SPEED

New Vistas in Chemical Product & Process Design

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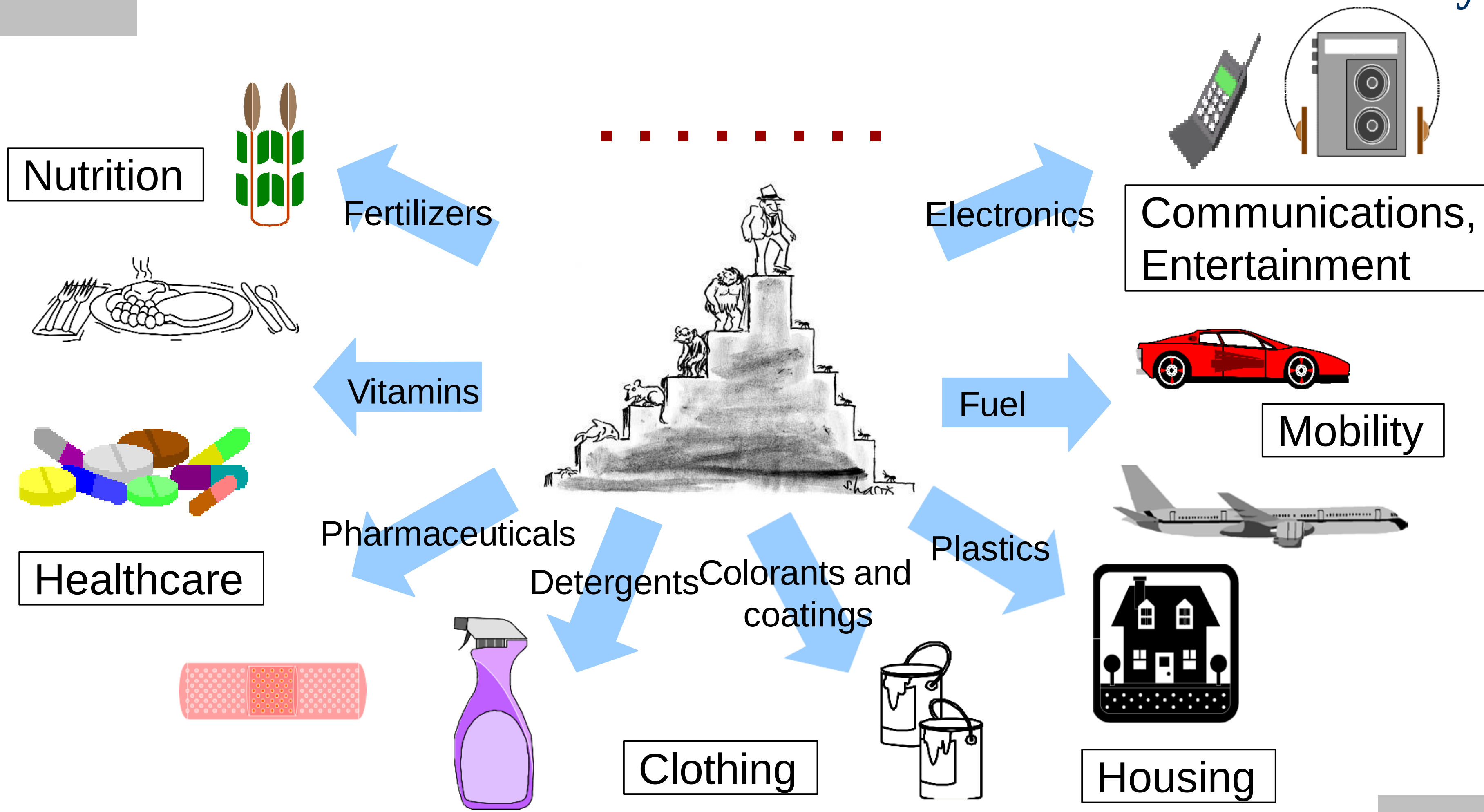
The big picture

