Chemical Product Centric Sustainable Process Design

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Workshop Overview

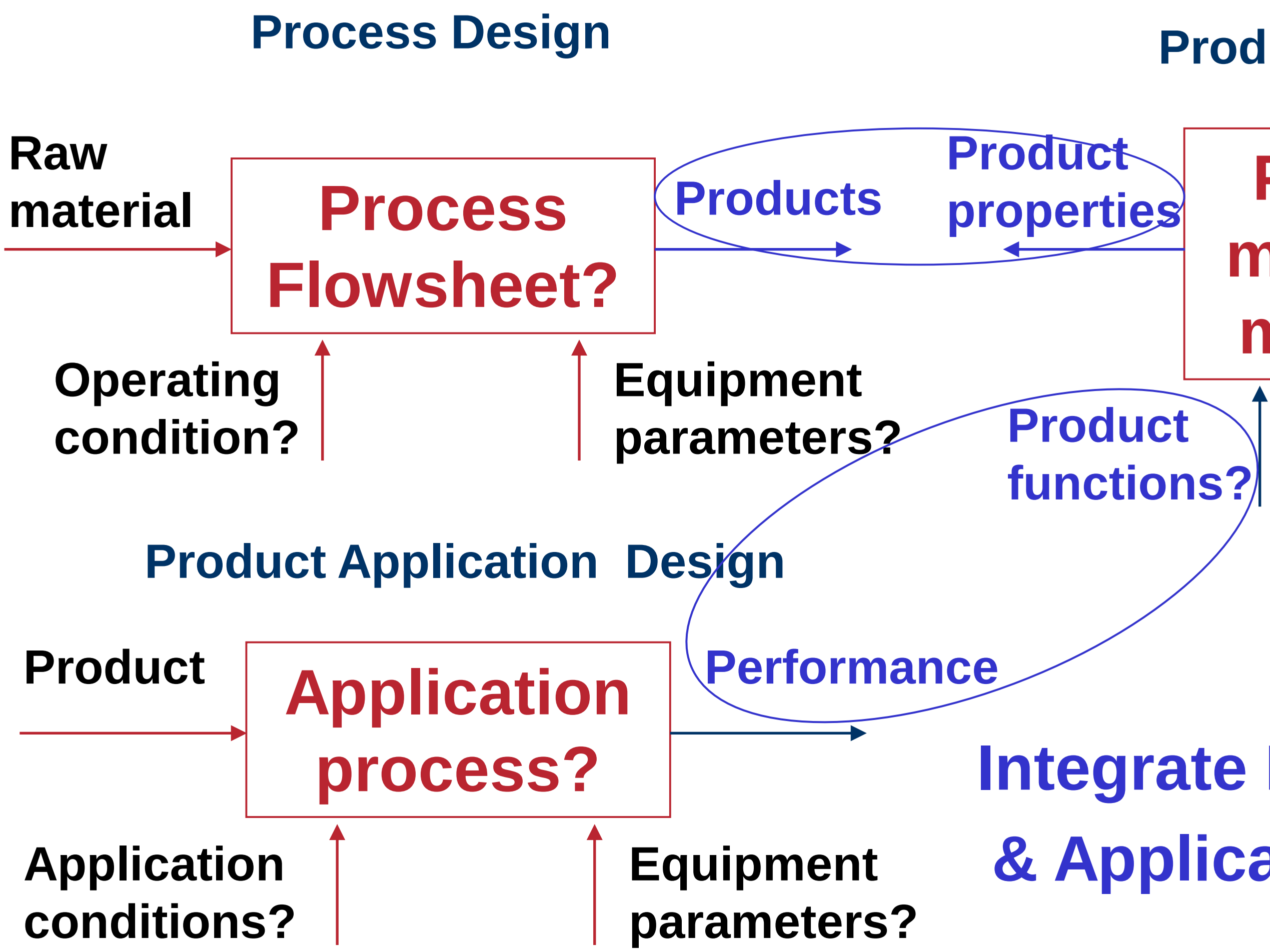
- **Lecture 1: Introduction & definition of concepts**
- **Lecture 2: Computer aided product (molecules & mixtures) design (case study as tutorial)**
- **Lecture 3: Targeted reverse process design & concept of process group based flowsheet synthesis (case study as tutorial)**
- **Lecture 4: Introduction to sustainable process design & the SustainPro software (case study-1 & case study-2)**
- **Lecture 5: (+ tutorials): Introduction to vPPDL; SustainPro**

Introduction & definition of concepts

- **Product centric process design**
  - **Chemical product design**
  - **Sustainable process design**
- **General problem definition**
- **Solution approaches**
  - **Reverse design**
  - **Decomposition**

Product centric chemical process design

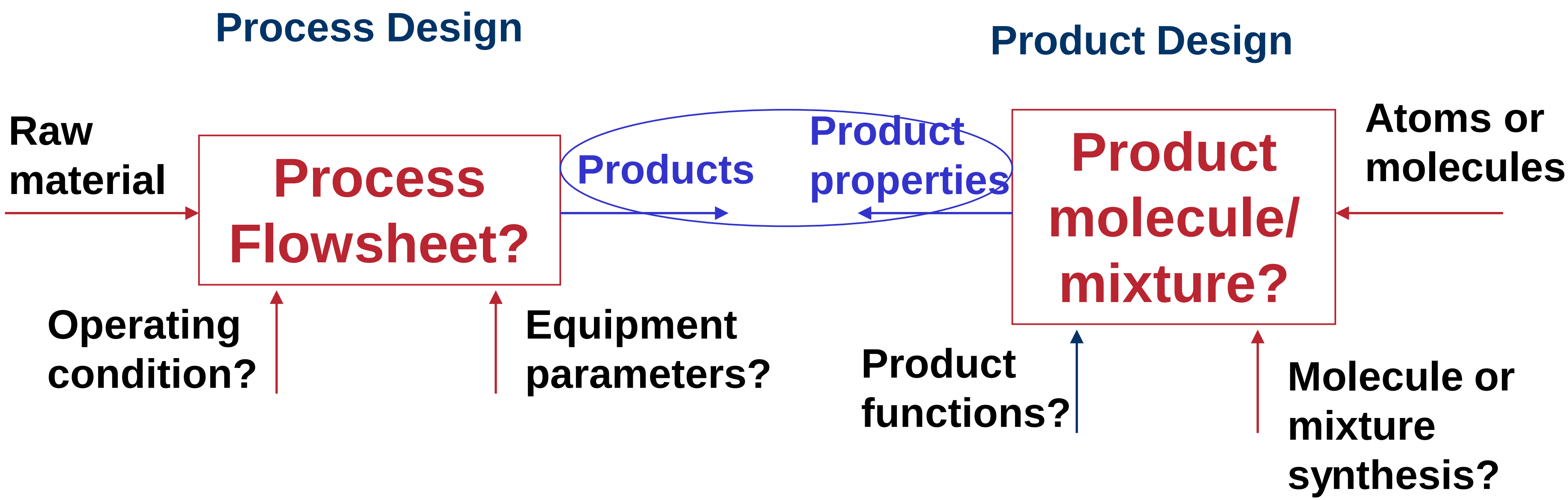
Problem Definition



Integrate Process-Product & Application

Product centric chemical process design

Examples of Product-Process Integration



- Petroleum blends & petroleum products — Routinely solved!
- Polymers & blends — Can be solved!
- Specialty chemicals (including drugs, ….) — Process role?

Examples of Product-Process Integration

For products such as drugs, pesticides, food, … delivery and application is important also needs to be validated

Product Design

Product properties ← **Product molecule/ mixture?** ← Atoms or molecules

Product functions? → Product molecule/ mixture?

Molecule or mixture synthesis? → Product molecule/ mixture?

