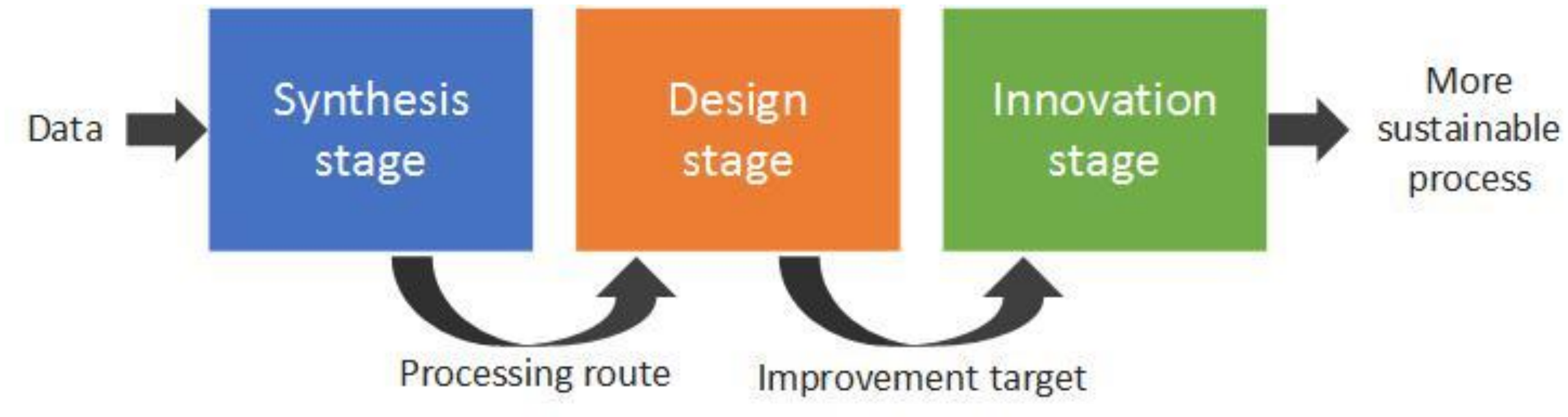
Simultaneous Product – Process Design (multiscale & multidiscipline)

4. Solution Approach

Decomposition based approach

Multi-stage sustainable design

3-Stages Innovative Design Methodology



- Synthesis Stage (find optimal processing route to convert raw materials to desired product)
- Design Stage (perform dtailed process simulation, analyses and identify targets for improvement)
- Innovation Stage (find new alternatives that match the targets for improvement)

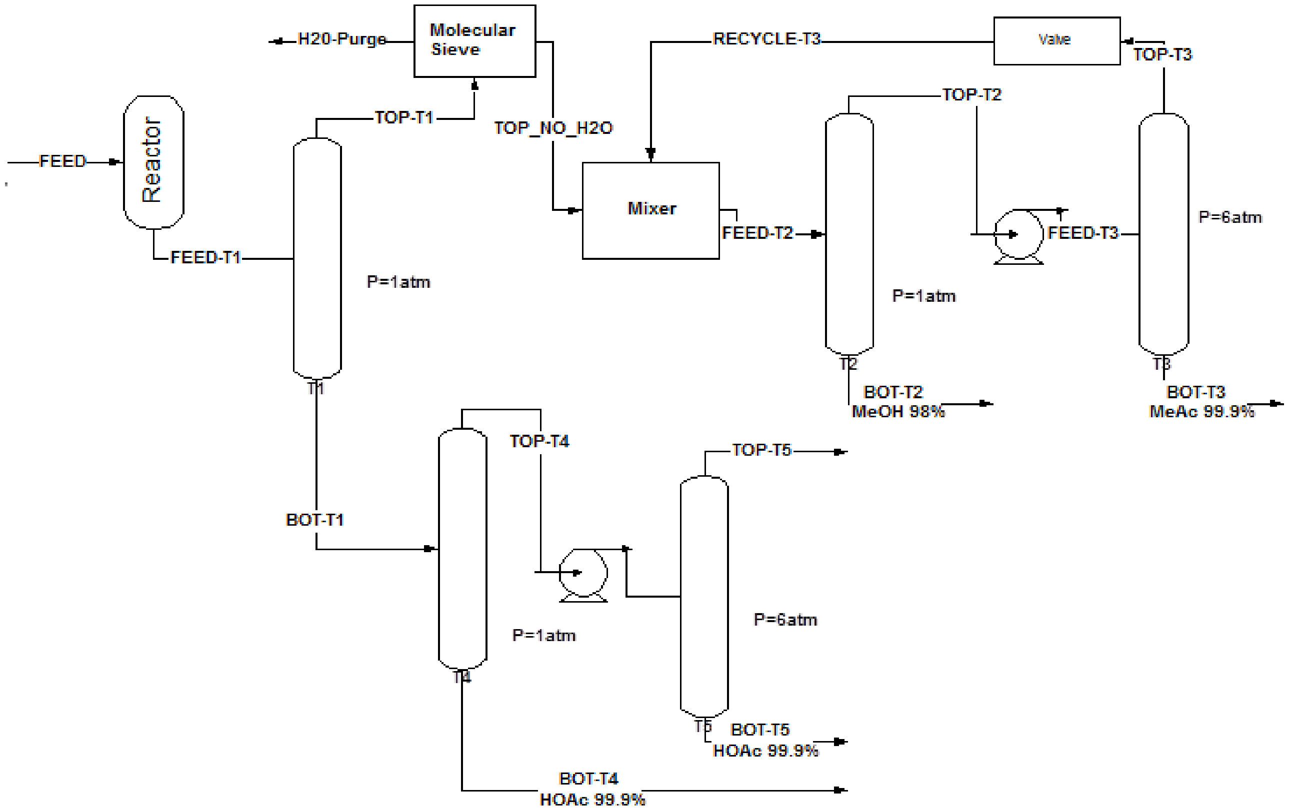
Stage-1: Generate & Test - Synthesis of processing routes-1

Step 1: Analyze problem

Step 2: Find building blocks to generate flowsheets

Step 3: Enumerate & rank all feasible flowsheets

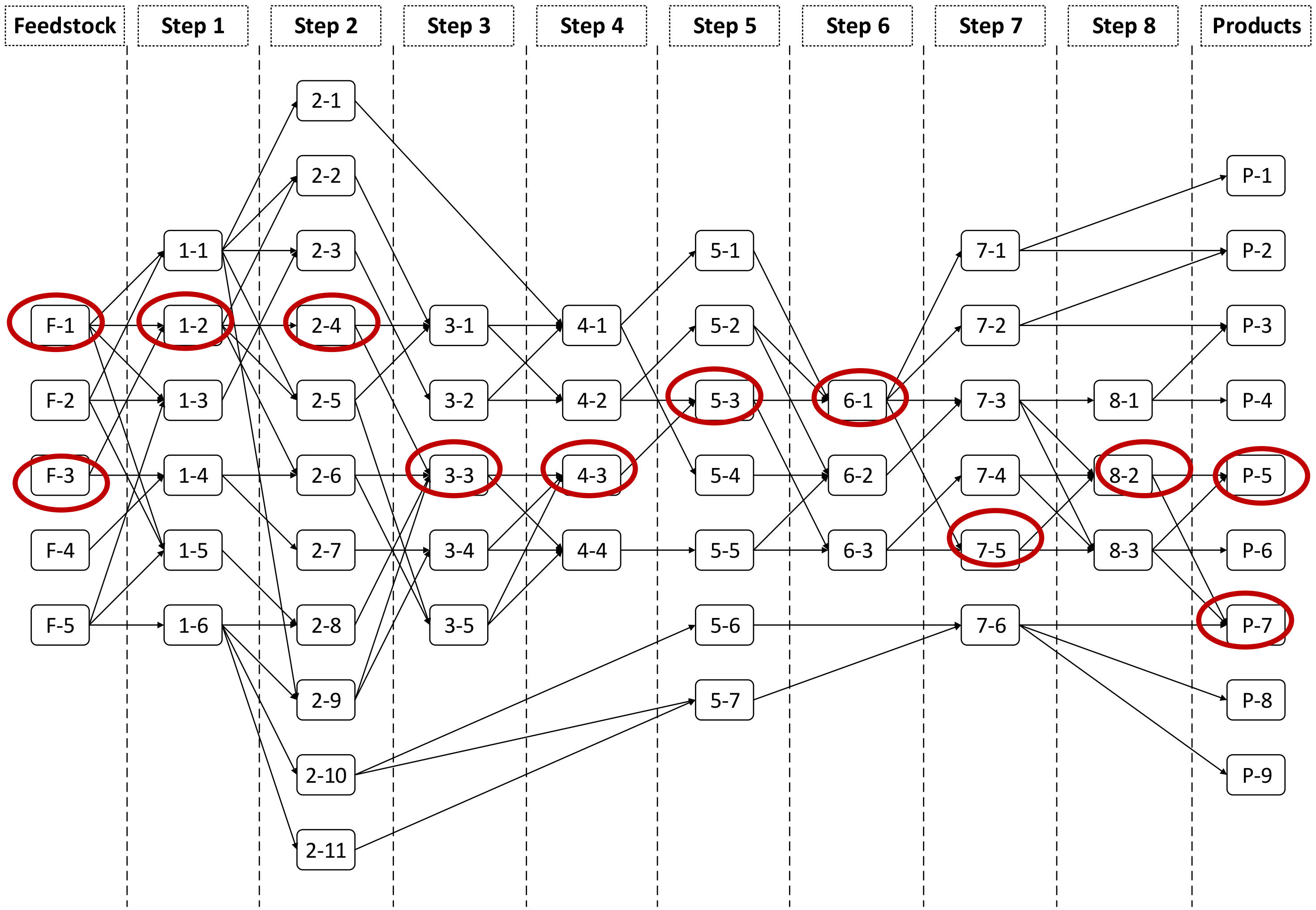
Step 4: Select highest ranked for detailed test



Advantage: Generates all possible flowsheets; identify the best very rapidly; can generate superstructure; apply also mathematical programming

Disadvantage: search space defined by known technologies only; needs a lot of data and/or predictive models

Stage-1: Generate & Test - Synthesis of processing routes-2



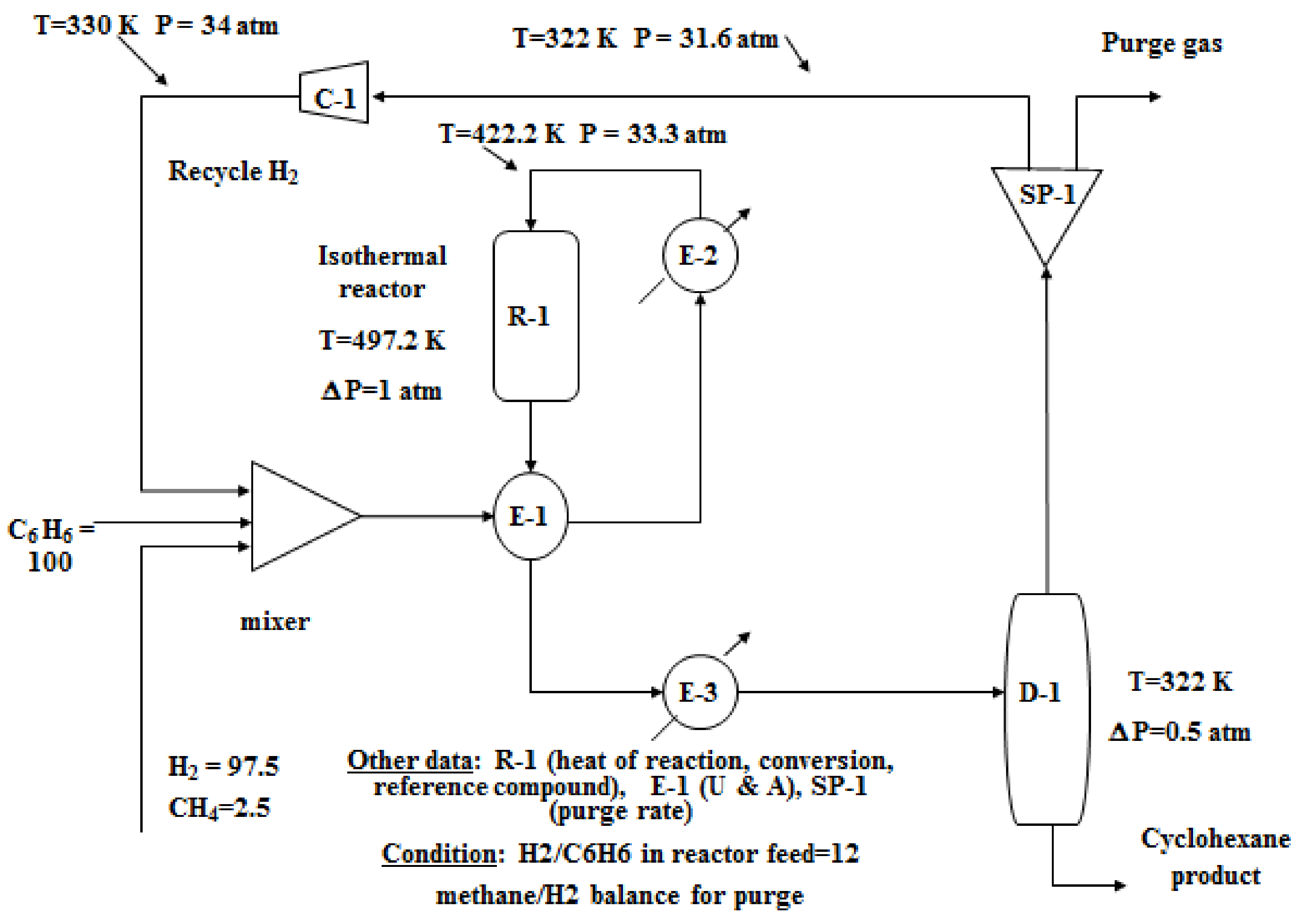
- **Represent alternatives as a network (superstructure)**
- **Develop mathematical models for the network**
- **Solve the mathematical programming problem**

Similar in concept to enumeration based method but employs mathematical programming techniques; can also employ enumeration & test