Product Application Design

Product → **Application process?** → Performance

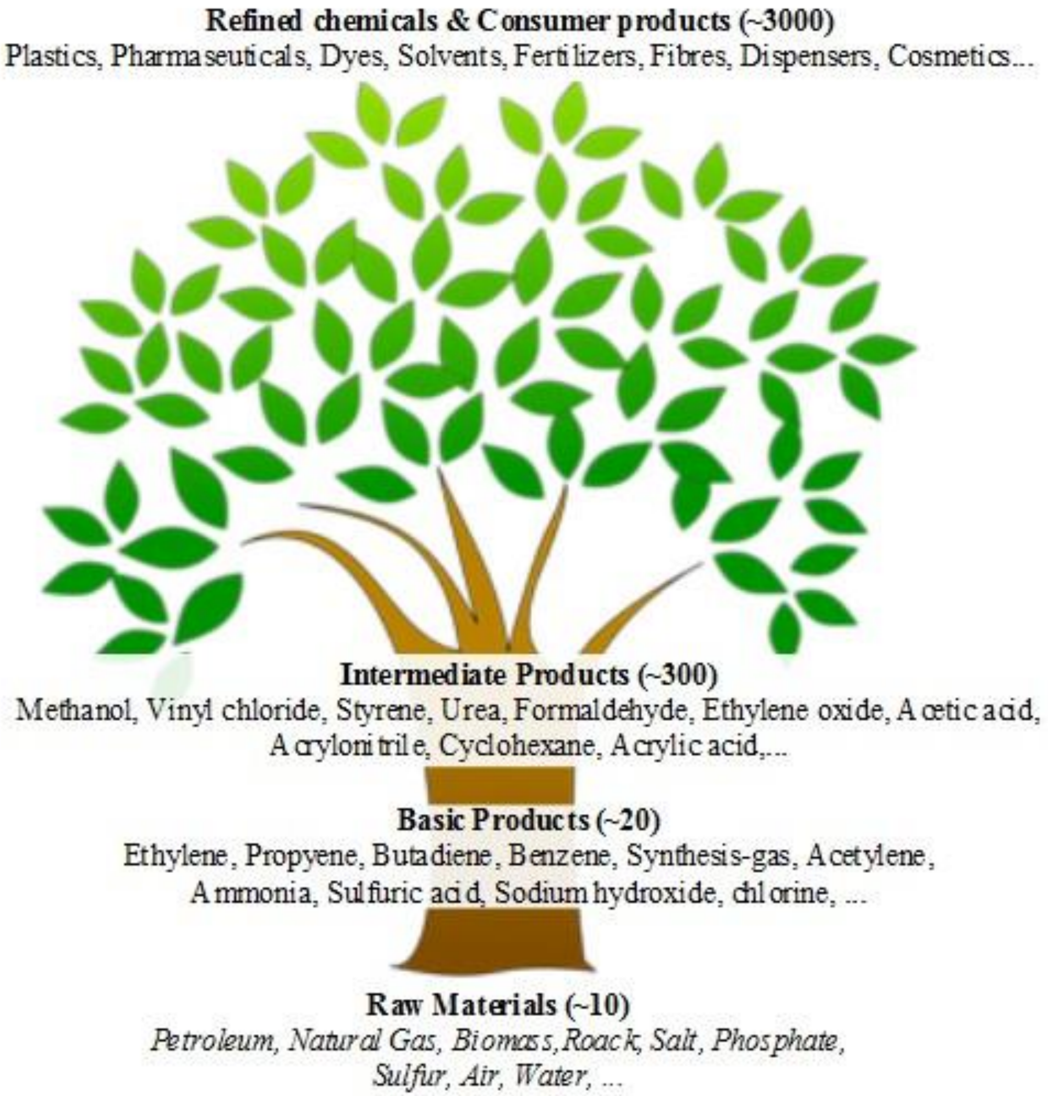
Application conditions? → Application process?

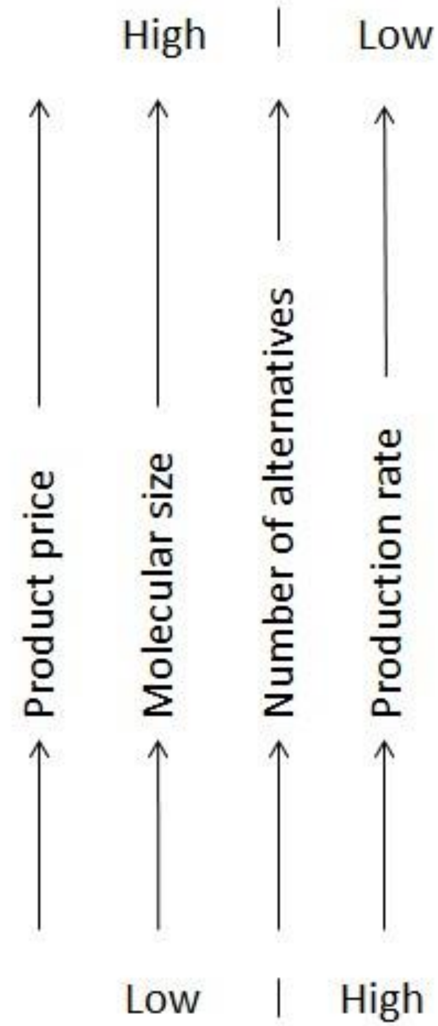
Equipment parameters? → Application process?

Production process needs to be reliable – first time right is important

The chemical product tree

Question of what, why & when (how)?





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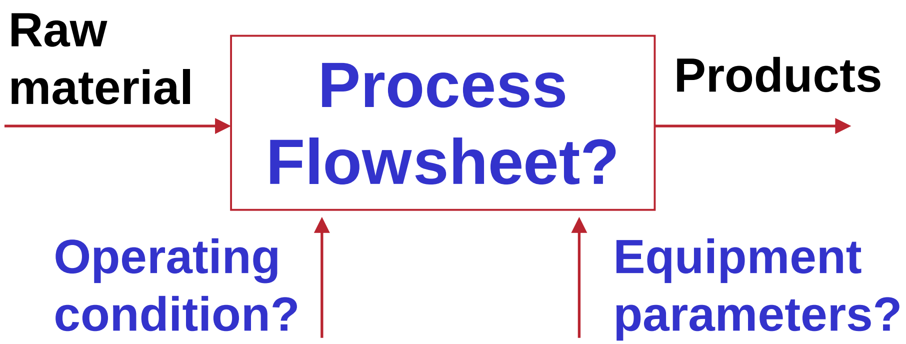
Chemical process design

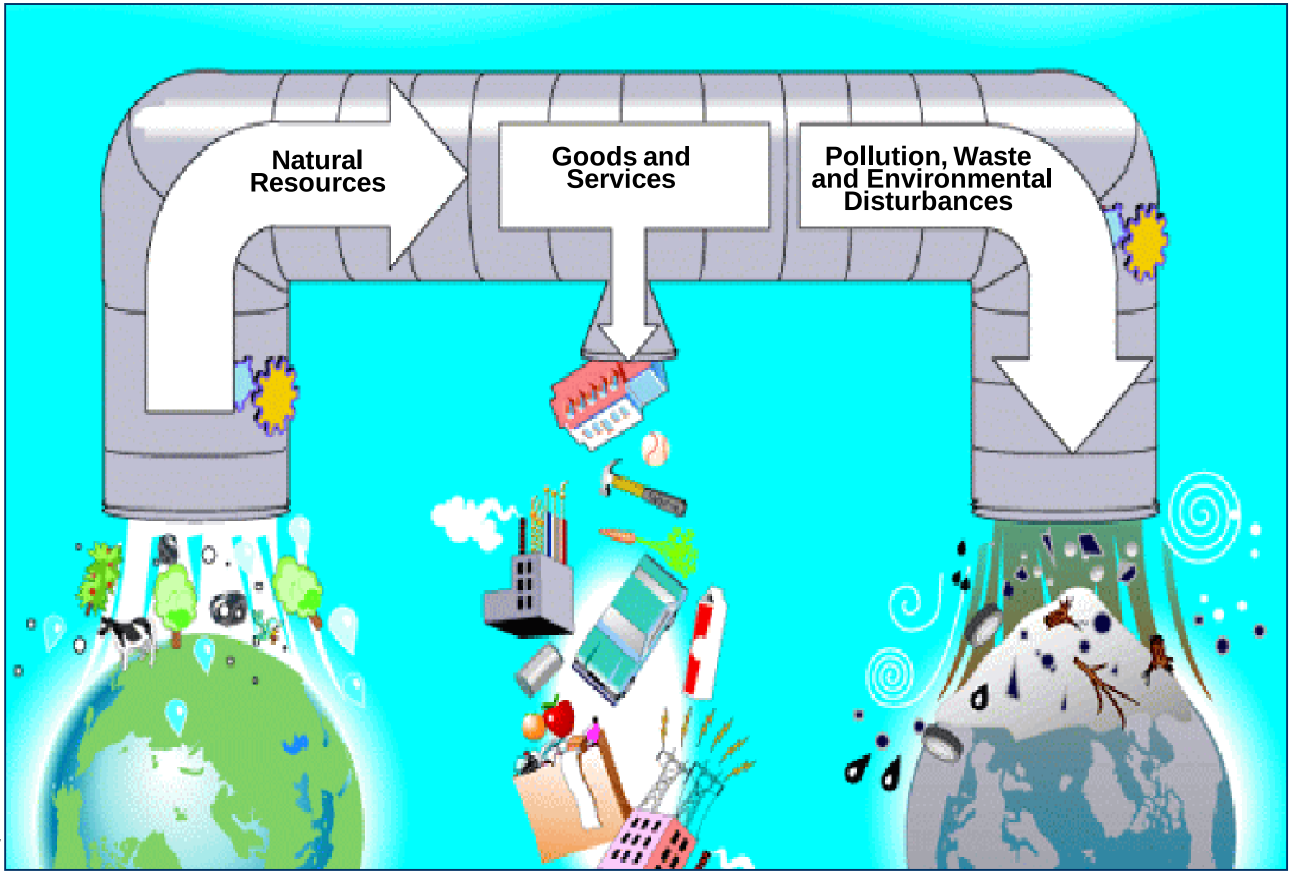


Chemical process design involves the determination of the process flowsheet and the corresponding condition of operation and equipment design that converts the selected raw materials to the desired products

Are our products & processes sustainable?

Need for significant improvement

Only 25 wt% of what goes into the pipe comes out as goods and services – scope for significant improvements



Adapted from Driolli, 2005

Without signficant improvements, our products-processes are not sustainable

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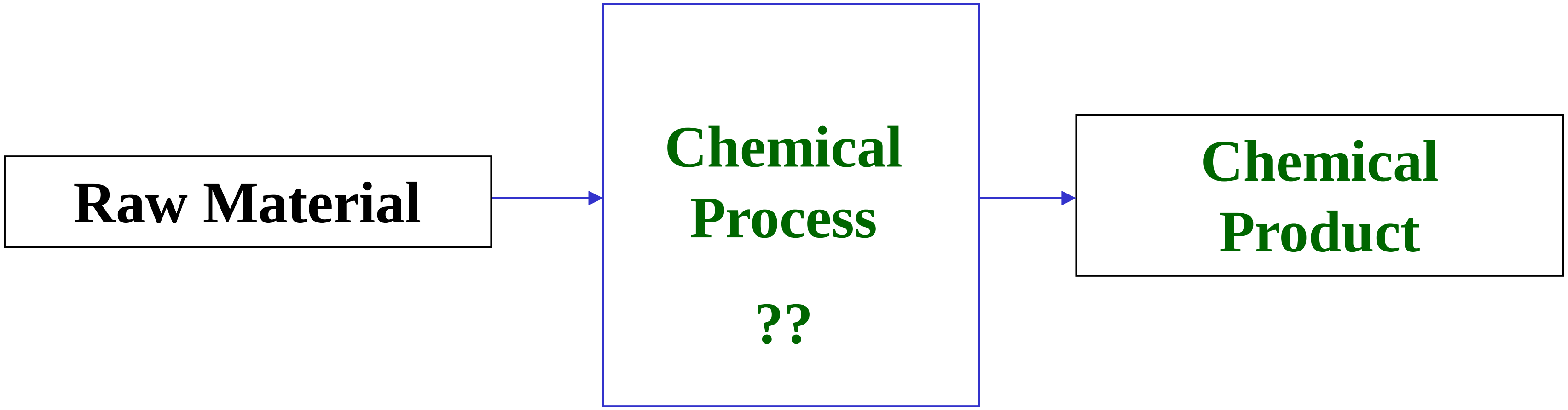
New definition of process design



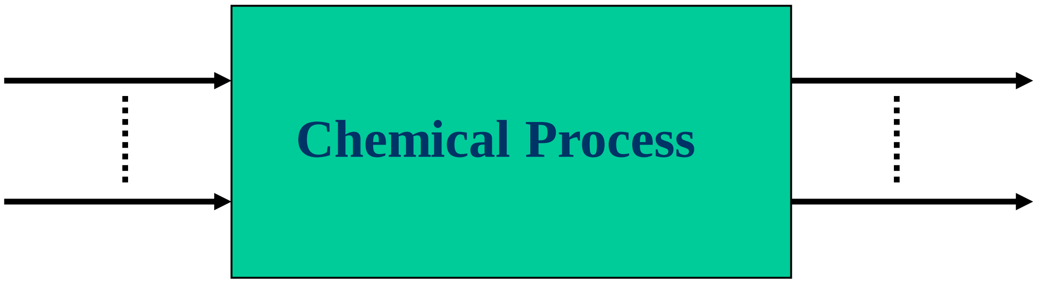
Chemical process design is about finding a sustainable process that can convert the raw materials to the desired chemical products

Sustainable: Economic, low environmental impact, low waste, efficient operation, correct raw material, …..

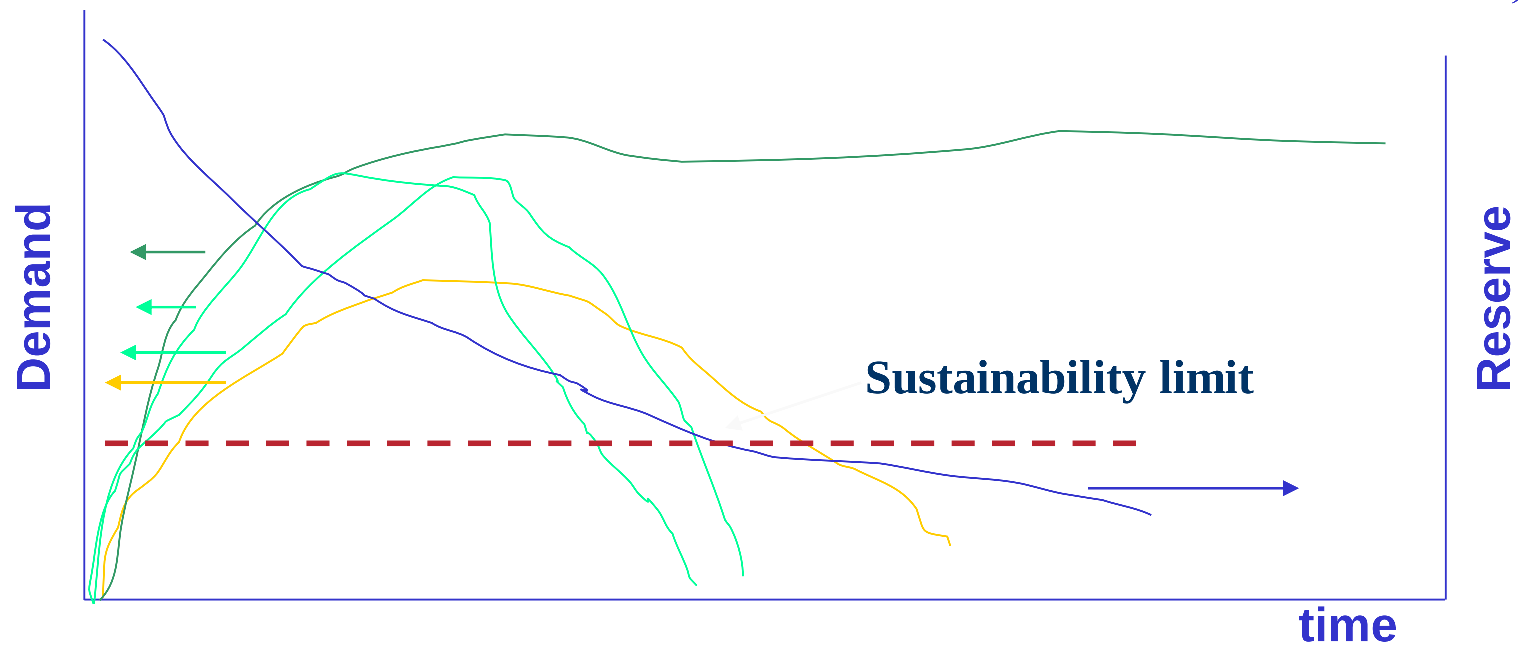
Concept of sustainability

Prolong the life of the process

Raw material, solvents, water, power, steam, …



Products, solvents, water, power, steam, unconverted materials, …

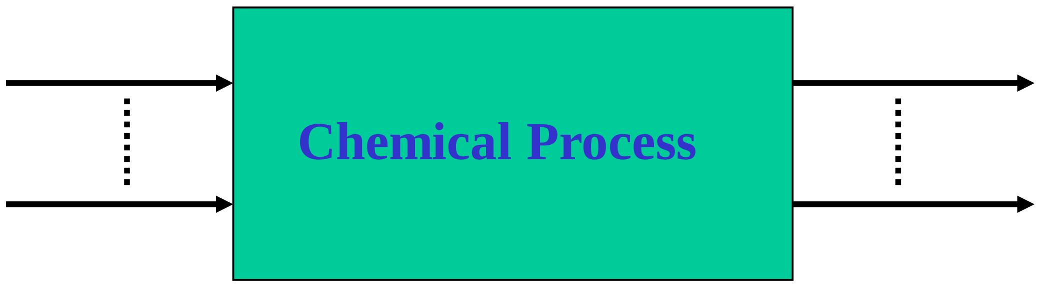


Sustainability of total system and sub-systems

Concept of Sustainabilty - II

Measure of sustainability

Raw material, solvents, water, power, steam, …



Products, solvents, water, power, steam, unconverted materials, …

- **Boundary:** process and its connections
- **Compared to a base-case design, generate alternatives that improve the following**
  - Operability, energy consumption, waste reduction, environmental impact, safety, cost, ….
- **Sustainability metrics** (as defined by IChemE): 49
  Environmental (resource usage; emissions, effluents, waste), economic (profit, value, tax; investments), societal (workplace, society)

Concept of Sustainabilty - III

How to achieve sustainability?