Design stage-2: Detailed design & analysis

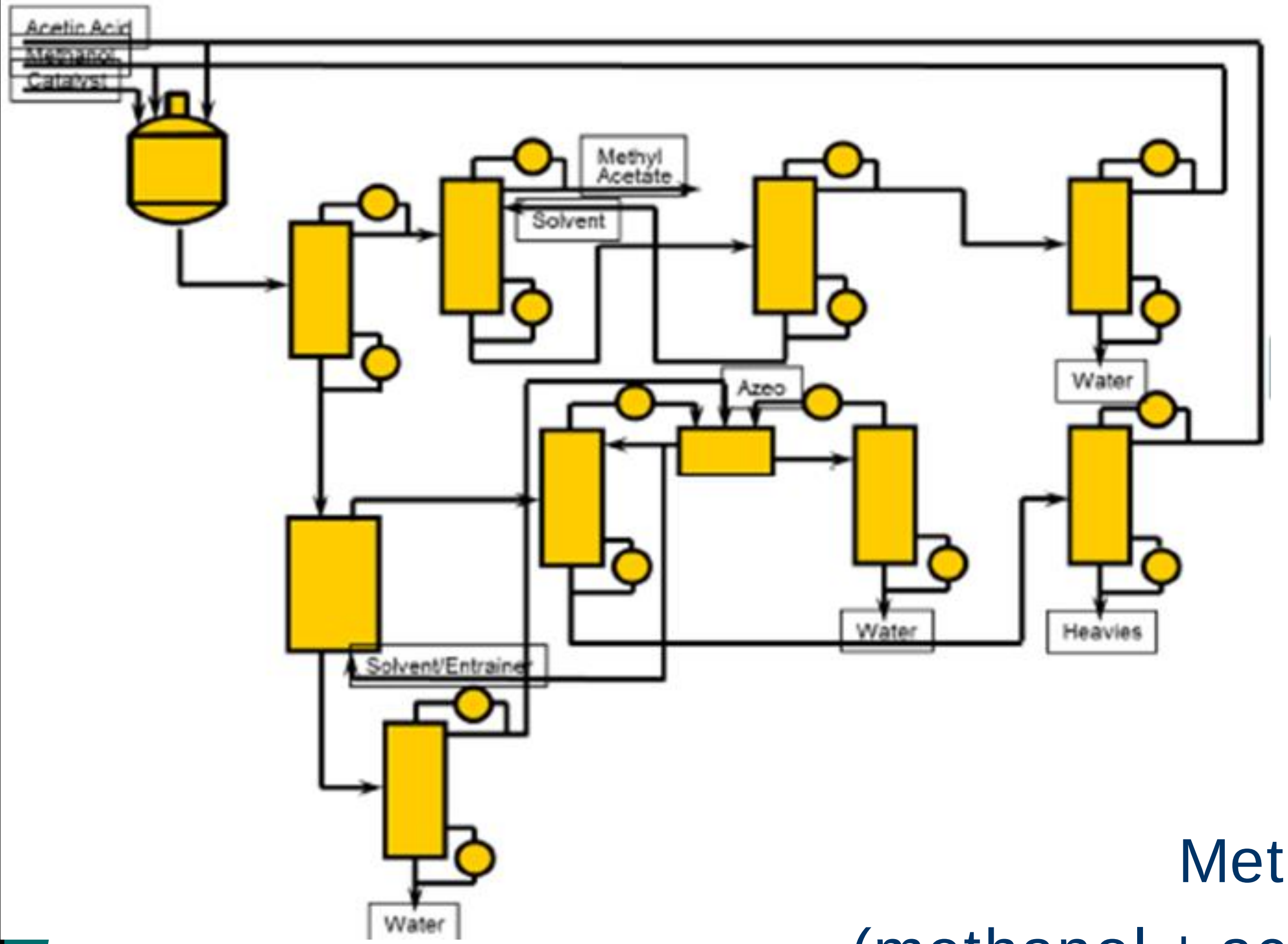
Perform detailed design calculations on the identified flowsheet

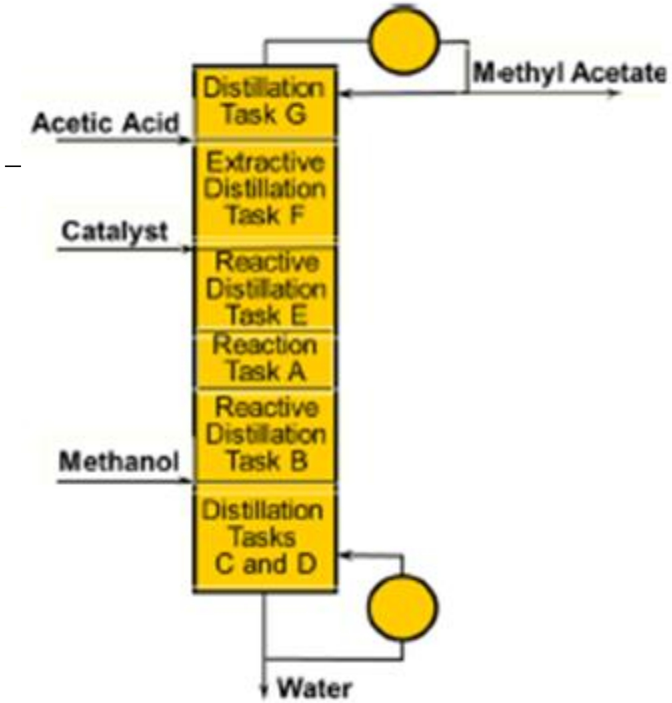
Flowsheet for cyclohexane production

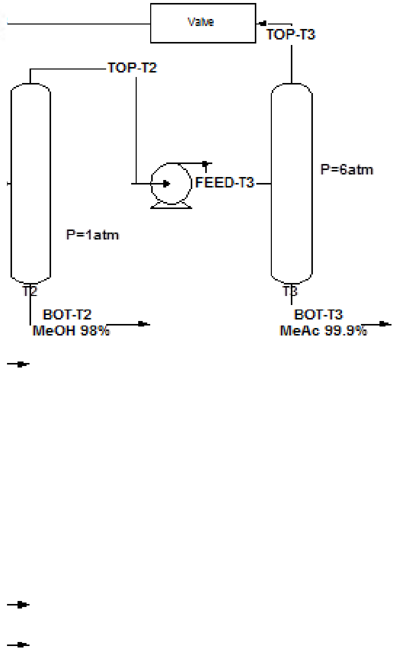


- **Determine the design variables of each task**
- **Perform analysis (economic; sustainability; LCA assessment)**
- Identify "process **hot-spots**"
- **Define targets for process improvement**

Stage-3: Innovative solution through process intensification





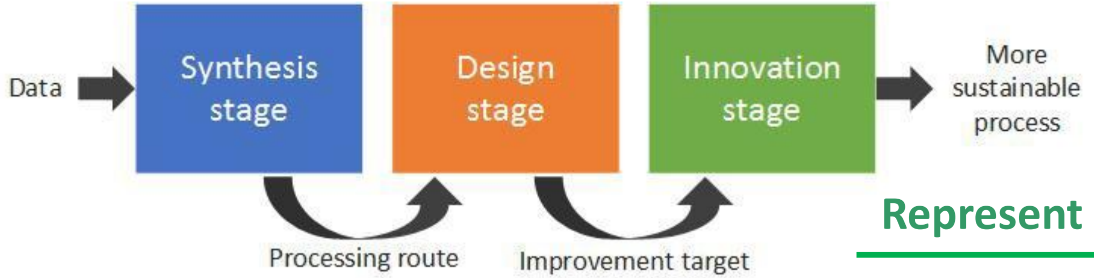


Methyl acetate production

(methanol + acetic acid = methyl acetate + water

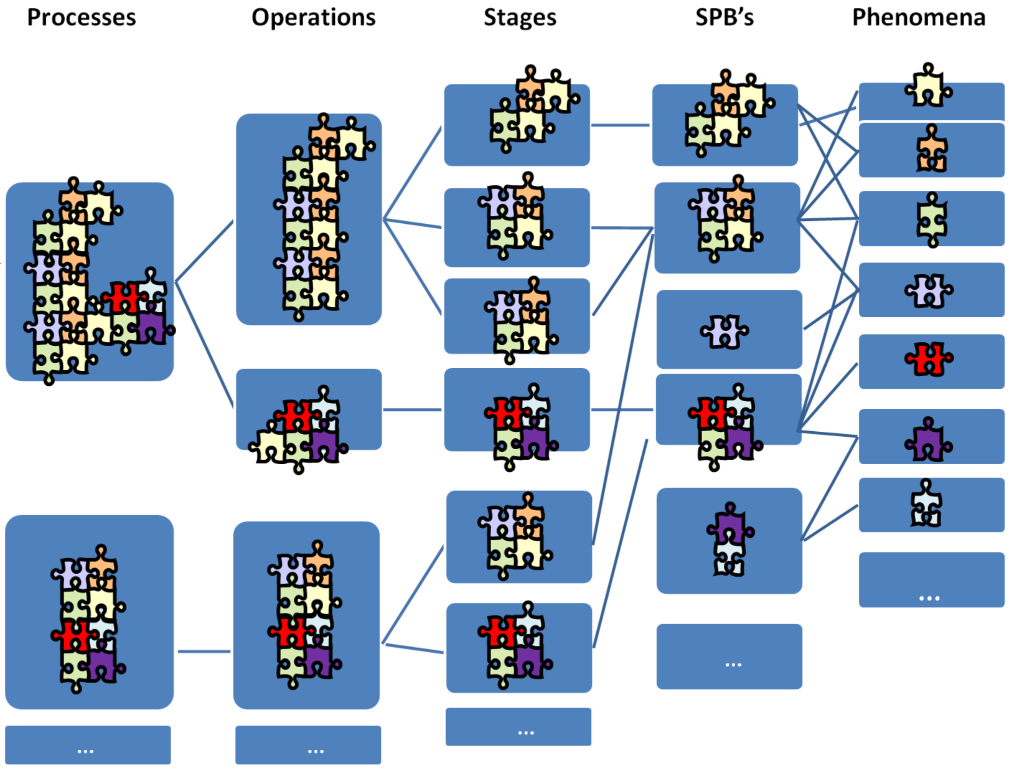
(Eastman Chemicals, Siirola, 1988)

S3: Sustainable process synthesis-design-intensification



CACE, PI-special issue, 2017; CACE, 81, 2015)

Represent base case process wrt to operations to phenomena



Recombine the phenomena to generate new intensified options

Intensification method:

Starting with a base case design (synthesis stage), set targets for improvement (design stage), generate new intensified options that match design targets and make the process more sustainable (innovation stage)

5a. Application Examples

Process synthesis

Process innovation

Tailor-made blend (product) design

General Problem Definition - Superstructure

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

Process model

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

Process constraints

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

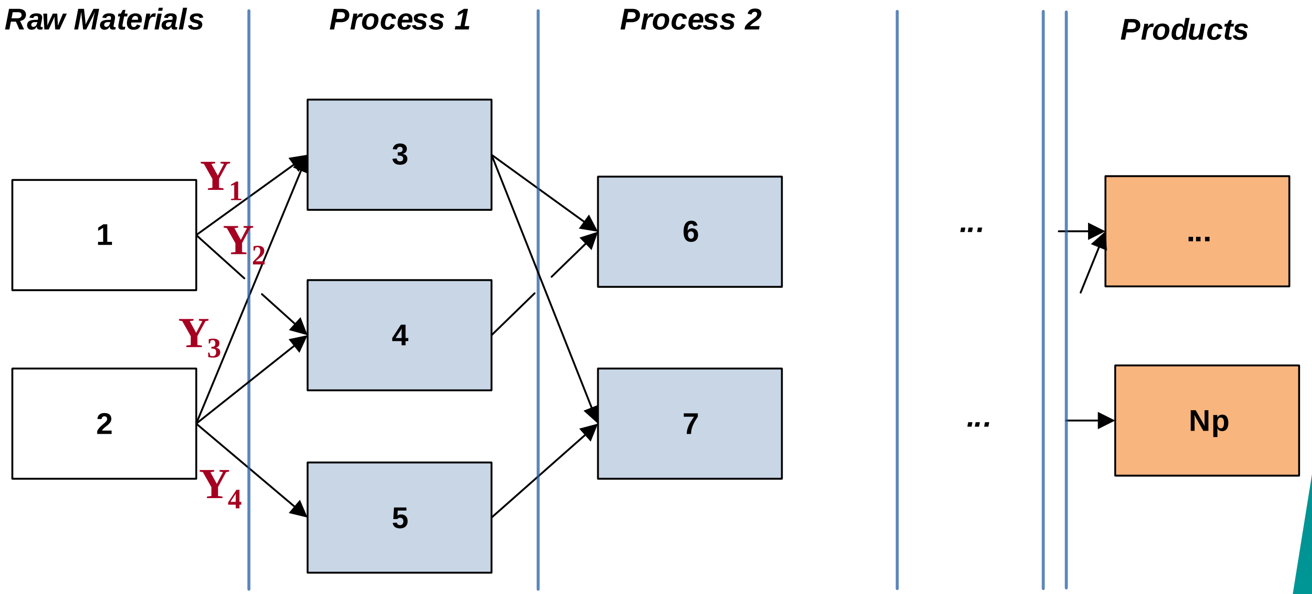
Equipment constraints

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

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

Flowsheet alternatives

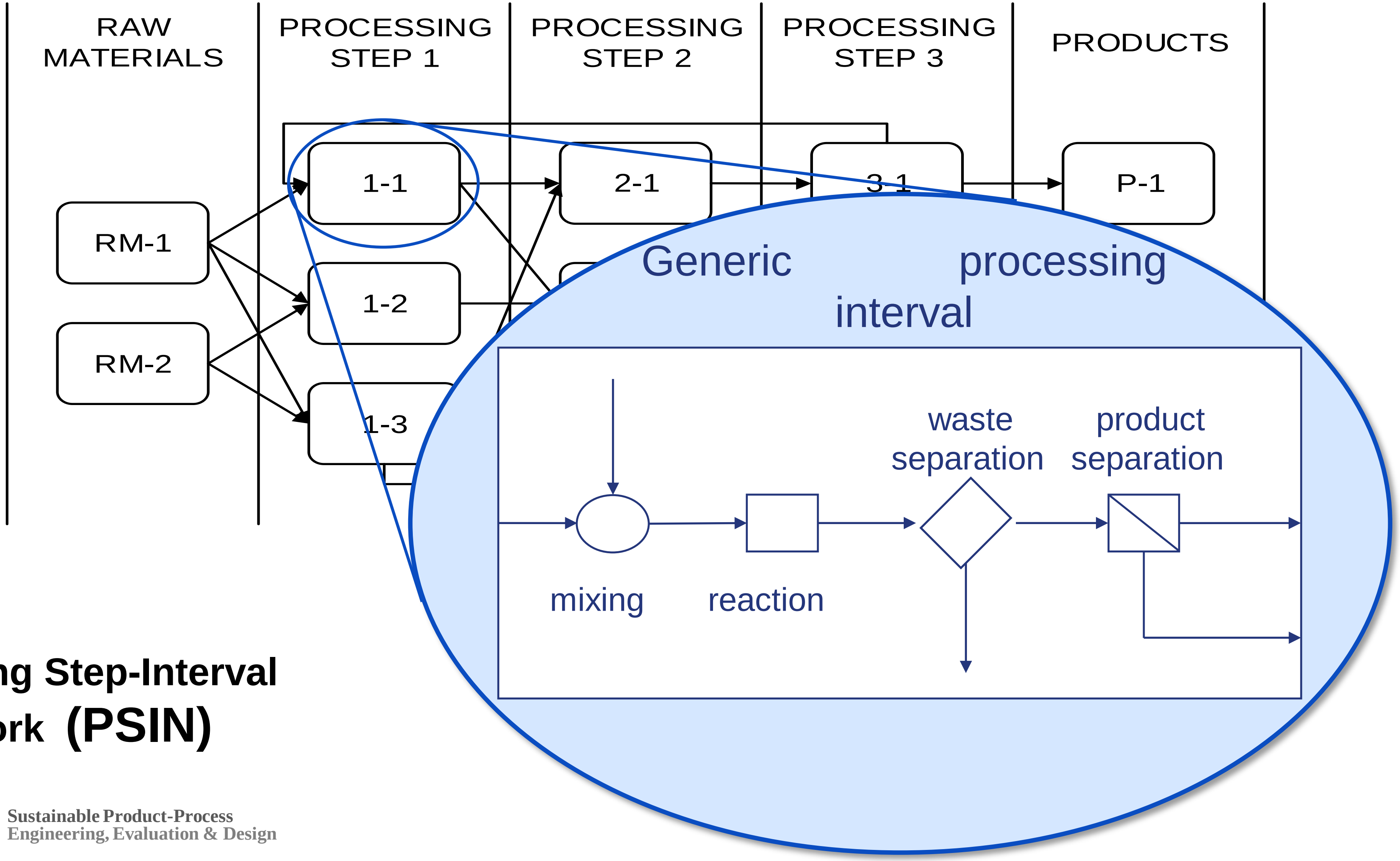
$$B\,\underline{x} + C^T\underline{y} \geq D$$



$\Sigma Y_i = 1$ or $1 \geq \Sigma Y_i \leq 2$ or set $Y_2 = 0$

Generic superstructure representation & model

The Processing Step-Interval Network representation is suitable for a wide range of problems



Processing Step-Interval Network (PSIN)