- **Improve one or more of the following**
    - **Operability, energy consumption, waste reduction, environmental impact, safety, cost, ….**
    - **Sustainability metrics (as defined by IChemE)**

Apply a systematic analysis of the mass and energy paths within the process to determine a set of mass and energy indicators that will help to define attainable targets for improvement; generate alternatives that meet these targets through a "reverse" approach

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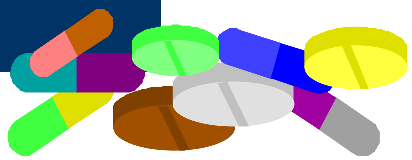
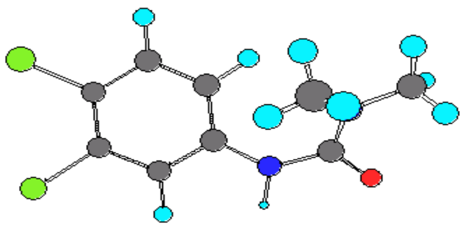
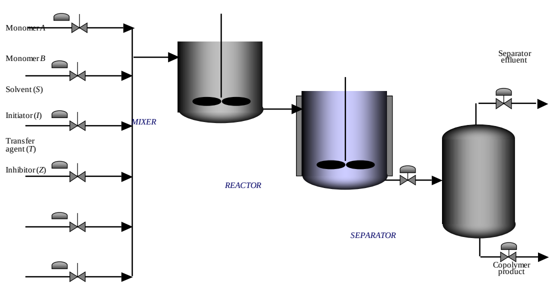
Chemical Product-Process Connection







Process development

Product

In-use properties

Product function

Physico-chemical properties

Process function

Process

Product development and manufacturing

General Problem Definition

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)

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

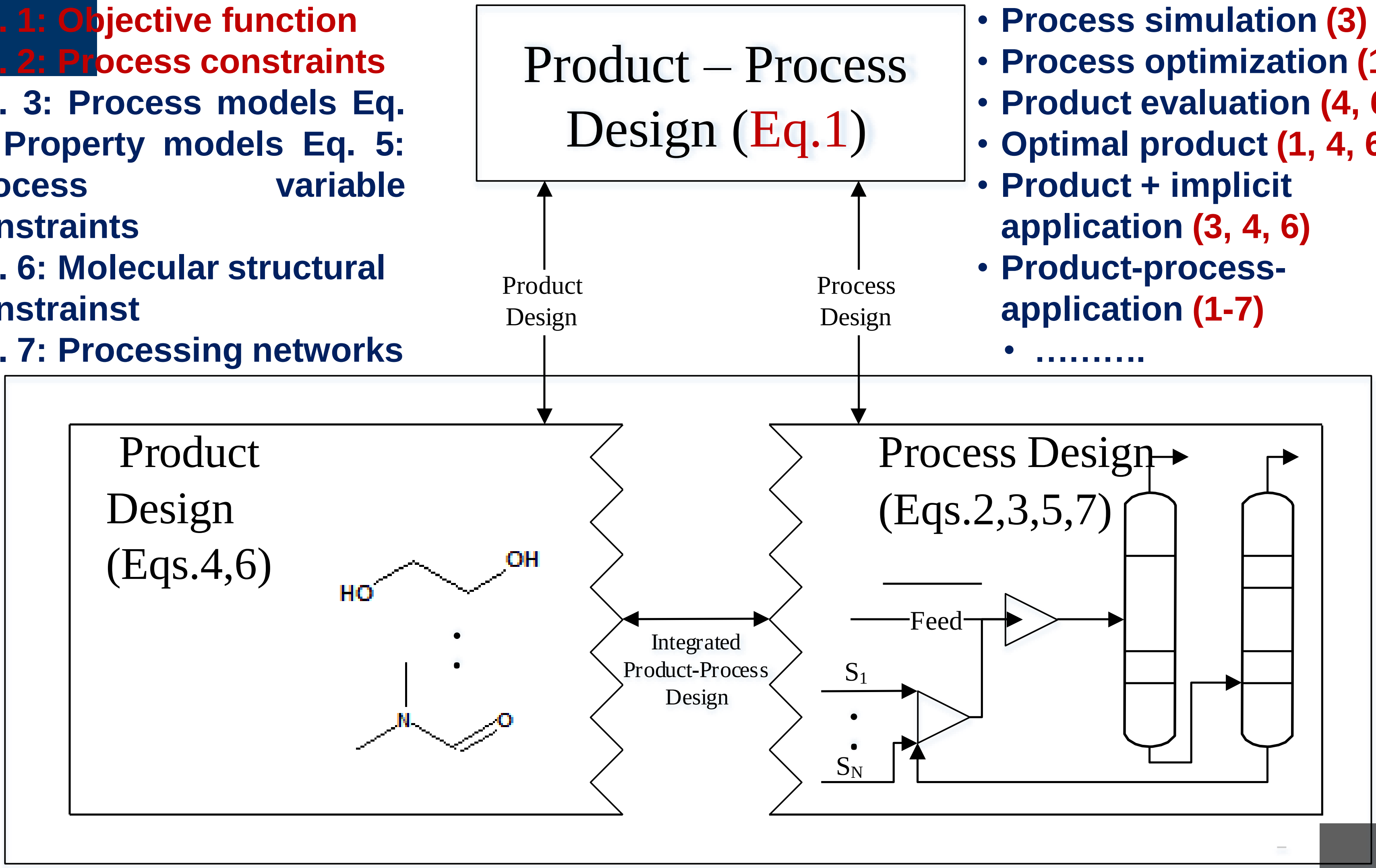
$l_2 \leq g_2(\underline{x}, \underline{y}) \leq u_2$ molecular structure constraints (Eq. 6)

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

General Problem Definition

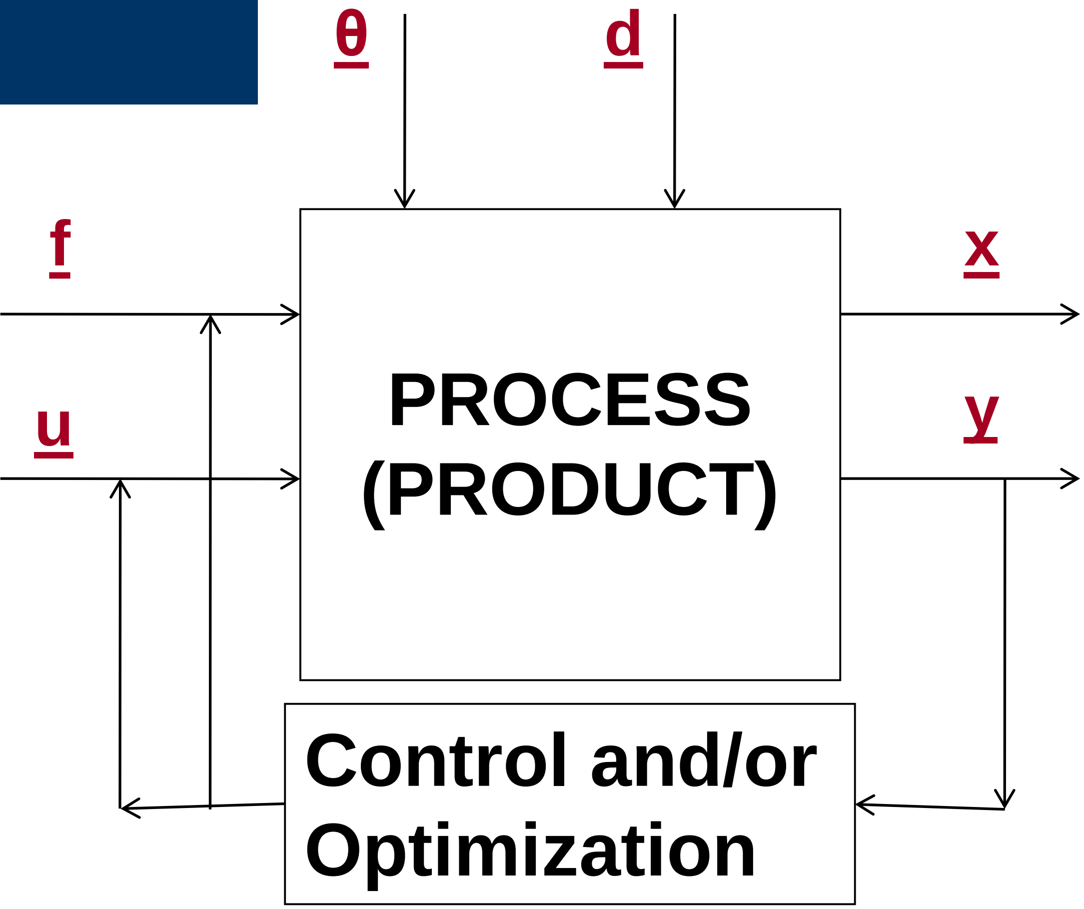
Eq. 1: Objective function
Eq. 2: Process constraints
Eq. 3: Process models Eq. 4: Property models Eq. 5: Process variable constraints
Eq. 6: Molecular structural constrainst
Eq. 7: Processing networks



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

Simultaneous Product – Process Design (multiscale & multidiscipline)

Models and relationships



Models:

Process/property

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

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

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

Sustainability Metrics

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

$\underline{S}_i = S_i\ (\underline{C}, \underline{f}, \underline{y})$

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

Safety & Hazards

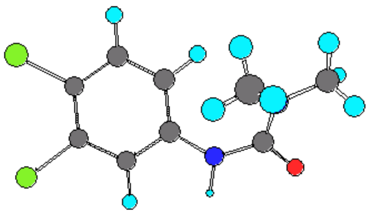
$\underline{H}_c = Hc\ (\underline{C}, \underline{f}, \underline{y}, \underline{d})$

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

Given: $\underline{\theta}$, $\underline{d}$, $\underline{f}$, $\underline{u}$; calculate $\underline{x}$, $\underline{y}$ (forward)

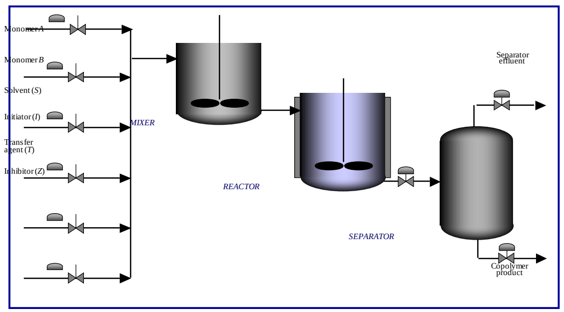
Given: $\underline{\theta}$, $\underline{d}_1$, $\underline{f}$, $\underline{u}_1$, $\underline{x}_1$, $\underline{y}_1$; calculate $\underline{x}_2$, $\underline{y}_2$, $\underline{d}_2$, $\underline{u}_2$ (reverse)

Example



Property models

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



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

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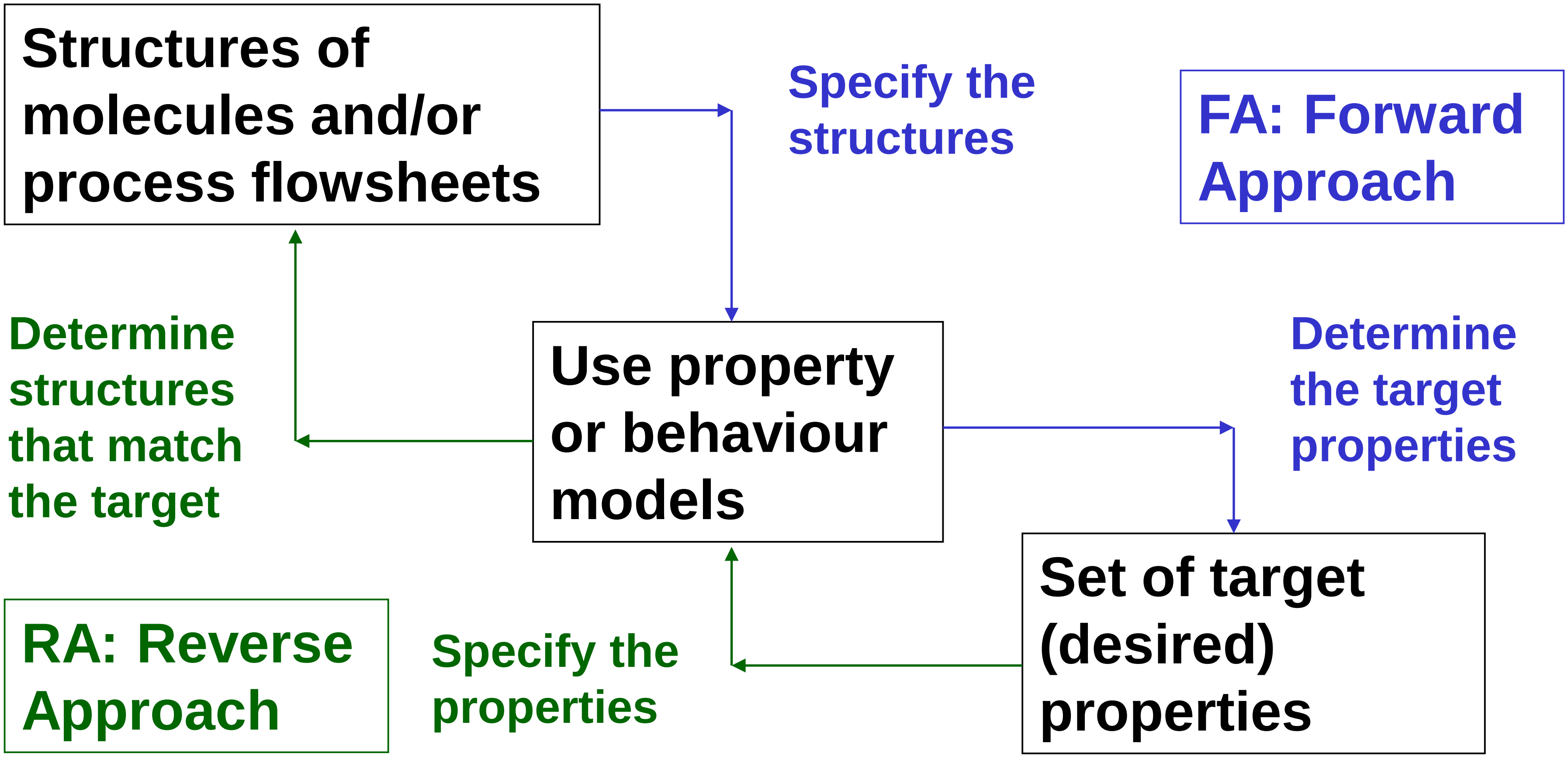
Solution Approach: Reverse Approach

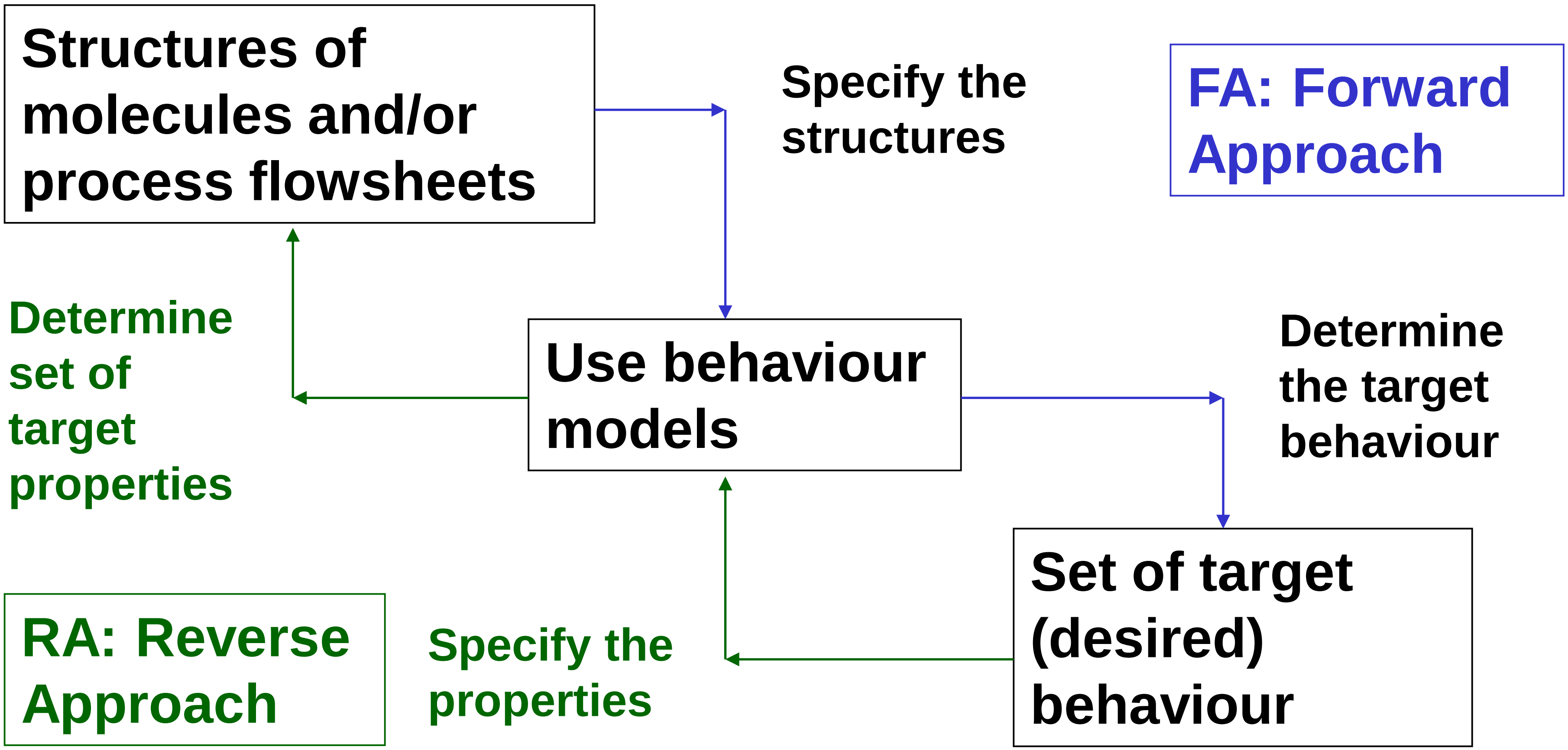
Property Based Design



Usually, FA used for process design while RA used for product design; why not RA & with property models for both?

Solution Approach: Concepts-2

Behaviour Based Analysis



Usually, FA used for both; why not FA for process analysis while RA used for product analysis?