Optimization Problem

A generic process model can represent multiple process options at various scales

Objective function

$$Z = S^{PROD} - C^{RAW} - C^{C} - C^{U} - C^{T} - CAPEX/\tau$$

$$S^{PROD} = \sum_{l}\sum_{k}\sum_{i} P^{PROD}_{k,l} f^{W}_{i,k} \qquad C^{RAW} = \sum_{l}\sum_{k}\sum_{i} P^{RAW}_{k,l} f^{W}_{i,k} \qquad C^{C} = \sum_{l}\sum_{k}\sum_{i} P^{C}_{i,l} g^{M}_{i,k} \qquad C^{U} = \sum_{l}\sum_{k}\sum_{ut} P^{U}_{ut,l} f^{UT}_{ut,k}$$

Process interval model

$$g^{M}_{i,k} = \sum_{ii} f^{IN}_{ii,k} \mu_{i,ii,k}$$

$$f^{M}_{i,k} = f^{IN}_{i,k} + g^{M}_{i,k}$$

$$f^{R}_{i,k} = f^{M}_{i,k} + \sum f^{M}_{react,k} \theta_{react,r,k} \gamma_{i,r,k} MW_{i}/MW_{react}$$

$$f^{W}_{i,k} = f^{R}_{i,k}\left(1 - \delta_{i,k}\right)$$

$$g^{W}_{i,k} = f^{R}_{i,k} - f^{W}_{i,k}$$

$$f^{OUT,1}_{i,k} = f^{W}_{i,k} \sigma_{i,k}$$

$$f^{OUT,2}_{i,k} = f^{W}_{i,k} - f^{OUT,1}_{i,k}$$

$$g^{U,1}_{ut,k} = \sum_{i} \beta^{1}_{ut,k} f^{IN}_{i,k}$$

Composition, availability and demand constraints

$$f^{W,LOC}_{i,k,l} = \phi_{i,k,l} F^{RAW}_{k,l}$$

$$F^{RAW}_{k,l} = \sum_{i} f^{W,LOC}_{i,k,l}$$

$$\sum_{i} F^{W,LOC}_{i,k,l} \leq AVAIL_{k,l}$$

$$\sum_{i} F^{W,LOC}_{i,k,l} \leq DEM_{k,l}$$

$$f^{P}_{i,k,kk}$$

$$f^{S}_{i,k,kk}$$

Superstructure connections

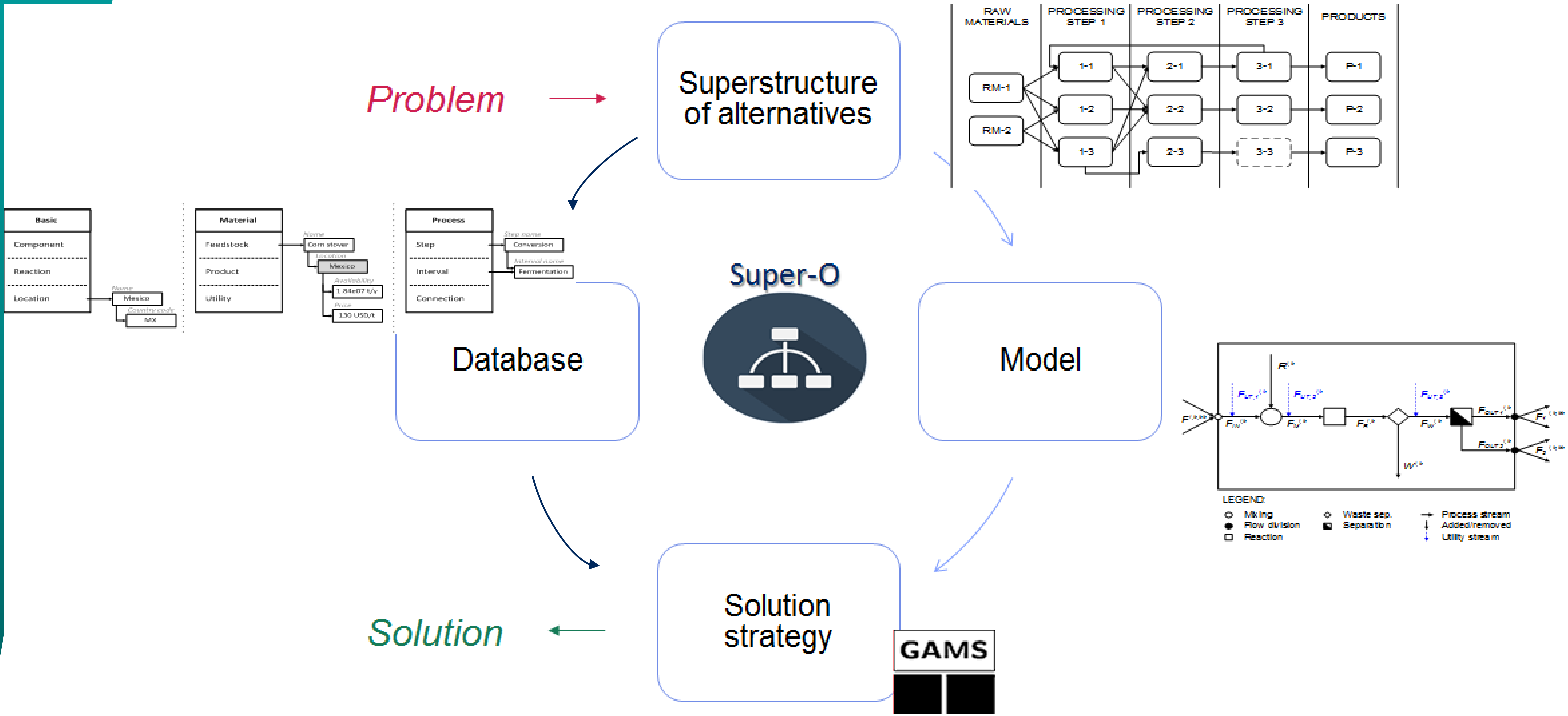
$$f^{1}_{i,k,kk} \leq f^{OUT,1}_{i,k} S^{P}_{k,kk}$$

$$f^{2}_{i,k,kk} \leq f^{OUT,2}_{i,k}\left(S_{k,kk} - S^{P}_{k,kk}\right)$$

Location dependent / Location independent

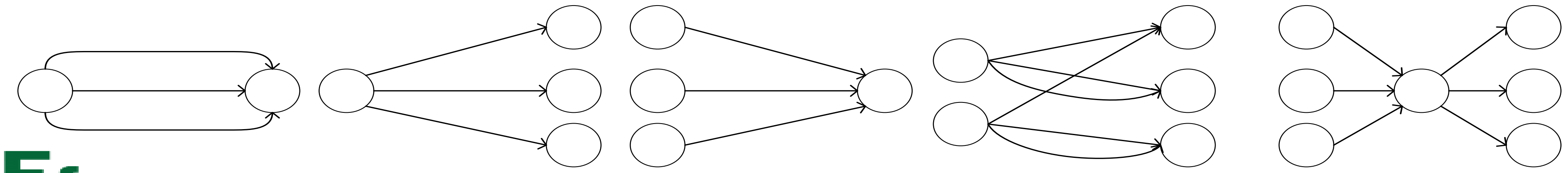
Synthesis Framework & Super-O (software)

Super-O: An interface for formulating and solving synthesis problems using superstructure optimization



Overview of problems & applications

Case (problem type)	Problem size							Model size		Reference
	NF	NP	NI	NC	NU	NR	NL	NEQ	NV (NDV)	
Network benchmark problem (d)	2	4	12	5	-	2	1	3,476	3,235 (120)	Quaglia et al. (2012)
Wastewater network (d)	2	6	24	15	-	37	1	112,147	108,742 (74)	Handani et al. (2014)
Sugarcane molasses biorefinery (b)	1	3	32	12	-	26	1	76,360	73,141 (52)	Bertran et al. (2015a)
DMC from CO_2 (a)	1	5	16	11	-	7	1	8,546	7,985 (26)	Frauzem et al. (2015)
Biodiesel biorefinery (d)	3	6	46	27	-	91	1	1,210,227	1,193,507 (182)	Bertran et al. (2015b)
MeOH, DME, DMC from CO_2 (b)	1	8	13	16	-	14	1	51,373	49,573 (60)	-
Bioethanol biorefinery (c)	6	1	35	34	3	47	7	175,383	162,798 (1,330)	Bertran et al. (2017)



(a) (b) (c) (d) (e)

Overview of problems & applications

The framework is applicable to a number of problem types across various application areas

	Process synthesis	Supply chain	Feed/product selection	Plant allocation	Equipment selection	Process retrofit	Blending
Chemical processes	☆		☆		☆		☆
Biorefineries	★	★	★	★			
Oil & Gas							
Pharma processes							
CO_2 utilization	☆		☆				
Wastewater management	☆				☆		

5b. Software Tools & Application Examples

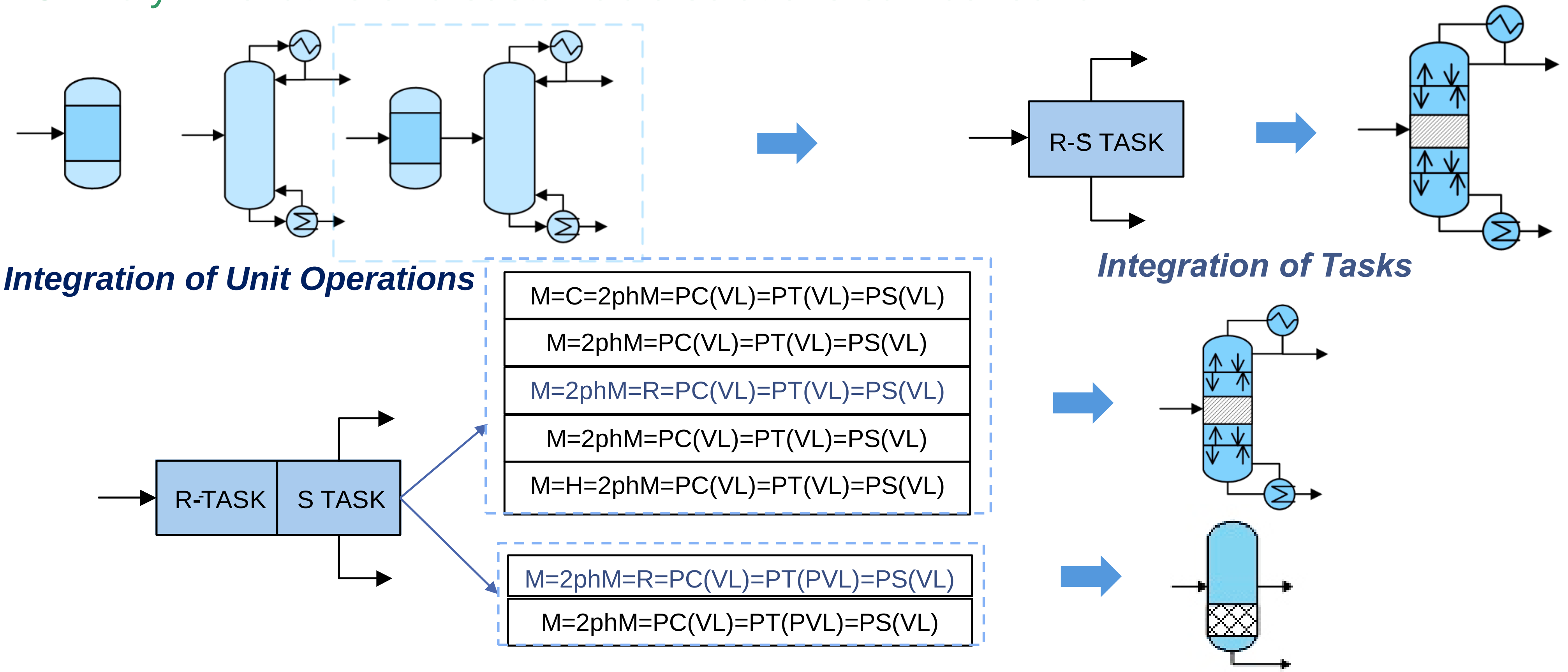
Process synthesis

Process innovation

Tailor-made blend (product) design

Integration: Process synthesis + Process intensification

- Performing Process Synthesis-Design and Process Intensification together in the early stages of process design
- Current search space of unit operations is extended by generating new unit operations
- Truly innovative and sustainable solutions can be found



*Integration and/or enhancement of phenomena**

Conversion of tasks to phenomena

R, M_I, M_T, M_R M_V, 2phM, PC(V-L), PT(V-L), PT(P:V-L), PS (V-L), D, H, C
13 in total

Reduced from 4017→58 using connectivity rules

Connectivity Rules:

1. **H+C should not exist in the same SPB**
2. **PC phenomena exists together with PT phenomena**
3. **SPB can contain simultaneous R and separation**

SPB	Interconnection Phenomena	In	Out
SPB.1	M	1..n(L)	1(L)
SPB2	M=R	1..n(L)	1(L)
SPB.7	M=R=2phM=PC=PT(VL)	1..n(L,VL)	1(V/L)
SPB.8	M=R=2phM=PC=PT(VL)=PS(VL)	1..n(L,VL)	2(V;L)
SPB.9	M=R=2phM=PC=PT(PVL)=PS(VL)	1..n(L,VL)	2(V;L)
SPB.58	D	1(L;VL,V)	1..n(L;V; VL)

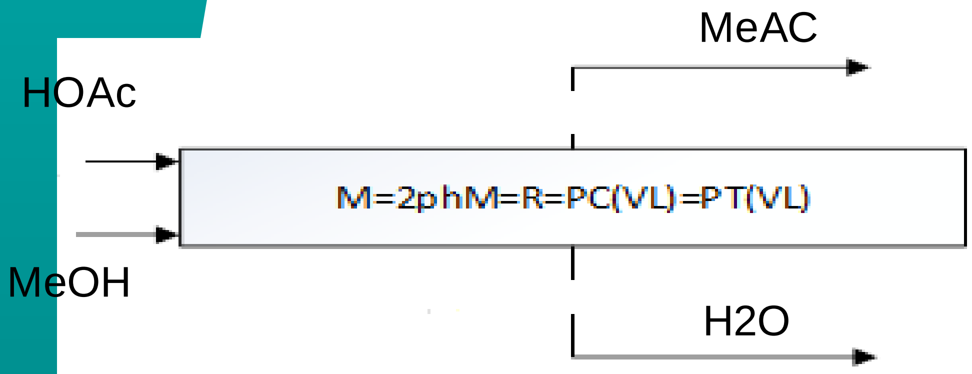
SPB	Interconnection Phenomena	In	Out
	~~M=R=H=C~~	~~1..n(L)~~	~~1(L)~~

SPB	Interconnection Phenomena	In	Out
SPB.7	M=R=2phM=PC=PT(VL)	1..n(L,VL)	1(V/L)

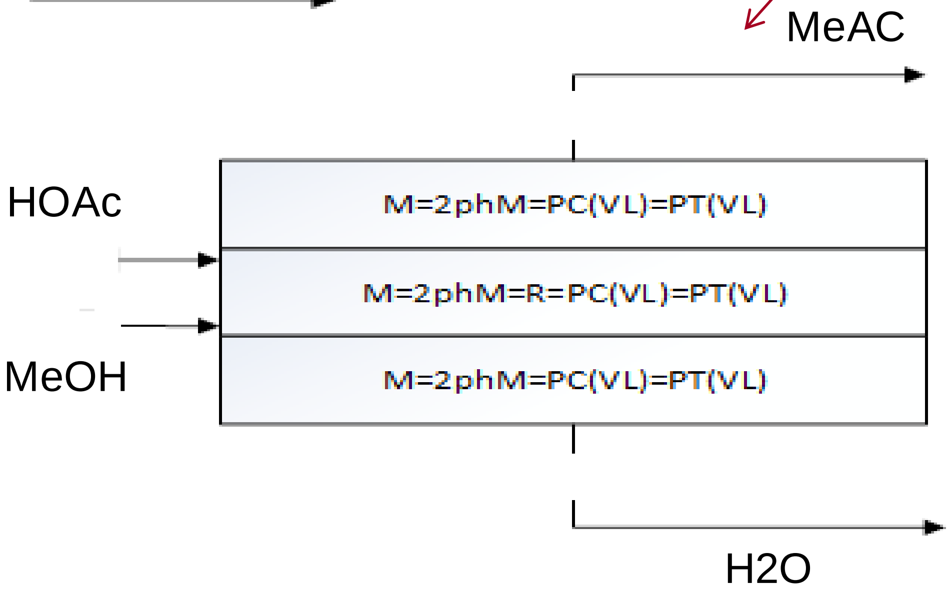
SPB	Interconnection Phenomena	In	Out
SPB.8	M=R=2phM=PC=PT(VL)=PS(VL)	1..n(L,VL)	2(V;L)
SPB.9	M=R=2phM=PC=PT(PVL)=PS(VL)	1..n(L,VL)	2(V;L)

Babi et al. (2015)

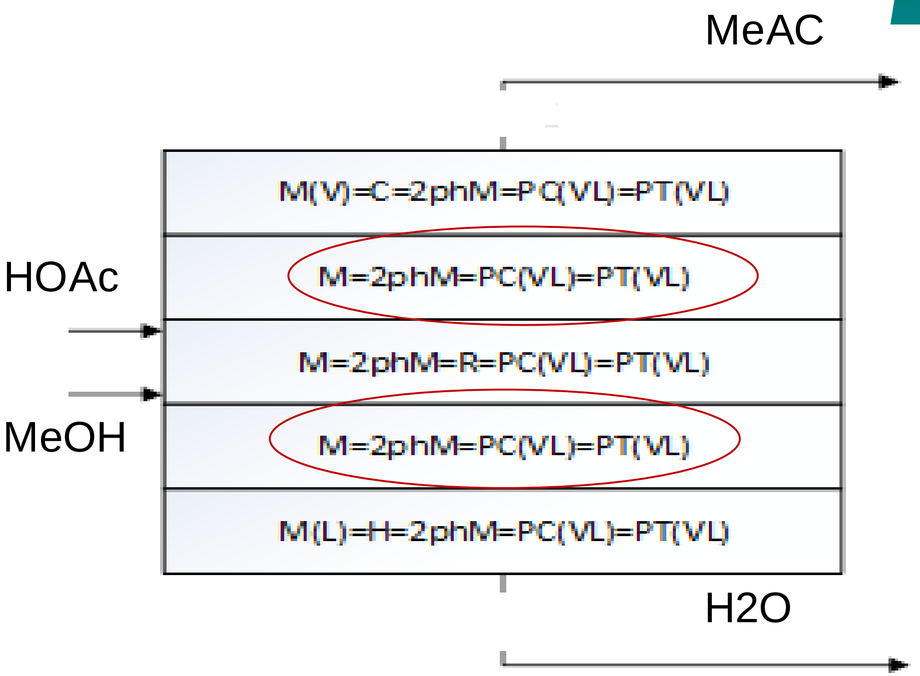
Combine phenomena: New unit operations



*Not feasible**

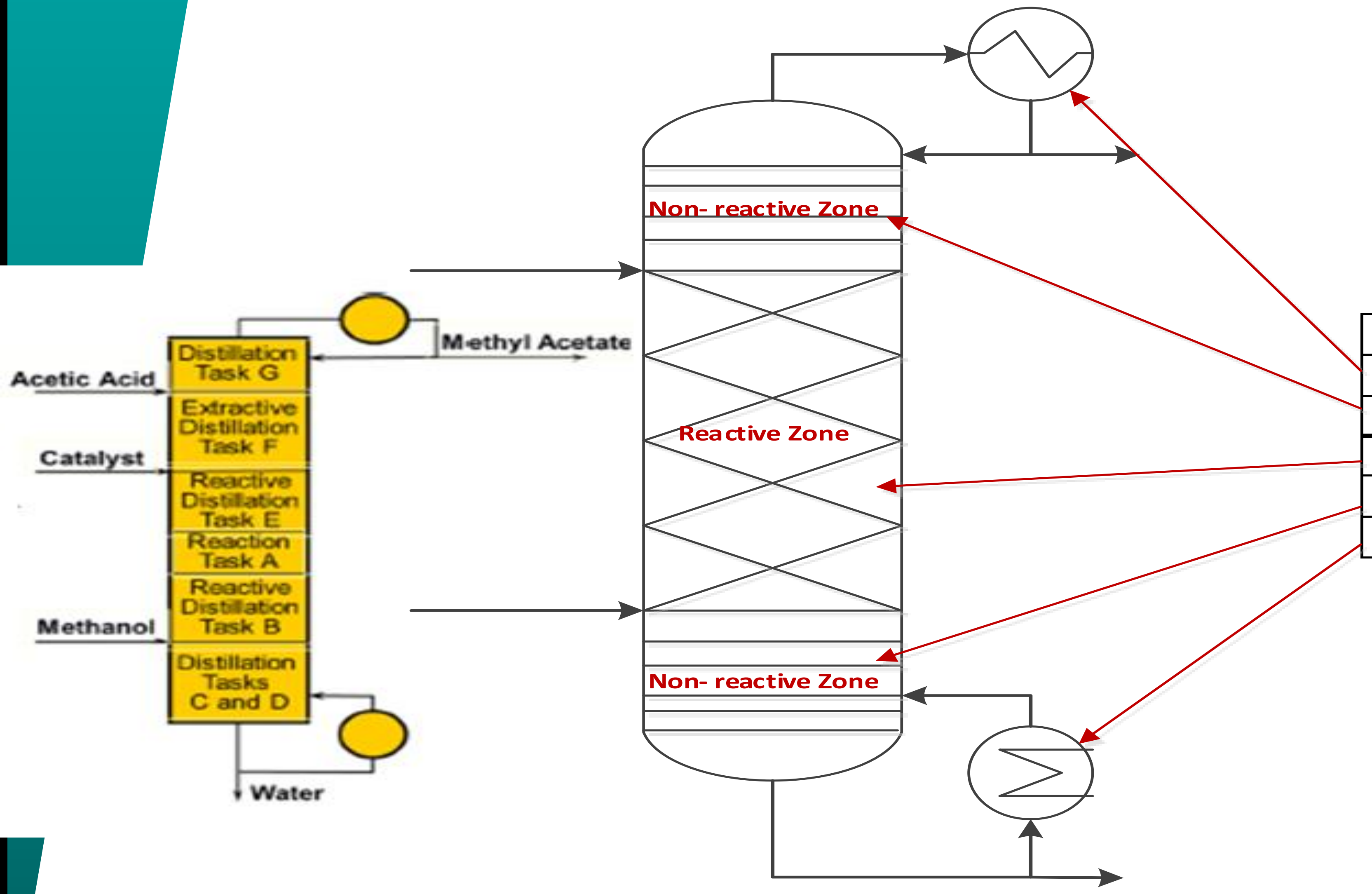


*Feasible**



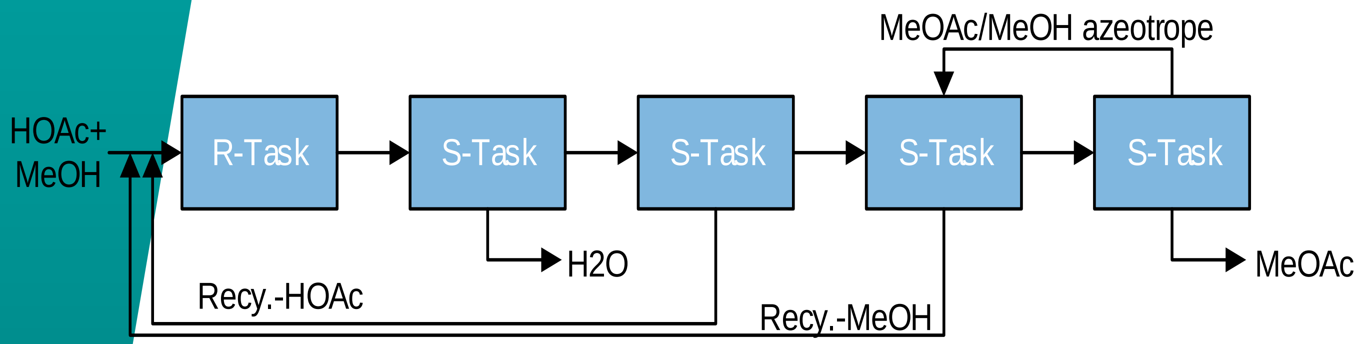
** With respect to defined targets*

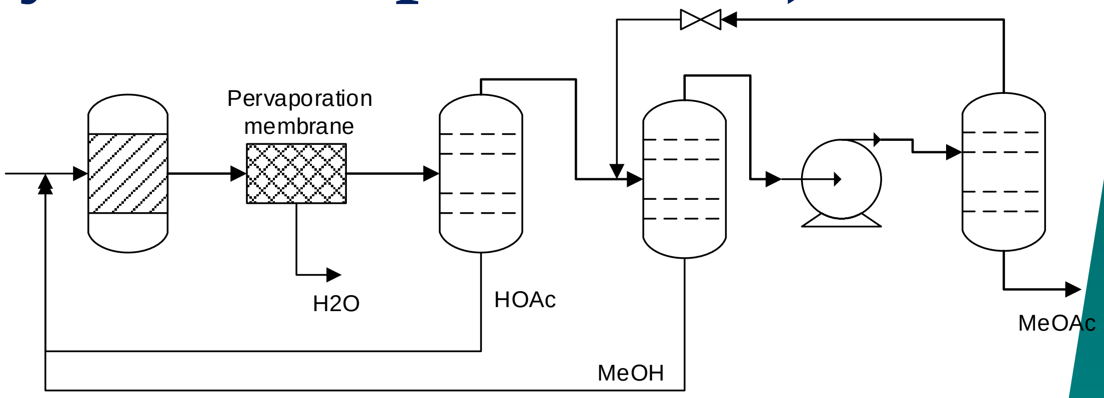
Innovative solution

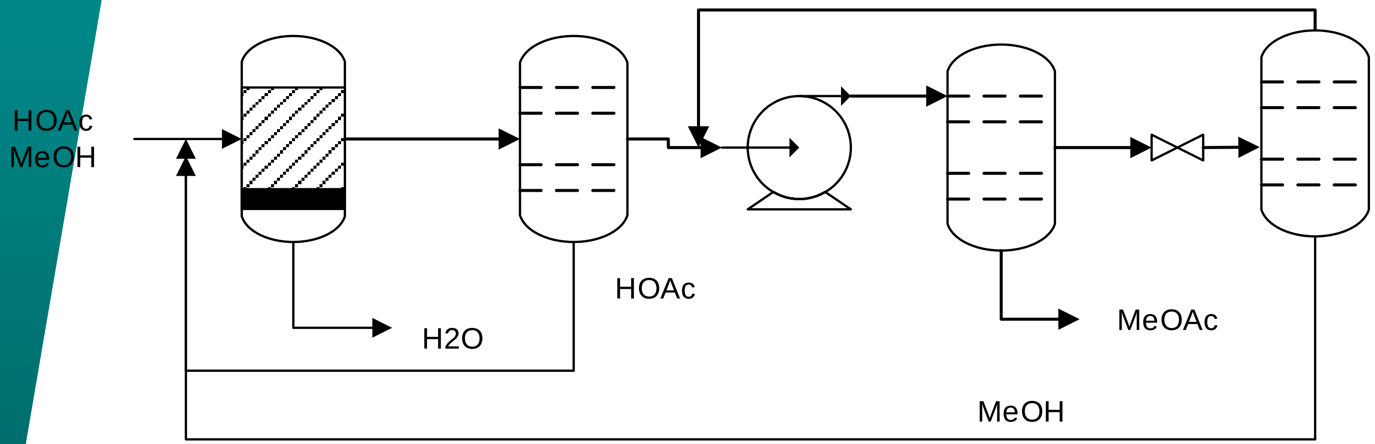


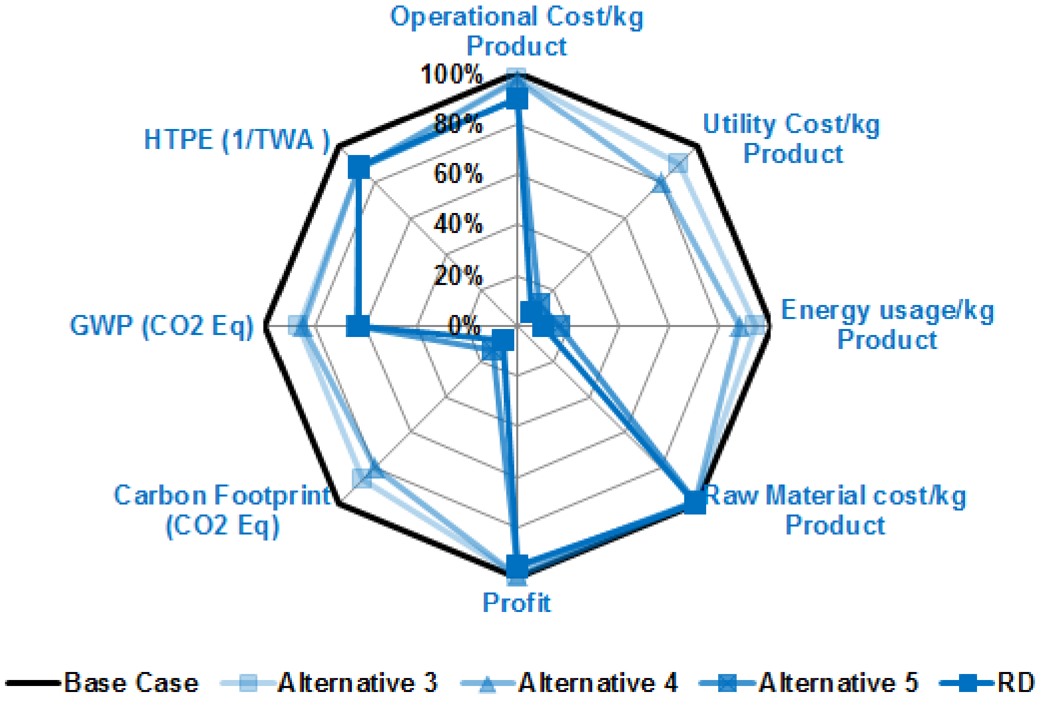
Operation
M(V)=C=2phM=PC(VL)=PT(VL)
M(V-L)=2phM=PC(VL)=PT(VL)
M(V-L)=R=2phM=PC(VL)=PT(VL)=PS(VL)
M(V-L)=2phM=PC(VL)=PT(VL)
M(L)=H=2phM=PC(VL)=PT(VL)

Other intensified options (methyl acetate production)