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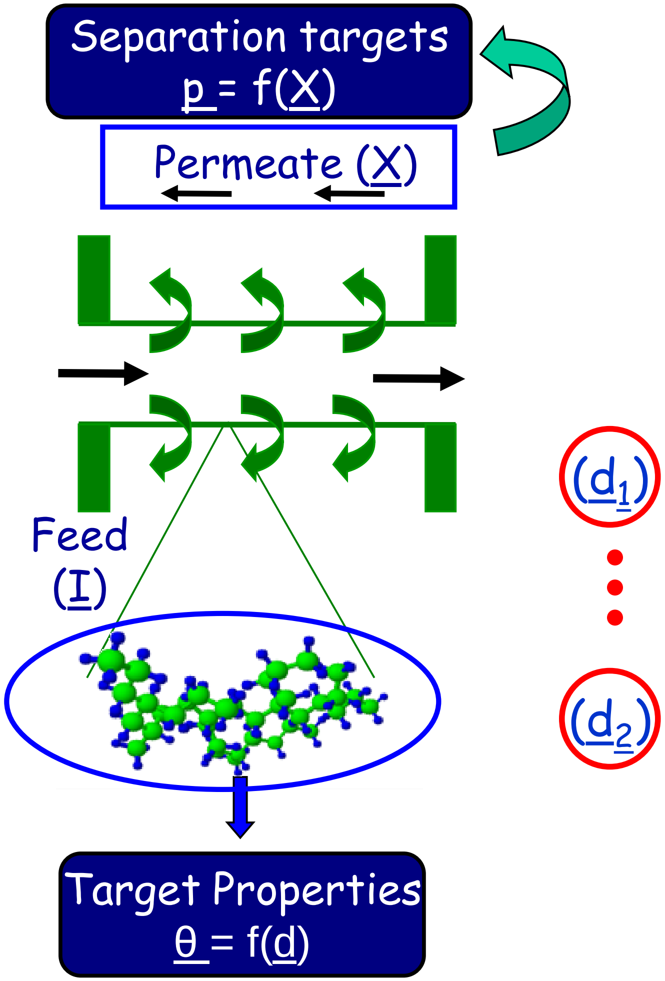
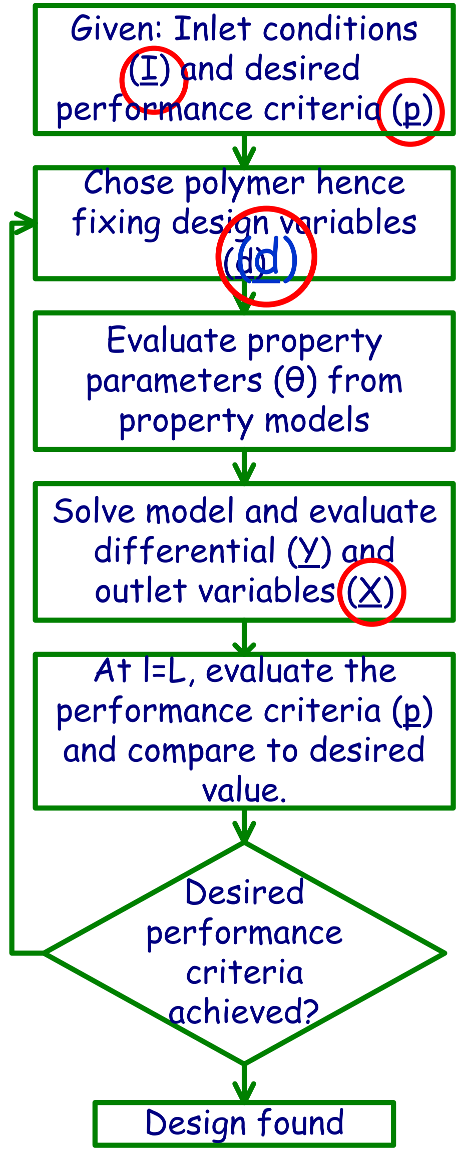
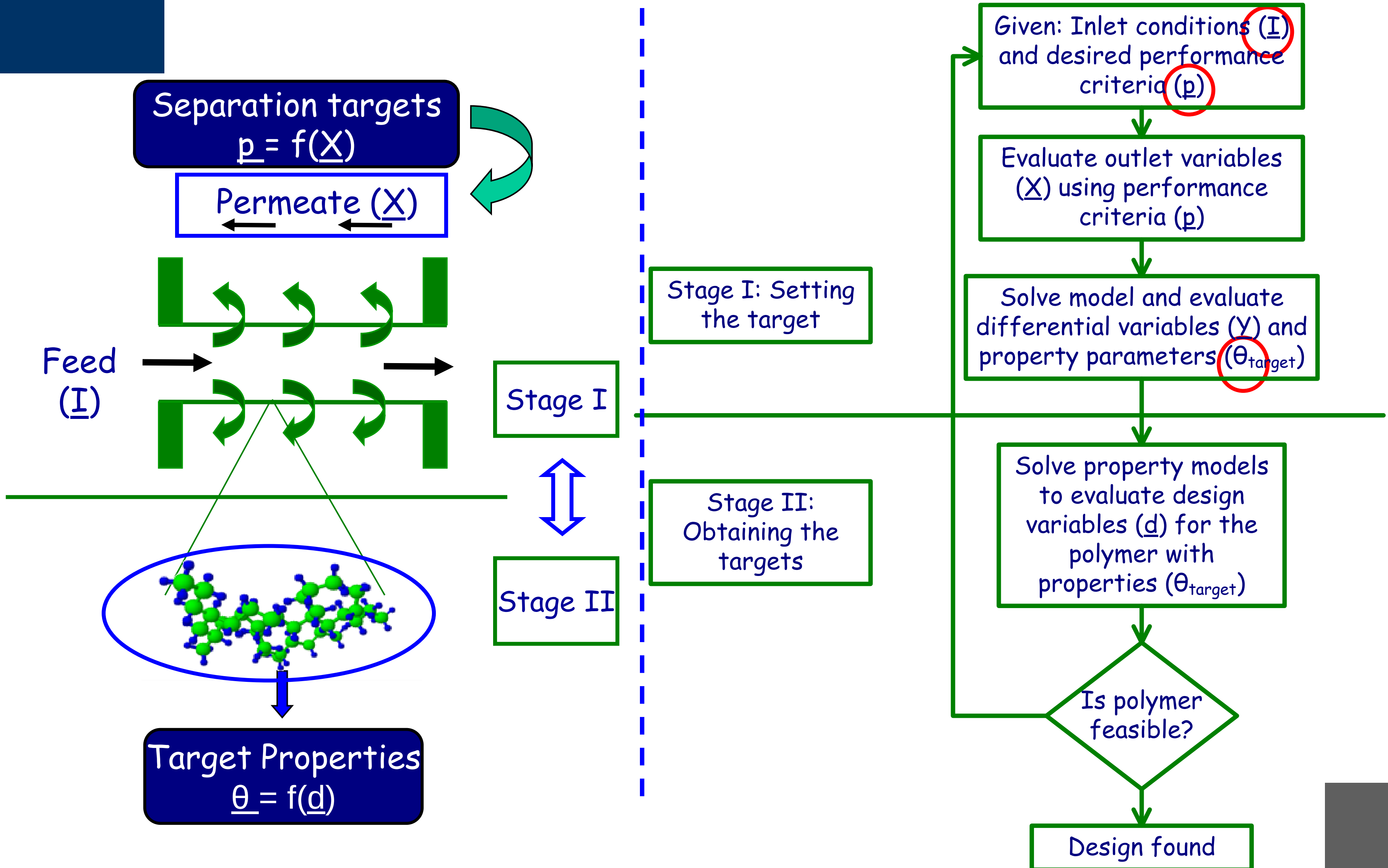
Forward Design Approach - Example





Design of a membrane-based separation process

Reverse Design Approach - Example



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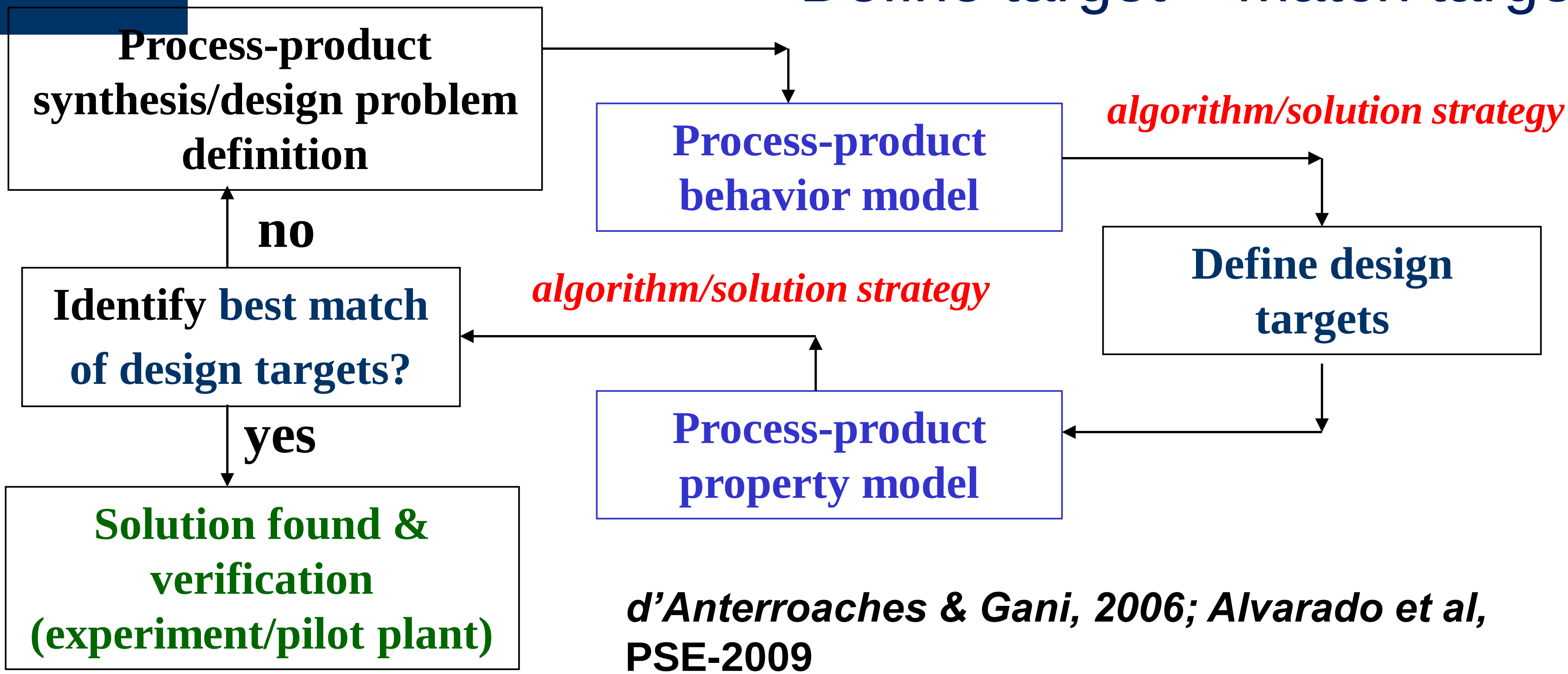
Decomposition-based approach: work flow

Define target – match target

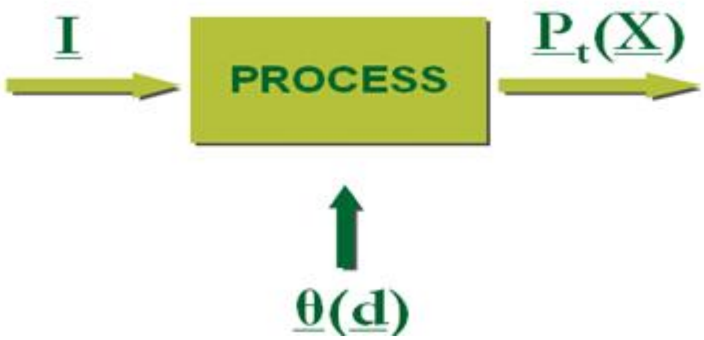


d'Anterroaches & Gani, 2006; Alvarado et al, **PSE-2009**

CAMD = CAFD; functional groups (molecules = process); property prediction (molecules = process)

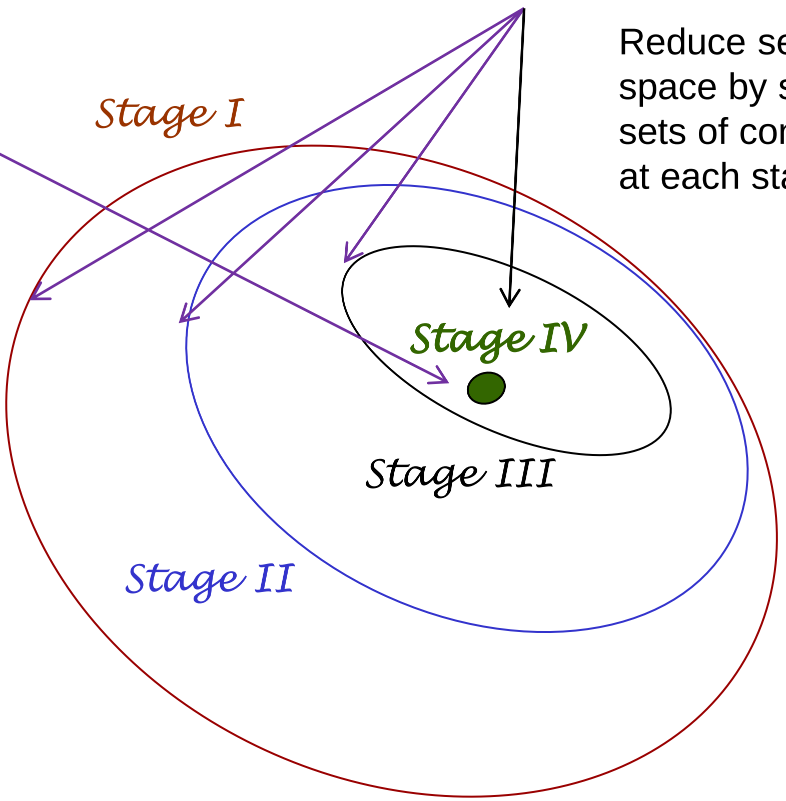
Targeted (Reverse) Approach

1. Define target



2. Match target

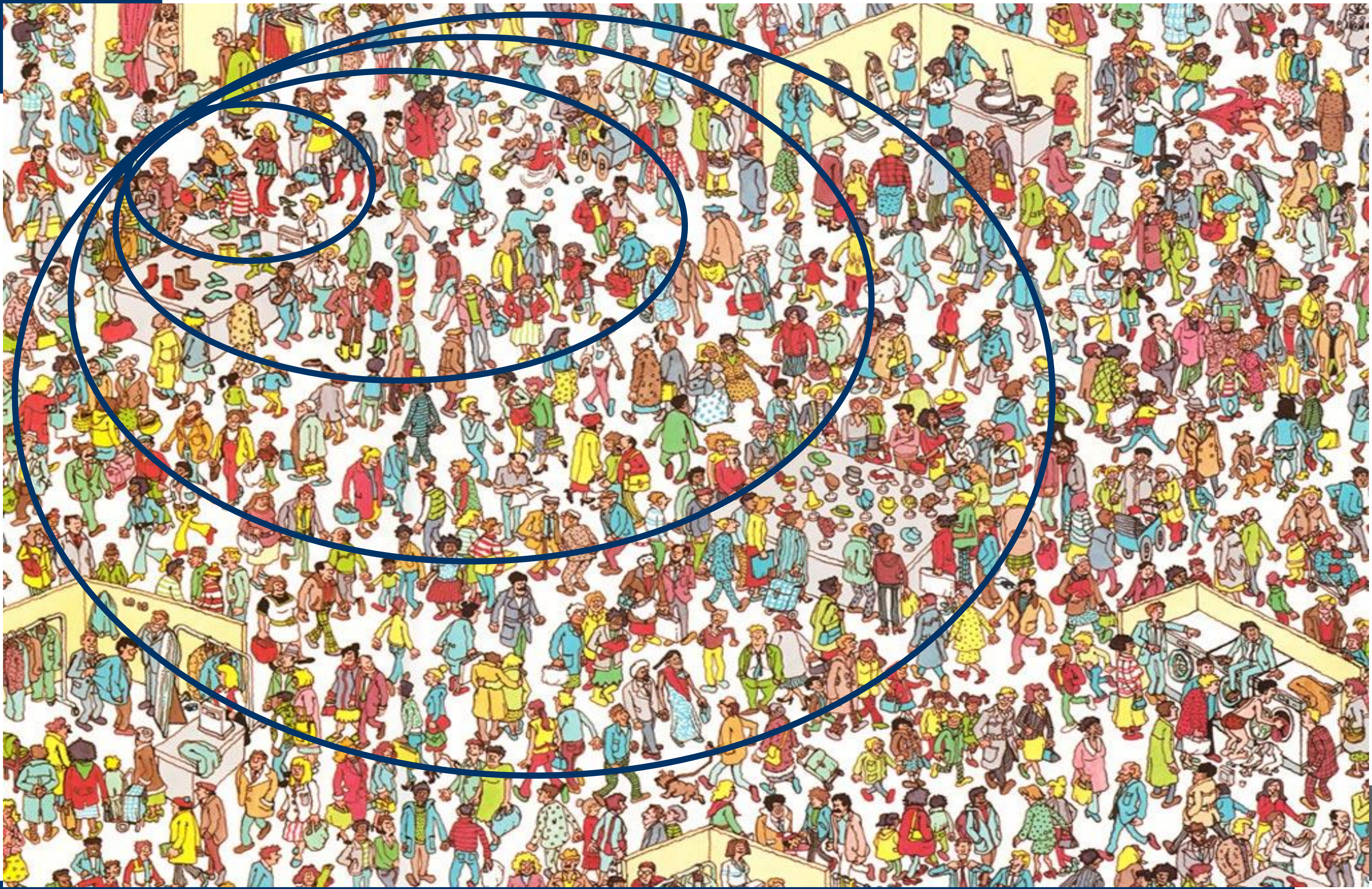
Reduce search space by satisfying sets of constraints at each stage



***Known*: I, X or $P_{t}(\underline{X})$**

***Calculate target*: d or θ (d)**

SPEED Locating the optimal product-pocess is like finding Wally



Manage the complexity by decomposition: example

Objective function

$$\min 2x_1 + 3x_2 + 1.5y_1 + 2y_2 - 0.5y_3 \quad \text{IV} \quad (1)$$

$s.t$

Process model

$$x_1^2 + y_1 = 1.25 \quad (2)$$

II

$$x_2^{1.5} + 1.5y_2 = 3.0 \quad (3)$$

Process constraints

$$x_1 + y_1 \leq 1.60 \quad (4)$$

III

$$1.333x_2 + y_2 \leq 3.00 \quad (5)$$

Flowsheet constraints

$$-y_1 - y_2 + y_3 \leq 0 \quad (6)$$

I

$$y_1 y_2 = 1 \quad (7)$$

Variable bounds

$$x_1, x_2 \geq 0 \quad (8)$$

$$y_1, y_2, y_3 = \{0,1\} \quad (9)$$

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)

Manage the complexity by decomposition: examples

$$\min 2x_1 + 3x_2 + 1.5y_1 + 2y_2 - 0.5y_3 \quad (1)$$

IV

$s.t.$

$$x_1^2 + y_1 = 1.25 \quad (2)$$

$$x_2^{1.5} + 1.5y_2 = 3.0 \quad (3)$$

II

$$x_1 + y_1 \le 1.60 \quad (4)$$

$$1.333x_2 + y_2 \le 3.00 \quad (5)$$

III

$$-y_1 - y_2 + y_3 \le 0 \quad (6)$$

$$y_1 y_2 = 1 \quad (7)$$

I

$$x_1, x_2 \ge 0 \quad (8)$$

$$y_1, y_2, y_3 = \{0,1\} \quad (9)$$

Can we do this for *real* problems?