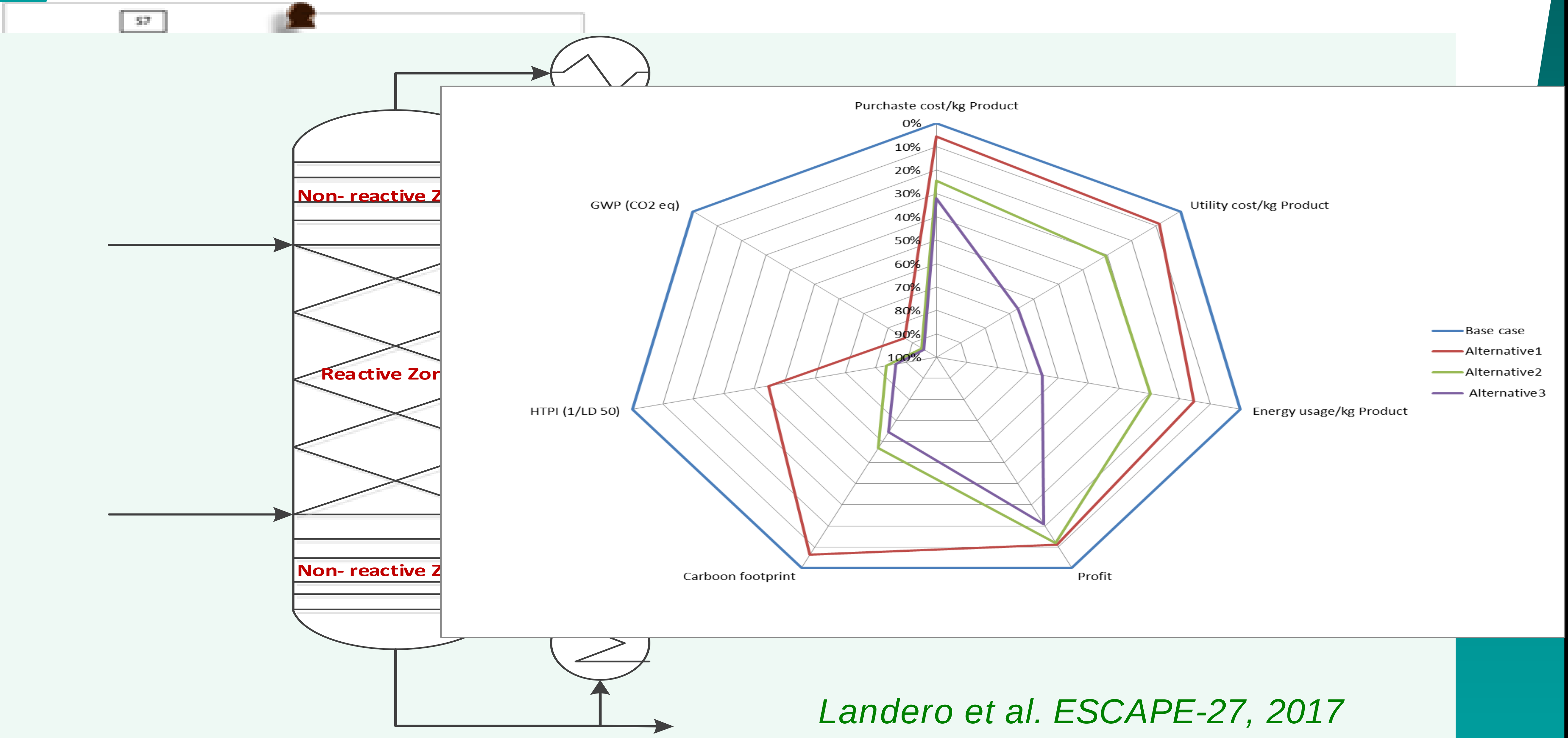








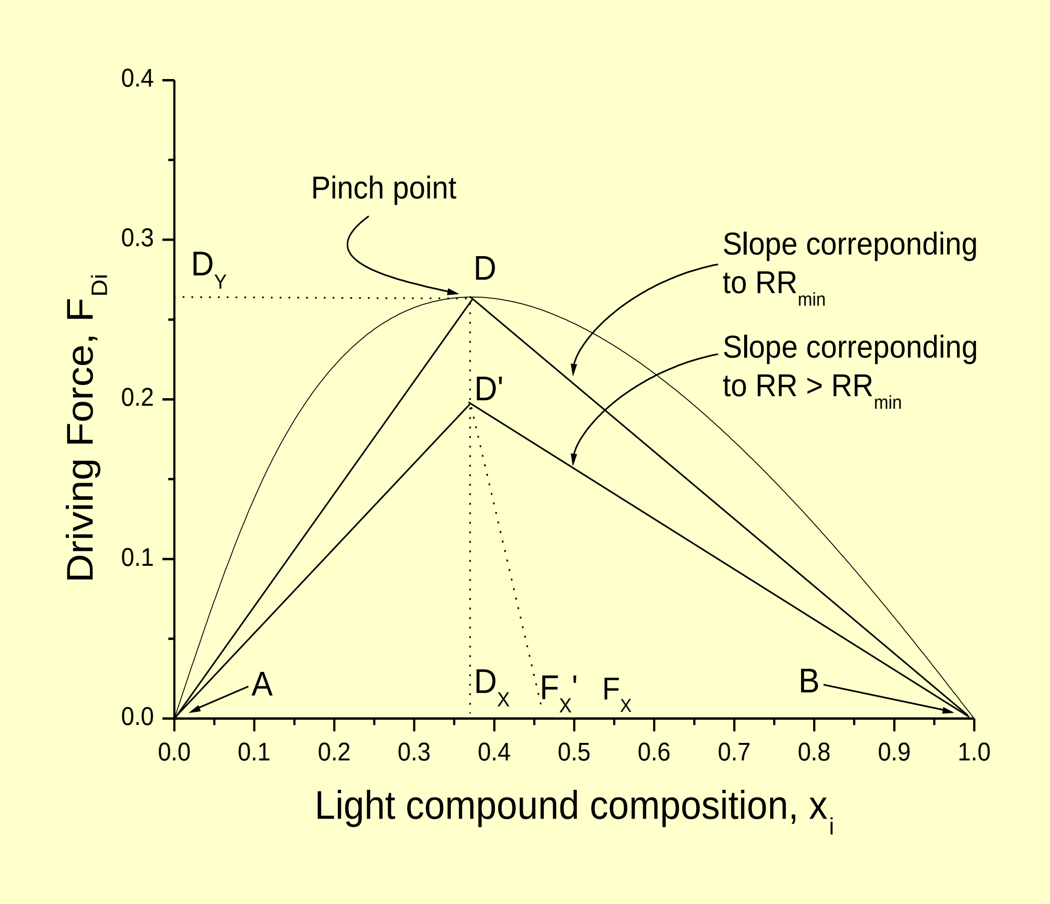
More examples (synthesis of dioxolane products)

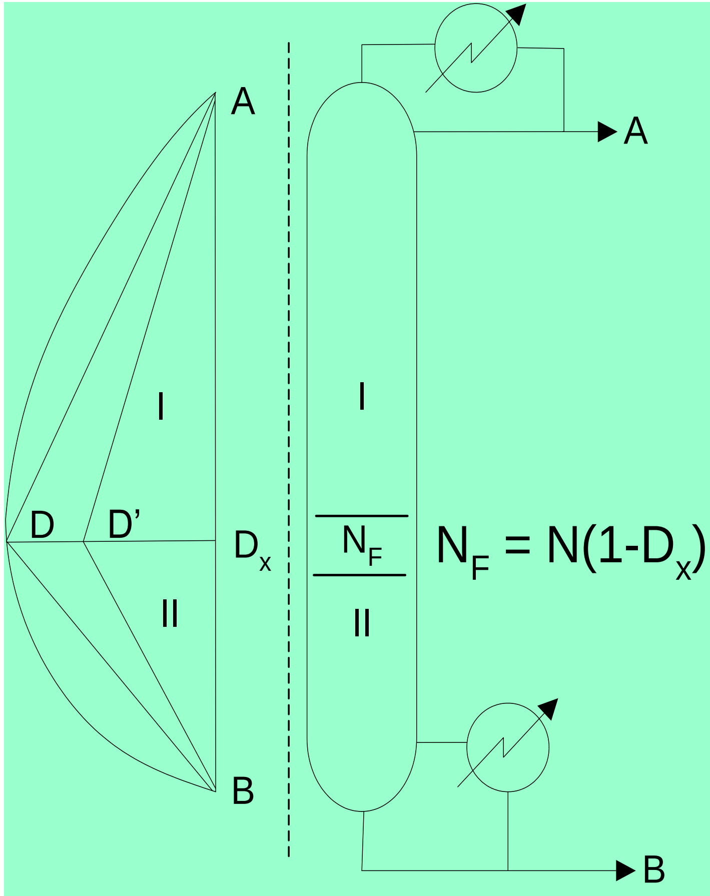


Landero et al. ESCAPE-27, 2017

What about operability and control?

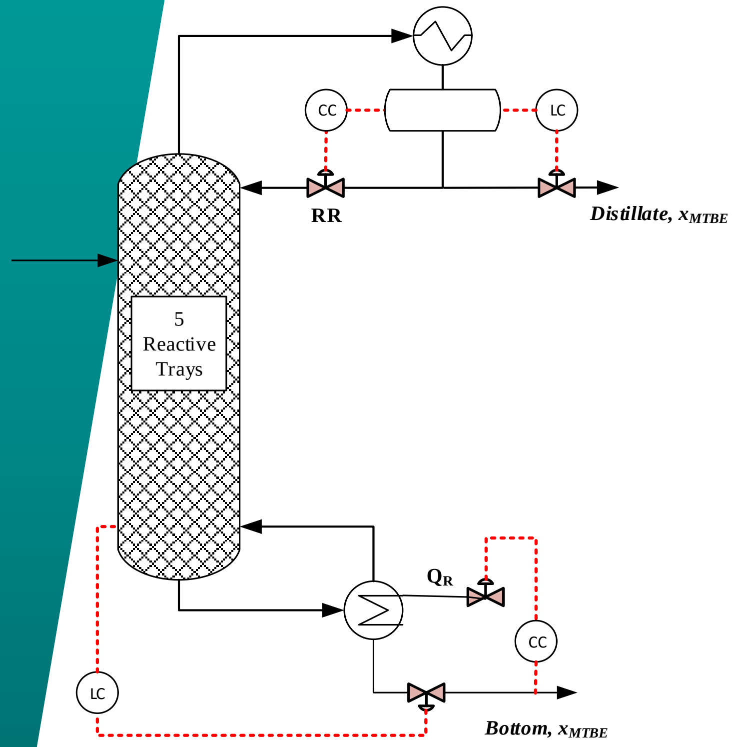
Given a mixture to be separated into two products in a distillation column with N trays. What is the optimal (with respect to the costs of operation) feed plate location and the corresponding reflux ratio for different product purity specifications ?





AIChE J. 1999 (design of distillation)
AIChE J. 2016 (design & control of distillation, including reactive distillation)

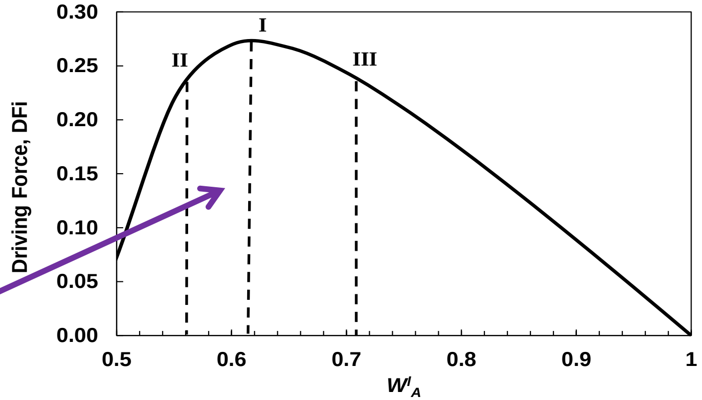
Controller design of reactive distillation columns



- **Controller structure verification**

- Controller structure at the maximum driving force:

$$\frac{dy}{du}=\begin{bmatrix}\frac{dW_A^d}{dRR} & \frac{dW_A^d}{dRB}\\ \frac{dW_A^B}{dRR} & \frac{dW_A^B}{dRB}\end{bmatrix}=\begin{bmatrix}DF_i & 0\\ 0 & -DF_i\end{bmatrix}$$



- The relative gain array (RGA):

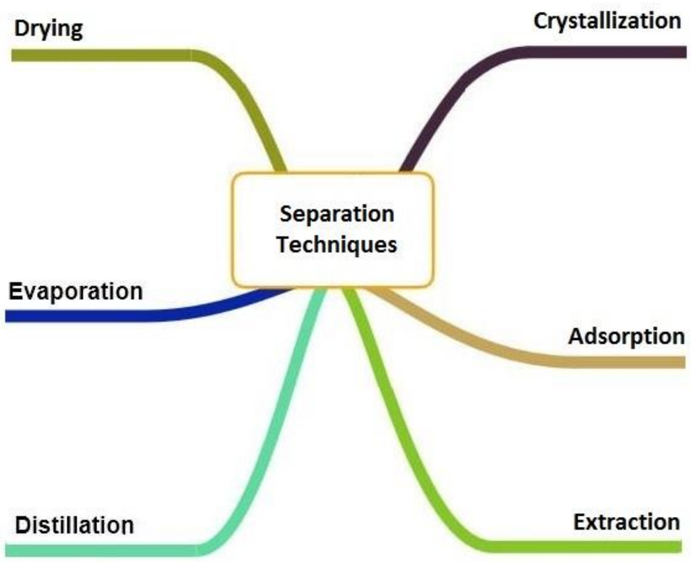
$$RGA_{(I)}=\begin{bmatrix}0.93 & 0.07\\ 0.07 & 0.93\end{bmatrix}, RGA_{(II)}=\begin{bmatrix}9.06 & -8.06\\ -8.06 & 9.06\end{bmatrix}, RGA_{(III)}=\begin{bmatrix}-0.28 & 1.28\\ 1.28 & -0.28\end{bmatrix}$$

Candidate design alternatives to the maximum driving force

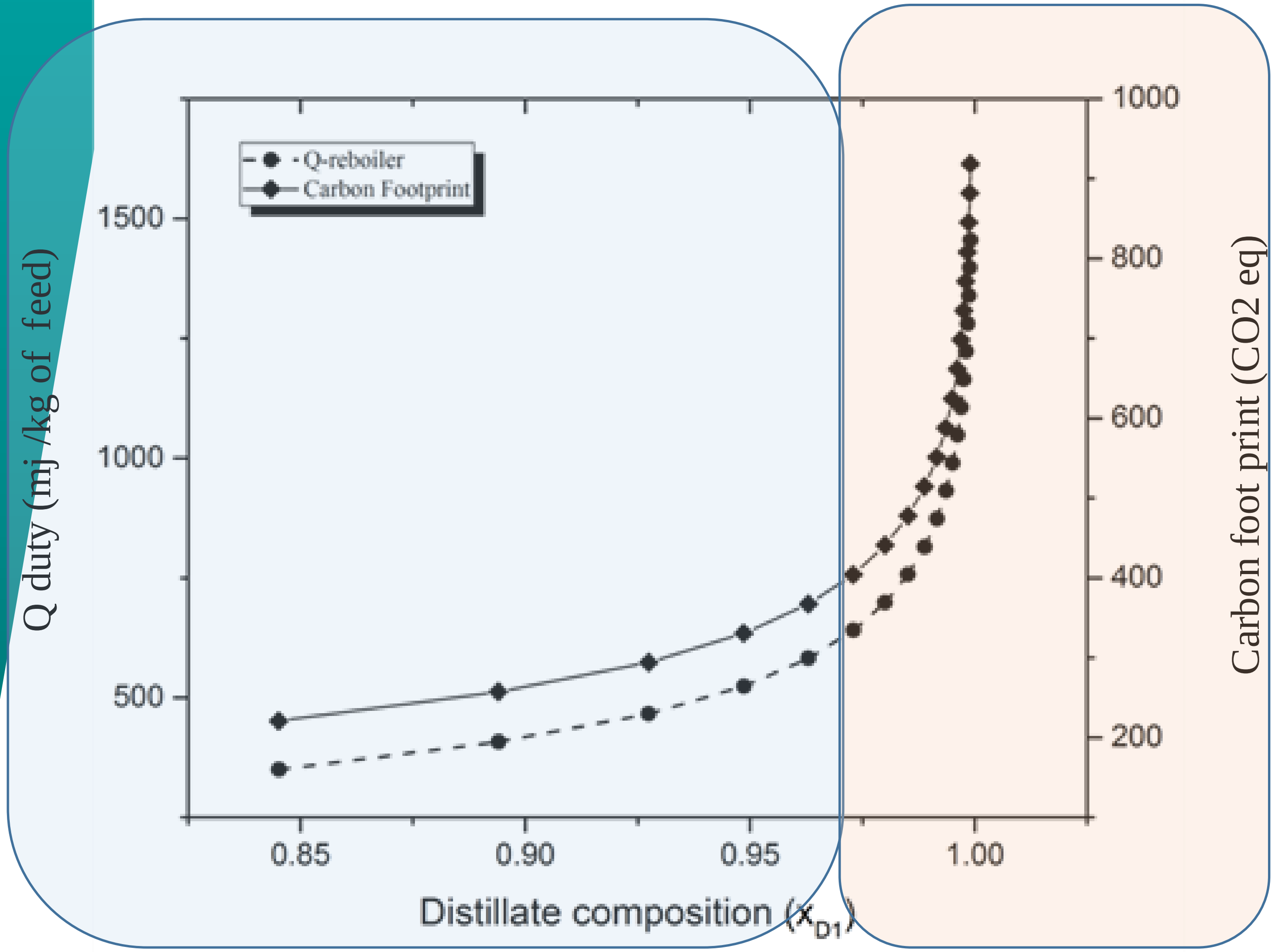
AIChE J. 2016 (design & control of distillation, including reactive distillation)