- **Computer-aided molecular design (1984- CACE, 32/10, 2008, PSE-2009)**
- **Formulation design (Conte et al, PSE-2009)**
- **Process flowsheet design & reverse approach (2006-2009)**
- **Integration of design-control (FOCAPD-2009)**
- **Sustainable process design (Carvalho et al, PSE-2009)**
- **Process intensification (CACE , 33/3, 2009)**

....

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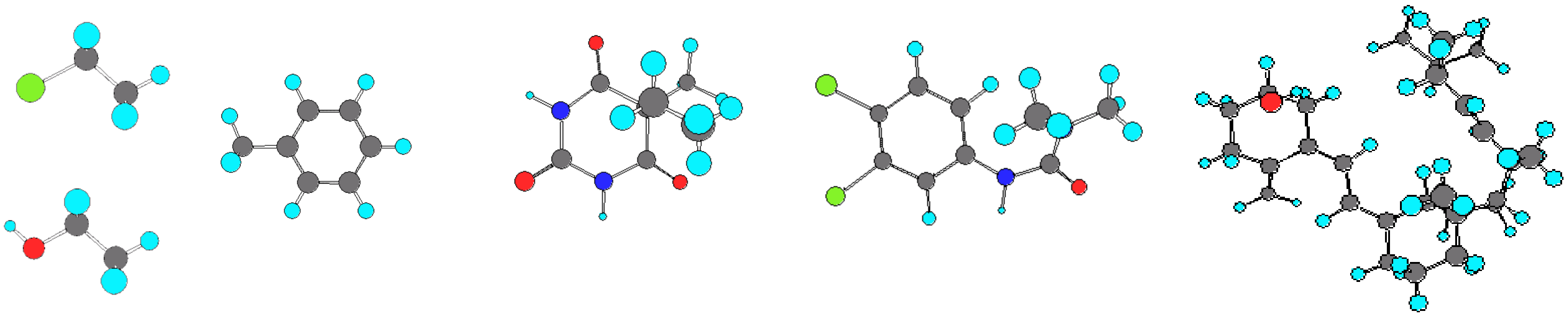
Different Types of Design Problems

1. Design of Molecules (CAMD)

Given, a set of target properties $\underline{\theta}$, find molecules or mixtures that match the target properties

solvents, fluids, … **drugs, pesticides, aroma, ….**

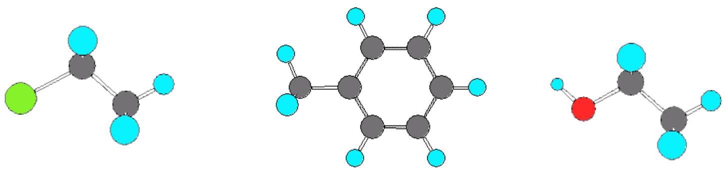


Low ←	**Value** →	**High**
Large ←	**Production rate** →	**Small**
Easy ←	**Finding candidates** →	**Difficult**

Different Types of Design Problems

2. Design of Mixtures (CAM^{b}D)

From a list of 250 solvents, find those that can be used as an oil-paint additive characterized by 25%-, 50%- & 75%-evaporation rate, solubility, viscosity and surface tension. Form the feasible set, find the optimal cost solvent mixture.



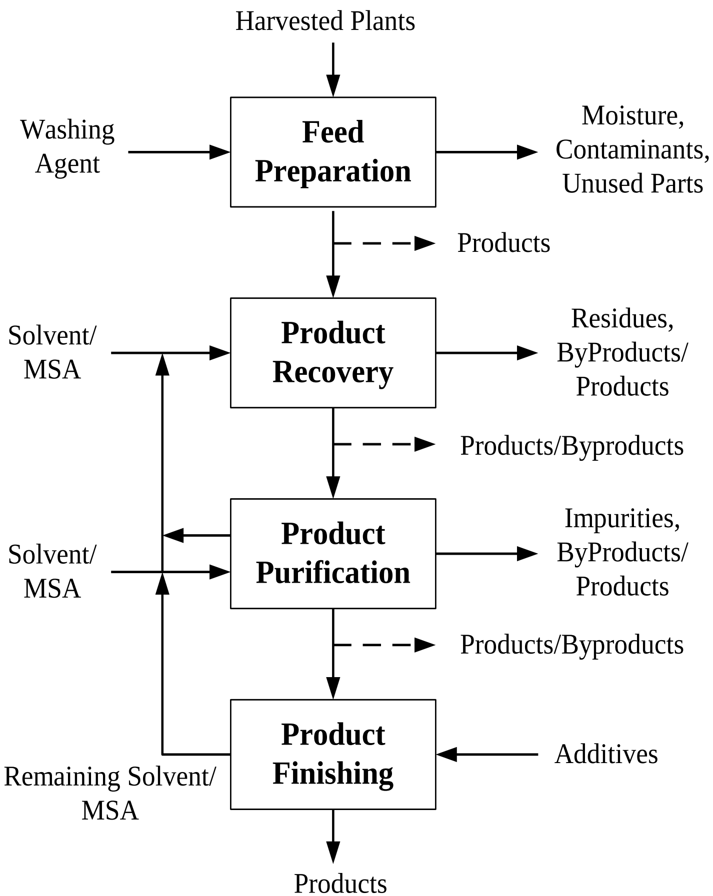
- **Synthesis method for mixtures**
- **Property models for solvents**
- **Evaporation models for solvents**
- **Cost = f(C_i, x_i)**

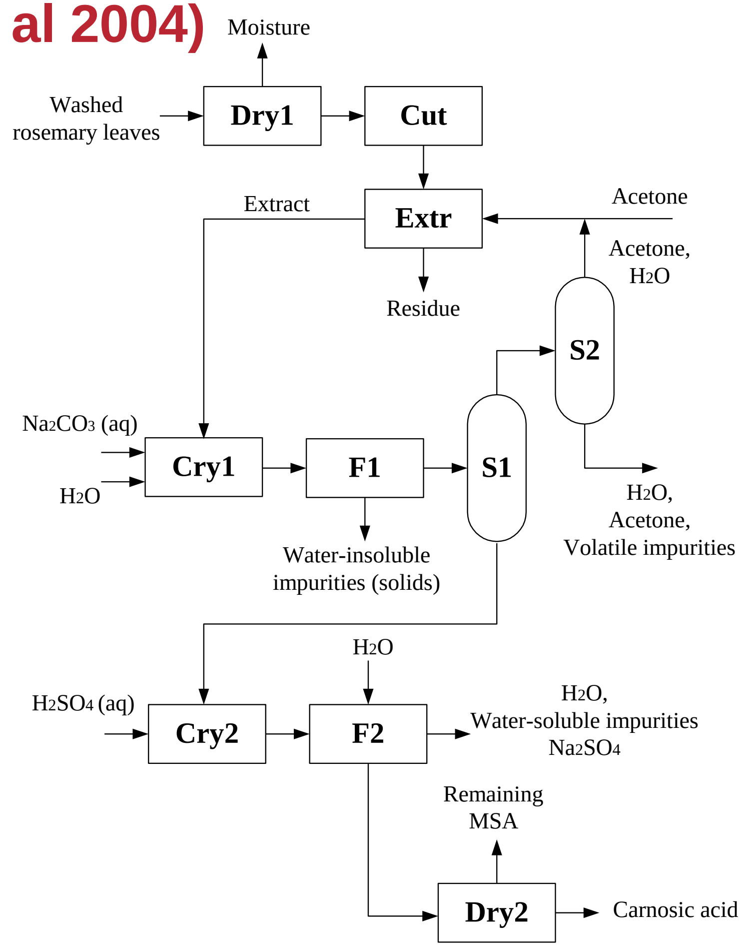
Note: Mixture design similar to oil-blend (petroleum, edible oil, ….), polymer blend, formulations, ….

Different Types of Design Problems

3. Design of Product-centric Process

Example: Manufacture of Carnosic acid by recovering it from popular herbs (Harjo et al 2004)





Different Types of Design Problems

4. Product-Process Evaluation

Given, a list of feasible candidates (product and/or process), the objective is to identify/select the most appropriate product-process based on a set of performance criteria.

For product design, this problem is similar to CAMD but without the generation step; also, similar to CAM^{b}D where additives are added to a product to significantly enhance the performance of the product

Examples

- **Select the optimal combination of pesticide and surfactants that match the needs of specific plants**
- **Select the optimal combination of drug/pesticide, solvent and polymeric microcapsule for controlled release of the product**
- **Increase the yield of a product by hybrid process operation**

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Summary

- Solution of different product-process design problems need a good understanding of the problems so that the available tools can be applied correctly and efficiently
- For computer aided product-process design, models are necessary
  - If appropriate models are available, almost all problems can be solved with an appropriate solution strategy
- Problems related to low-value products are easier to solve than the high-value products
  - The limiting factors for these problems are availability of data and appropriate models