Energy consumption reduction

- **Separation Processes are indispensable in chemical industry.**
- **Distillation is one of most used separation techniques among all**
- **80 % of all the vapor-liquid separations are performed by distillation.**
- **Distillation is among highly energy intensive techniques with lower thermal efficiency .**
- **More than 40,000 distillation units alone in US (2005) using nearly 75 million KW of energy**



Distillation Analysis – Energy Efficiency



High efficient region

Low efficient region

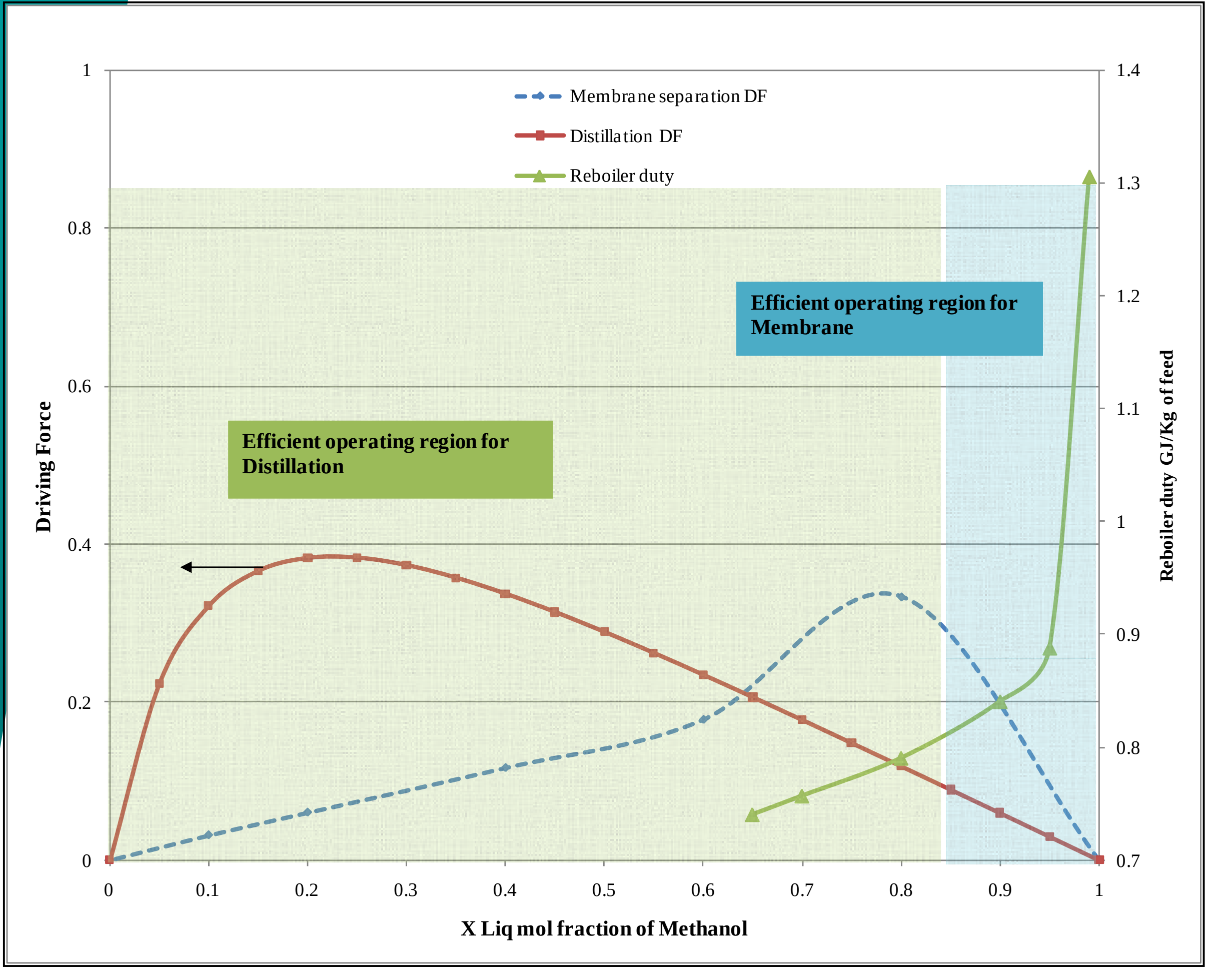
- Product purity ∝ Energy requirement ∝ Operating cost
- Reboiler duty increases exponentially during last 5-10 % of purity

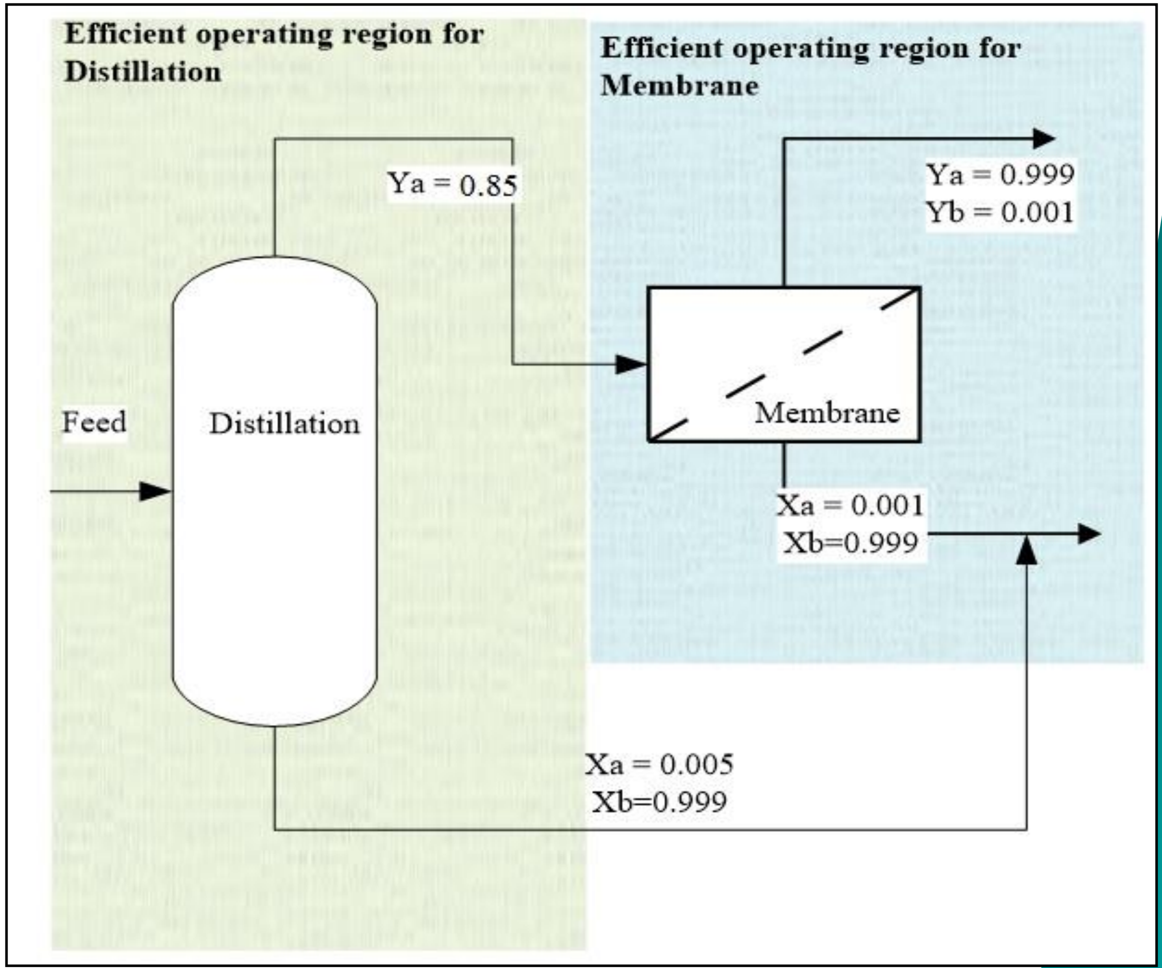
Tula et al. CACE, 105, 2017

Sustainable Product-Process Engineering, Evaluation & Design

Synthesis of Hybrid Scheme

Principle: Use separation techniques at their highest efficiencies

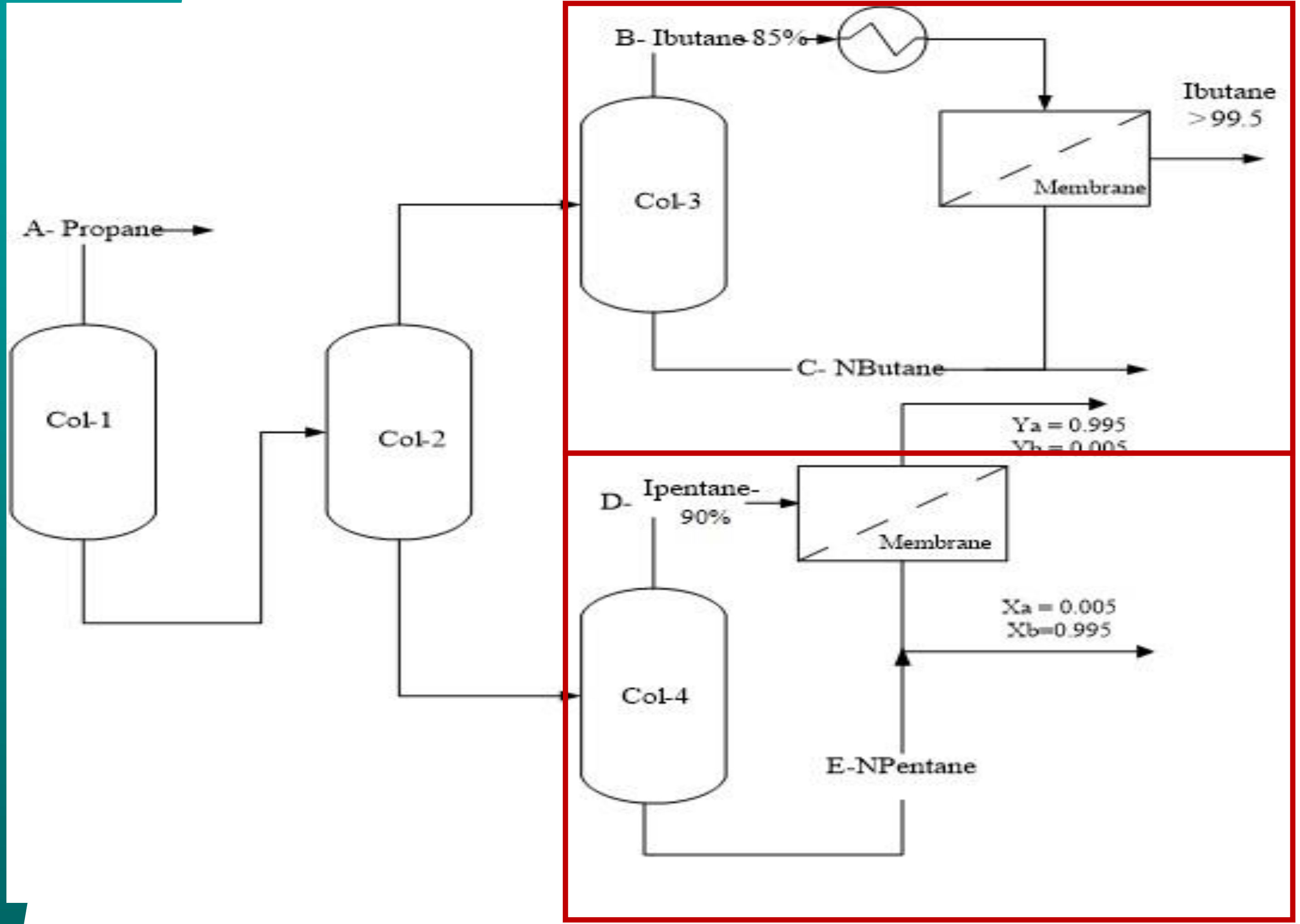




Tula et al. CACE, 105, 2017

PSE for SPEED Sustainable Product-Process Engineering, Evaluation & Design

Application of hybrid scheme



Rigorous Simulation data (GJ/hr)			
	Distillation	**Distillation (Region 1)**	**Savings %**
Energy (C4 col)	32.33	17.98	44.4
Energy (C5 col)	89	55.5	37.6

Tula et al. CACE, 105, 2017

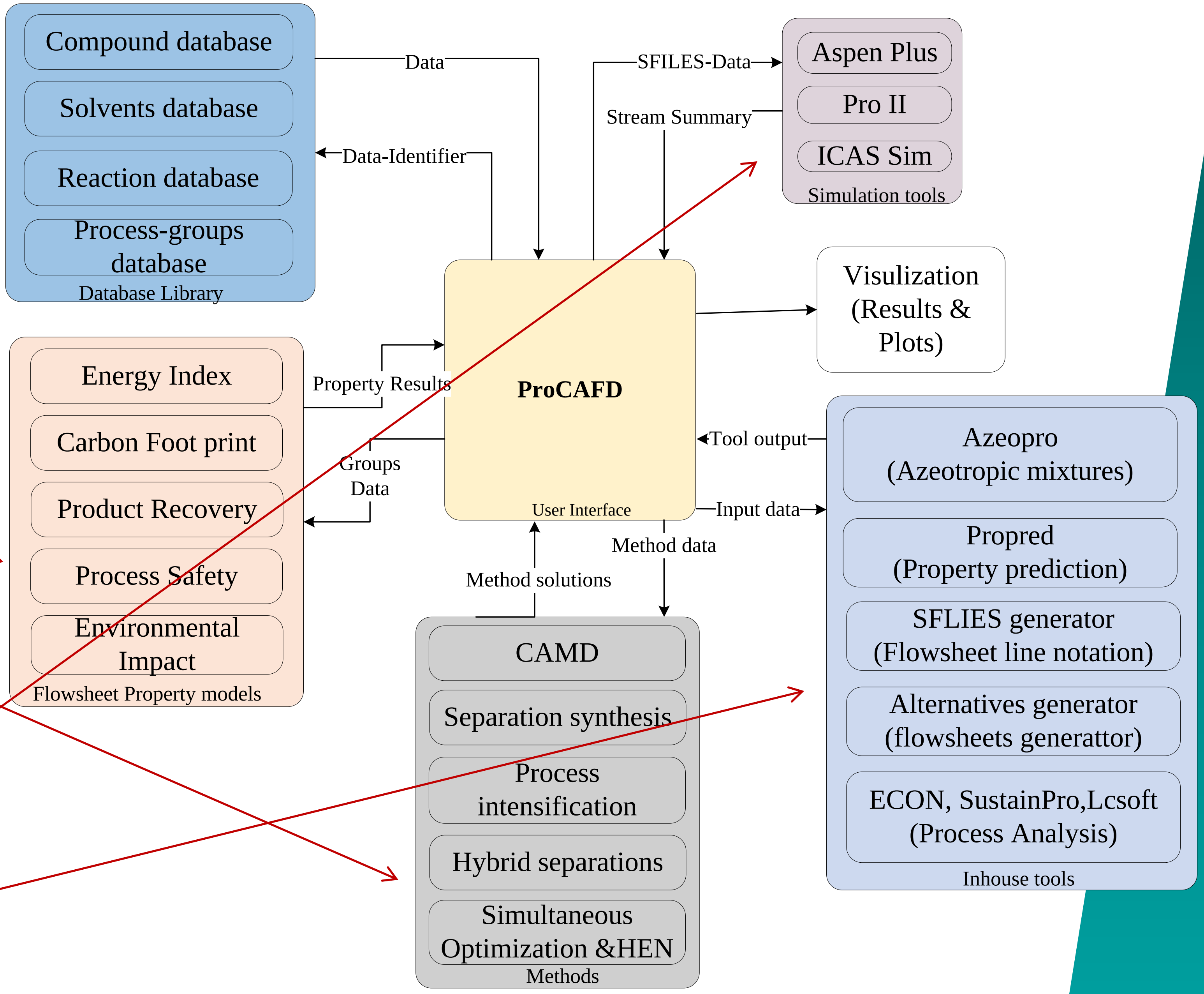
6a. Software Tools

ProCAFD (process synthesis, design, analysis, improvement)

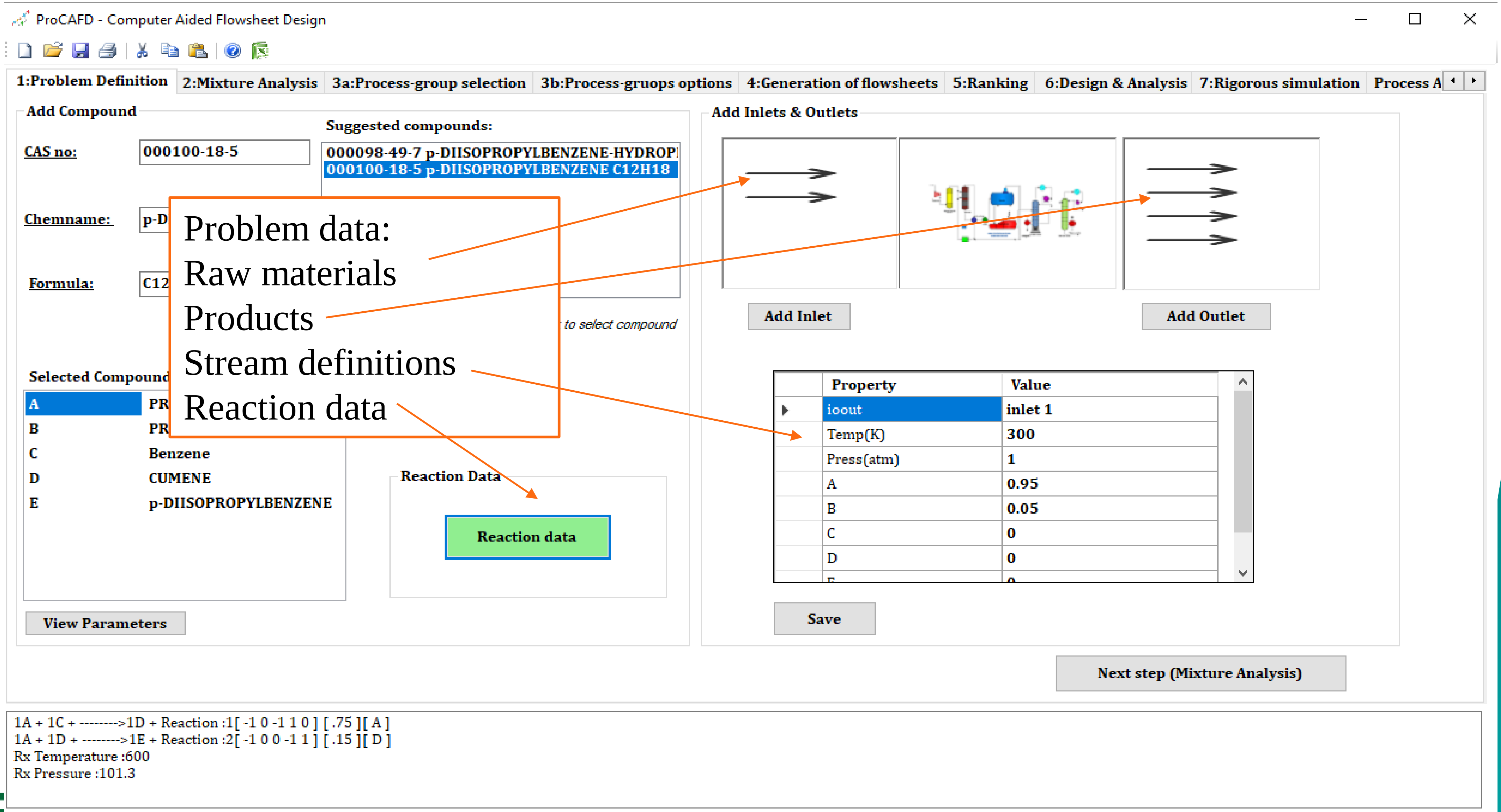
ProCAFD (software tool)

Integrated software tool for process synthesis, design, analysis

- Database library
- Flowsheet property models
- Synthesis, design, PI methods
- Process simulation
- Utility tools (LCA, ECON, ProPred, etc.)



Integration of ProCAFD & Super-O: problem definition in ProCAFD



Integration of ProCAFD & Super-O: problem definition in ProCAFD

ProCAFD - Computer Aided Flowsheet Design

3a:Process-group selection | 3b:Process-gruops options | 4:Generation of flowsheets | 5:Ranking | 6:Design & Analysis | 7:Rigorous simulation | Process Analysis | Process Integration | Settings

Porcess-group	Process.group Type	Process-group desc
iAB	Inlet Process-group	Process Inlet stream AB
iC	Inlet Process-group	Process Inlet stream C
oAB	Outlet Process-group	Process Outlet stream AB
oC	Outlet Process-group	Process Outlet stream C
oD	Outlet Process-group	Process Outlet stream D
oE	Outlet Process-group	Process Outlet stream E
reABC/ABCDE	Reactor Process-group	Reactor unit op ABC/ABCDE
dlE/DABC	Separation Process-gr...	Distillation separation task to separate E/DABC
dlE/DBC	Separation Process-gr...	Distillation separation task to separate E/DBC
dlE/DAC	Separation Process-gr...	Distillation separation task to separate E/DAC
dlE/DC	Separation Process-gr...	Distillation separation task to separate E/DC
dlE/DAB	Separation Process-gr...	Distillation separation task to separate E/DAB
dlE/DB	Separation Process-gr...	Distillation separation task to separate E/DB
dlE/DA	Separation Process-gr...	Distillation separation task to separate E/DA
dlE/D	Separation Process-gr...	Distillation separation task to separate E/D
laE/DABC	Separation Process-gr...	Liquid Adsoption separation task to separate E/DABC
laE/DBC	Separation Process-gr...	Liquid Adsoption separation task to separate E/DBC
laE/DAC	Separation Process-gr...	Liquid Adsoption separation task to separate E/DAC
laE/DC	Separation Process-gr...	Liquid Adsoption separation task to separate E/DC
laE/DAB	Separation Process-gr...	Liquid Adsoption separation task to separate E/DAB
laE/DB	Separation Process-gr...	Liquid Adsoption separation task to separate E/DB
laE/DA	Separation Process-gr...	Liquid Adsoption separation task to separate E/DA
laE/D	Separation Process-gr...	Liquid Adsoption separation task to separate E/D
pvCD/EAB	Separation Process-gr...	Pervaporation separation task to separate CD/EAB
pvCD/EB	Separation Process-gr...	Pervaporation separation task to separate CD/EB

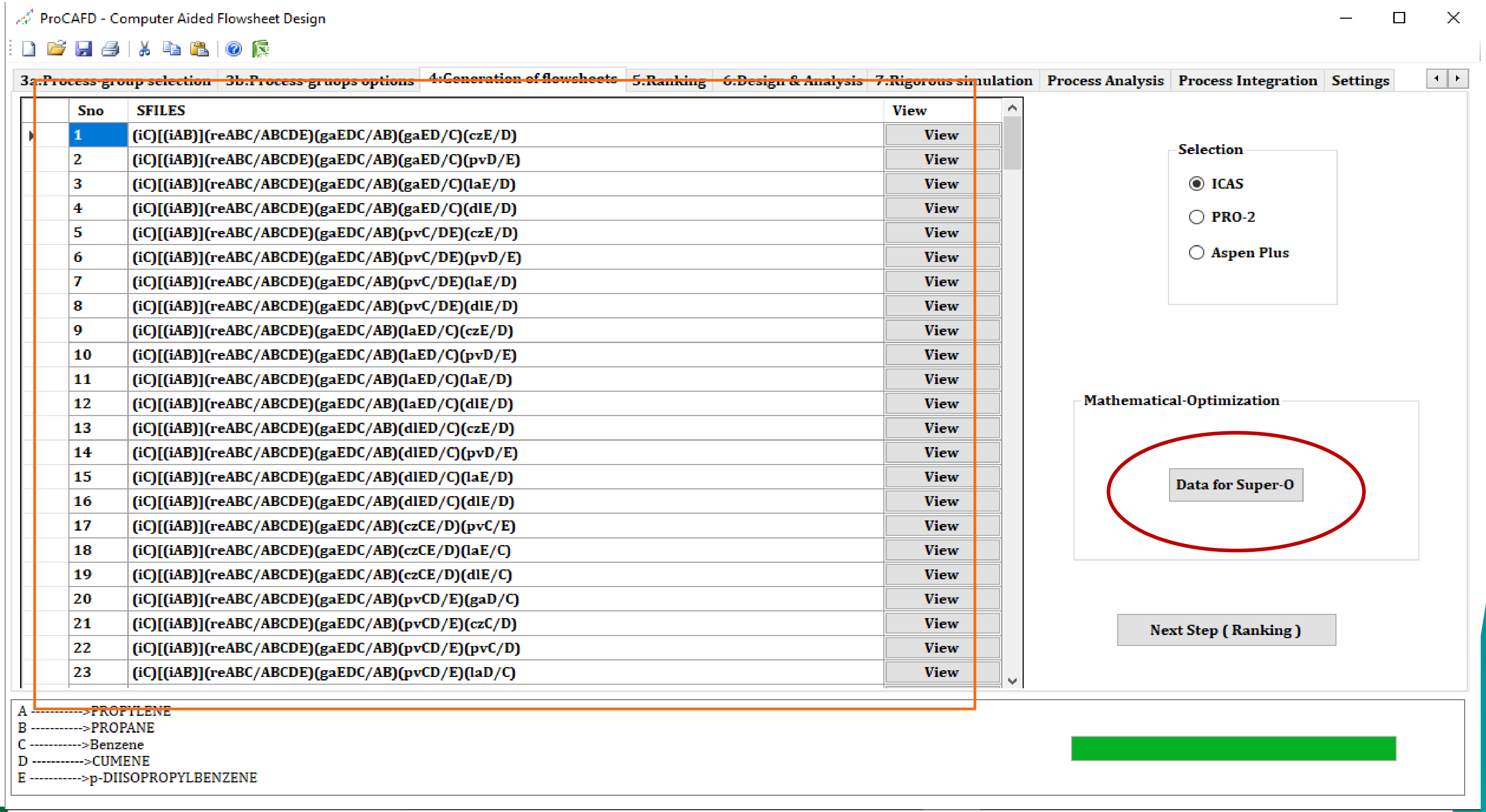
Inlet/Outlet PG's	6
Separation PG's	148
Reaction PG's	1
Total PG's	155

Total number of flowsheet combinations : 3176376

Next Step
(Process-Group options)

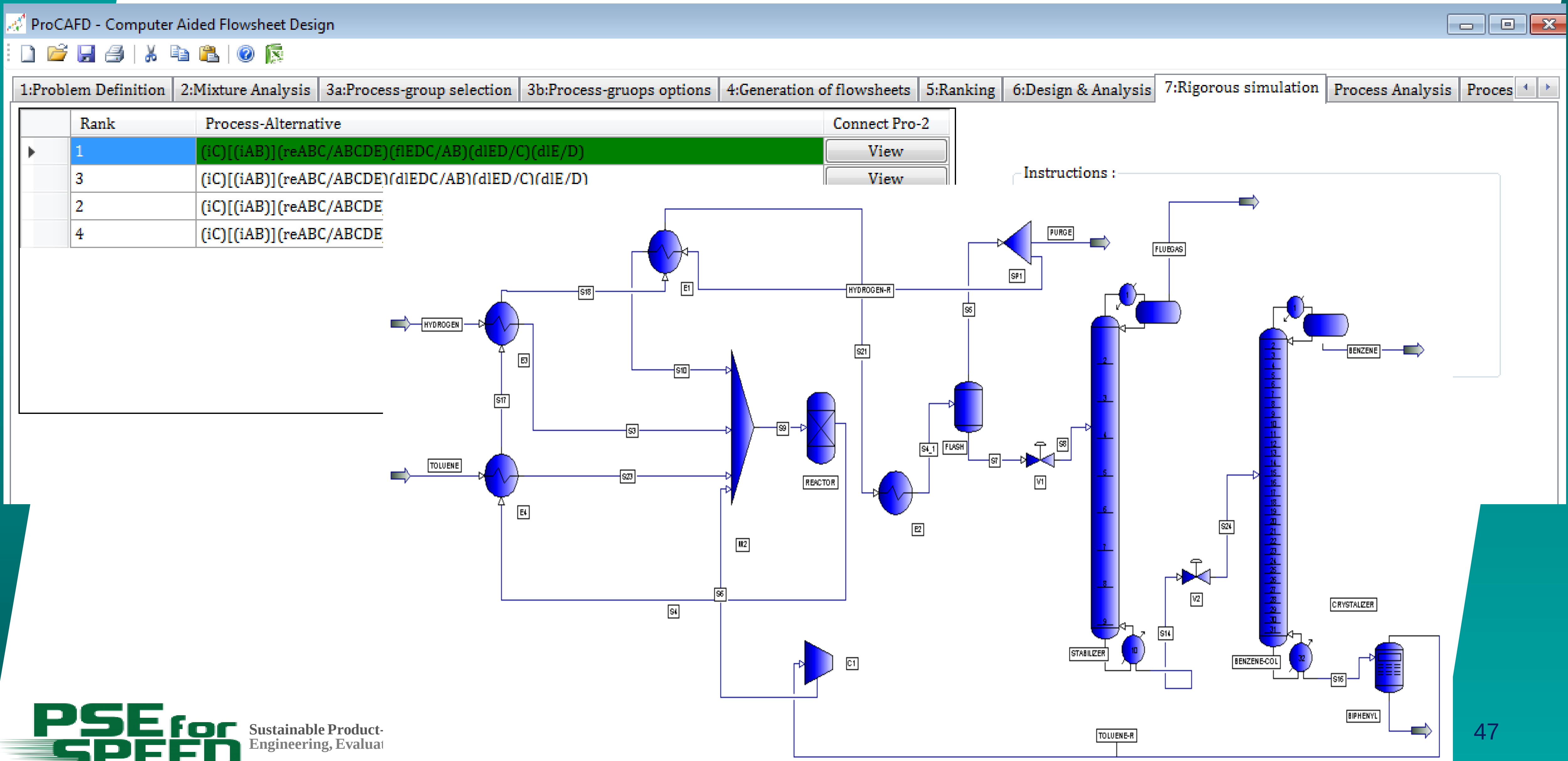
A ----------->PROPYLENE
B ----------->PROPANE
C ----------->Benzene
D ----------->CUMENE
E ----------->p-DIISOPROPYLBENZENE

Integration of ProCAFD & Super-O: Export data to Super-O



Sno	SFILES	View
1	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(gaED/C)(czE/D)	View
2	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(gaED/C)(pvD/E)	View
3	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(gaED/C)(laE/D)	View
4	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(gaED/C)(dlE/D)	View
5	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(pvC/DE)(czE/D)	View
6	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(pvC/DE)(pvD/E)	View
7	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(pvC/DE)(laE/D)	View
8	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(pvC/DE)(dlE/D)	View
9	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(laED/C)(czE/D)	View
10	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(laED/C)(pvD/E)	View
11	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(laED/C)(laE/D)	View
12	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(laED/C)(dlE/D)	View
13	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(dlED/C)(czE/D)	View
14	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(dlED/C)(pvD/E)	View
15	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(dlED/C)(laE/D)	View
16	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(dlED/C)(dlE/D)	View
17	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(czCE/D)(pvC/E)	View
18	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(czCE/D)(laE/C)	View
19	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(czCE/D)(dlE/C)	View
20	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(pvCD/E)(gaD/C)	View
21	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(pvCD/E)(czC/D)	View
22	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(pvCD/E)(pvC/D)	View
23	(iC)[(iAB)](reABC/ABCDE)(gaEDC/AB)(pvCD/E)(laD/C)	View

Integration of ProCAFD & Super-O: problem definition in ProCAFD

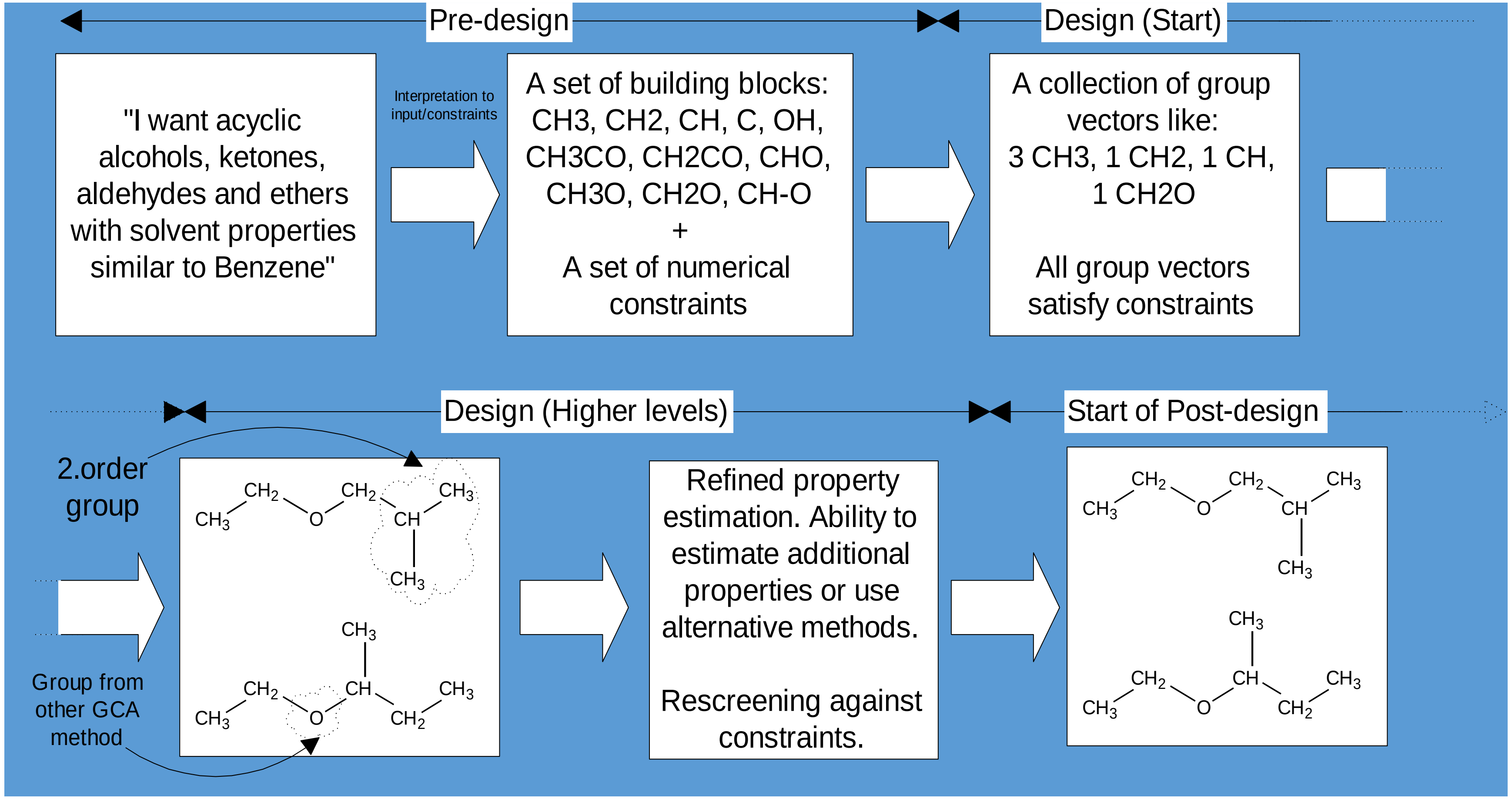


Sustainable Product-
Engineering, Evaluat

6b. Software Tools

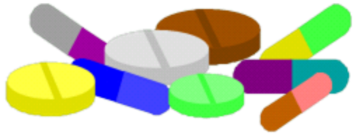
ProCAPD (product synthesis, design, analysis, improvement)

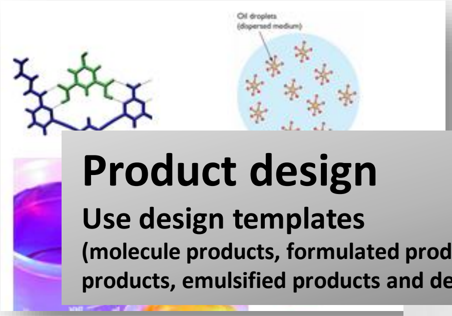
Multi-level generate & test according to a predefined sequence (chemical substitution)



ProCAPD – The product simulator

There is a need for a product simulator with the same and more useful features than a typical process simulator. Based on available data, models, methods and analysis tools, the first chemical product simulator has been developed: ProCAPD





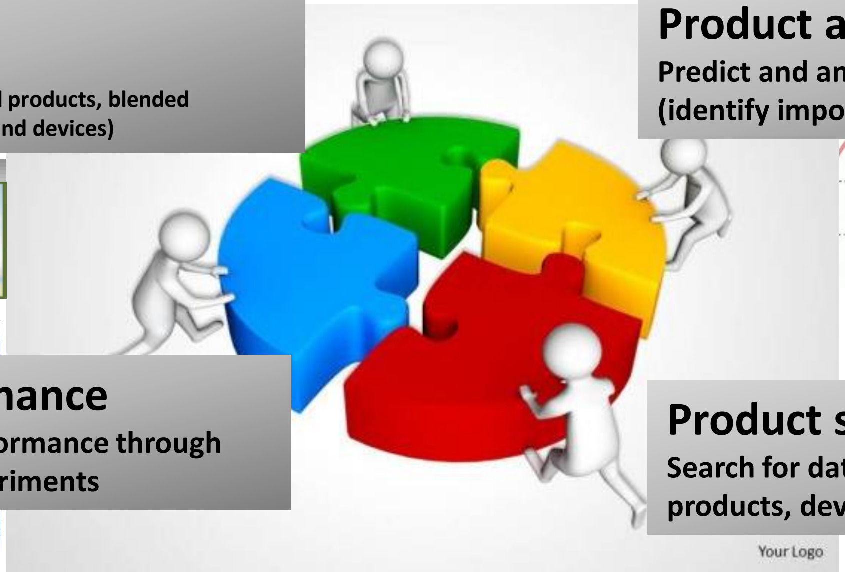
Product design

Use design templates

(molecule products, formulated products, blended products, emulsified products and devices)

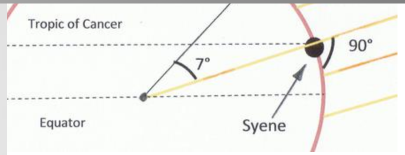
Product performance

Simulated product performance through virtual application experiments



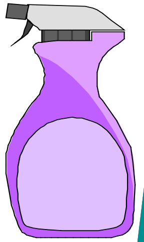
Product analysis

Predict and analyze product behavior (identify important product properties)



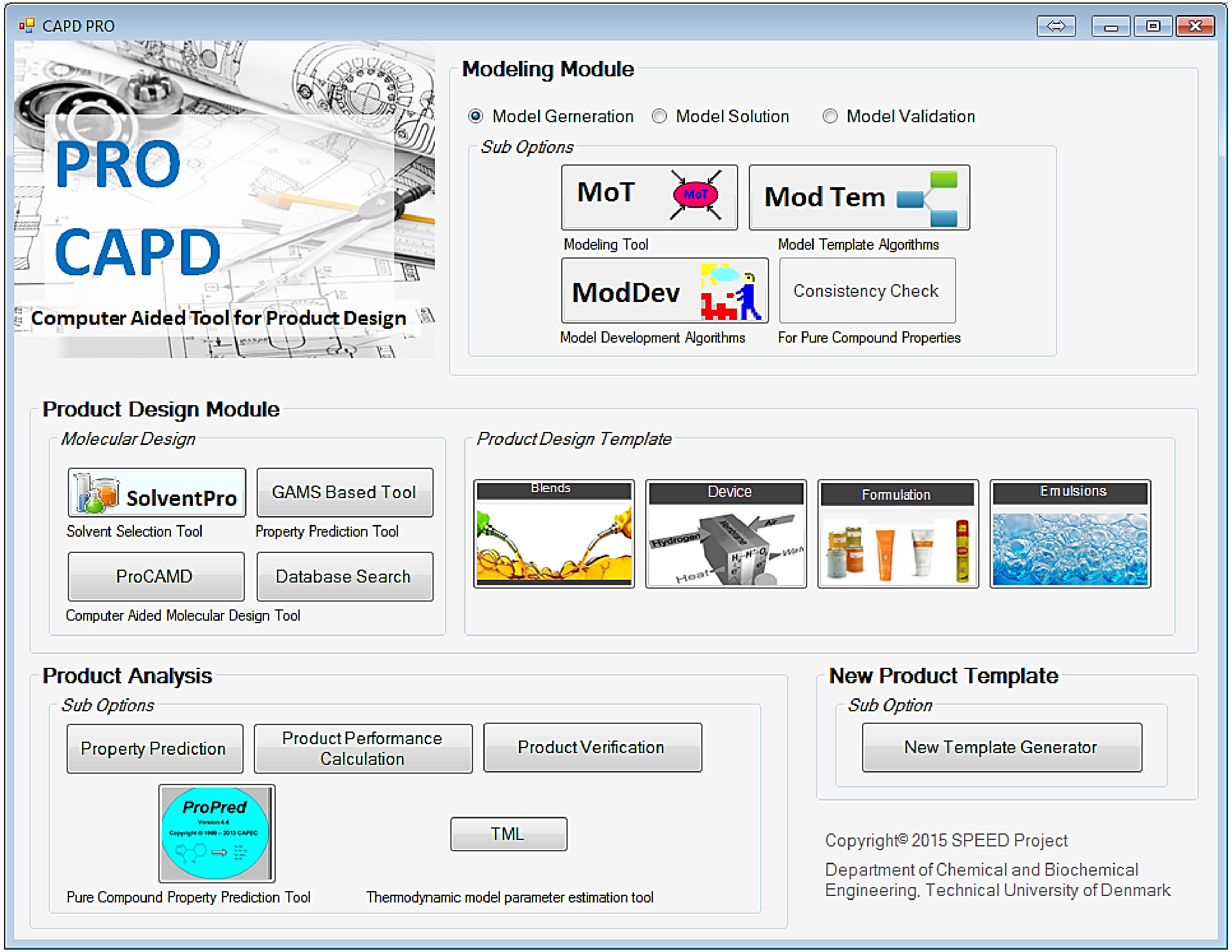
Product search

Search for data, models, properties, products, devices, etc.



Gasoline blend

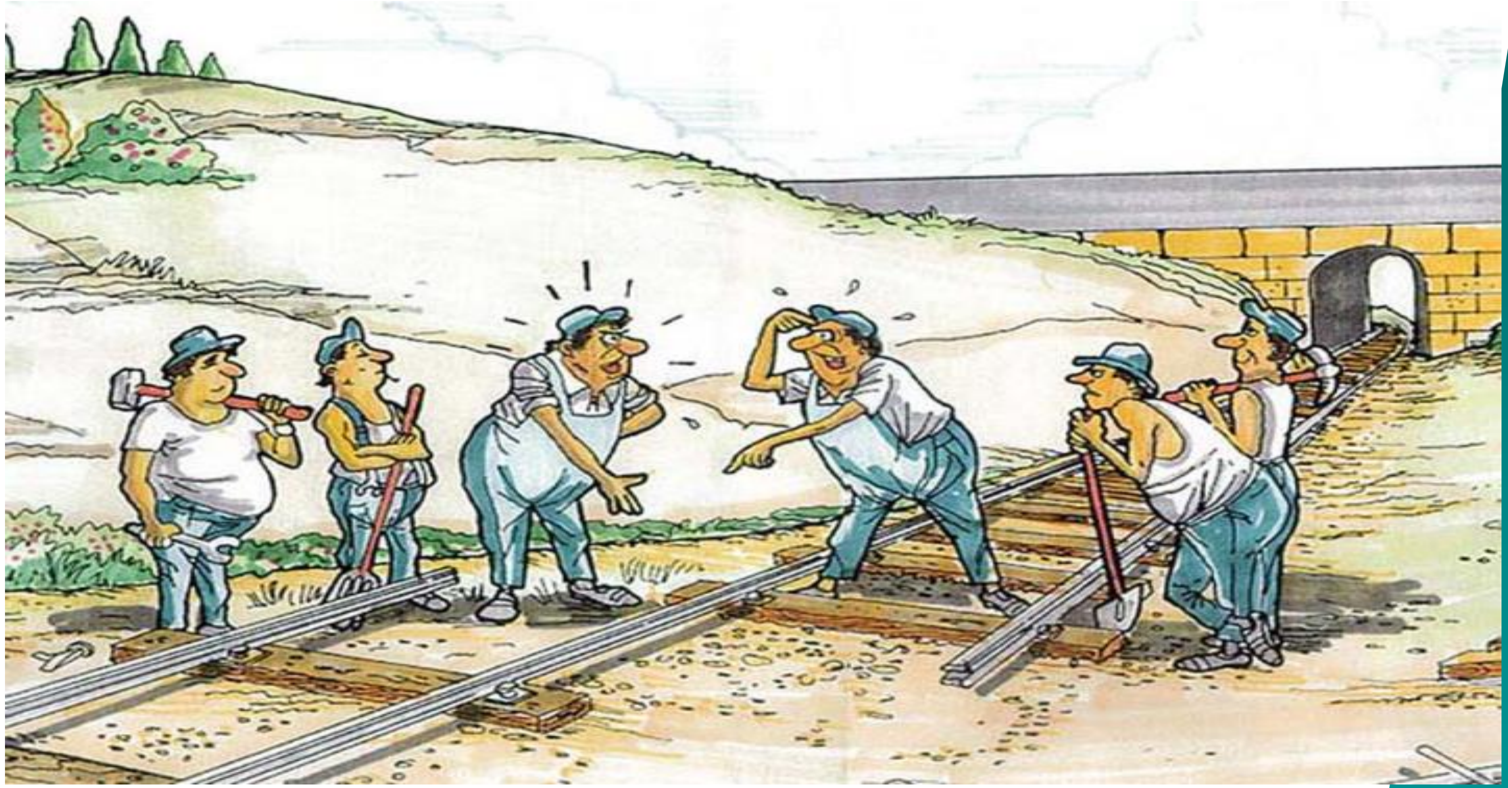
ProCAPD – Features & Options



ProCAPD: for design, analysis of single molecular product; blend (surrogate fuels); formulated products (paints, cosmetics, detergents); & devices

Conclusions

- It is possible to find new innovative solutions
- Issues related to uncertainty of data & models are important and need to be considered
- Mutli-disciplinary nature of problems need to be handled



- Golden Era for Chemical Engineering (Westmoreland, 2014) – do something!
- Focused team-effort needed to meet the challenges