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

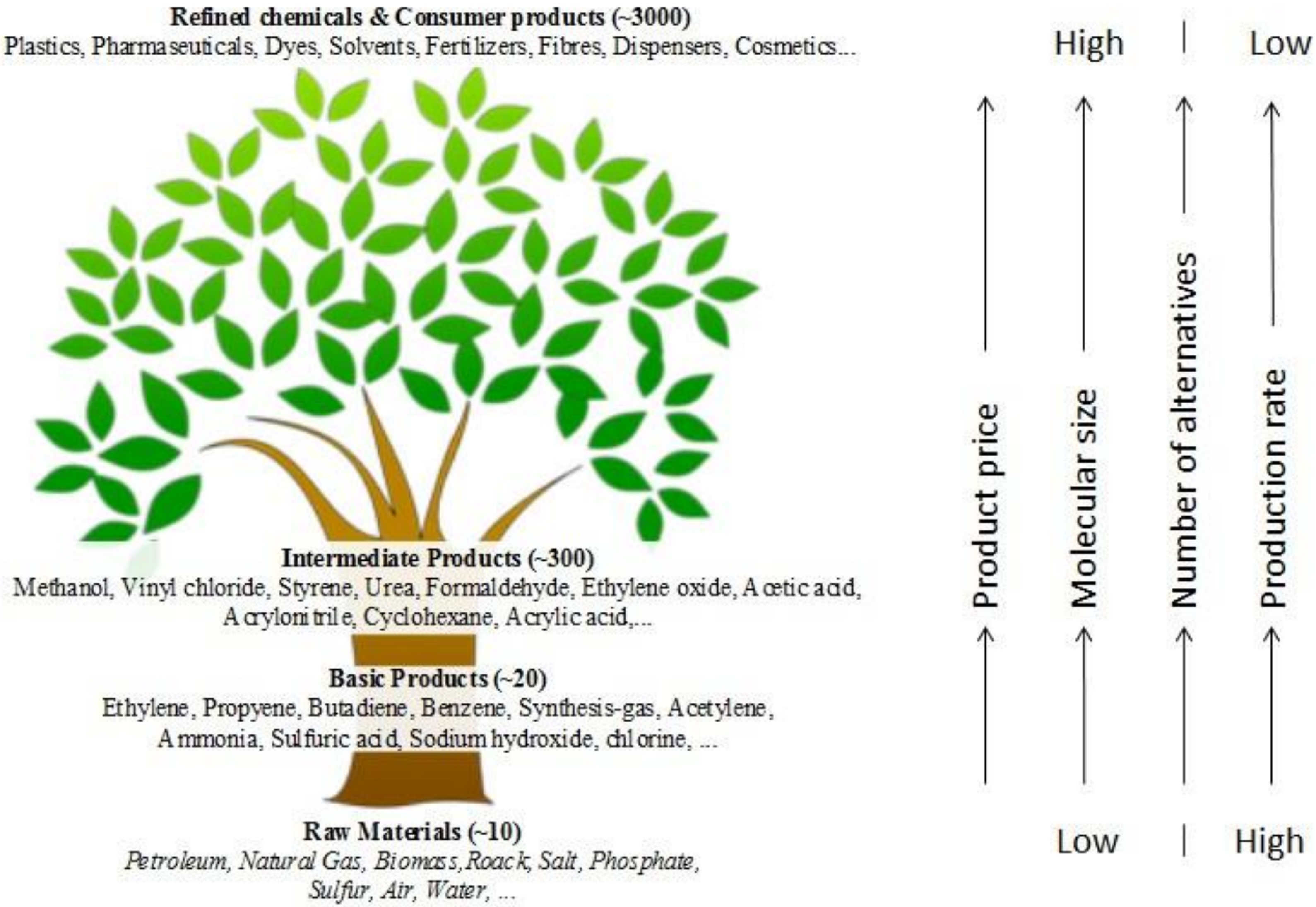
Positive contributions to society



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

The chemical product tree

Question of what, why & when (how)?



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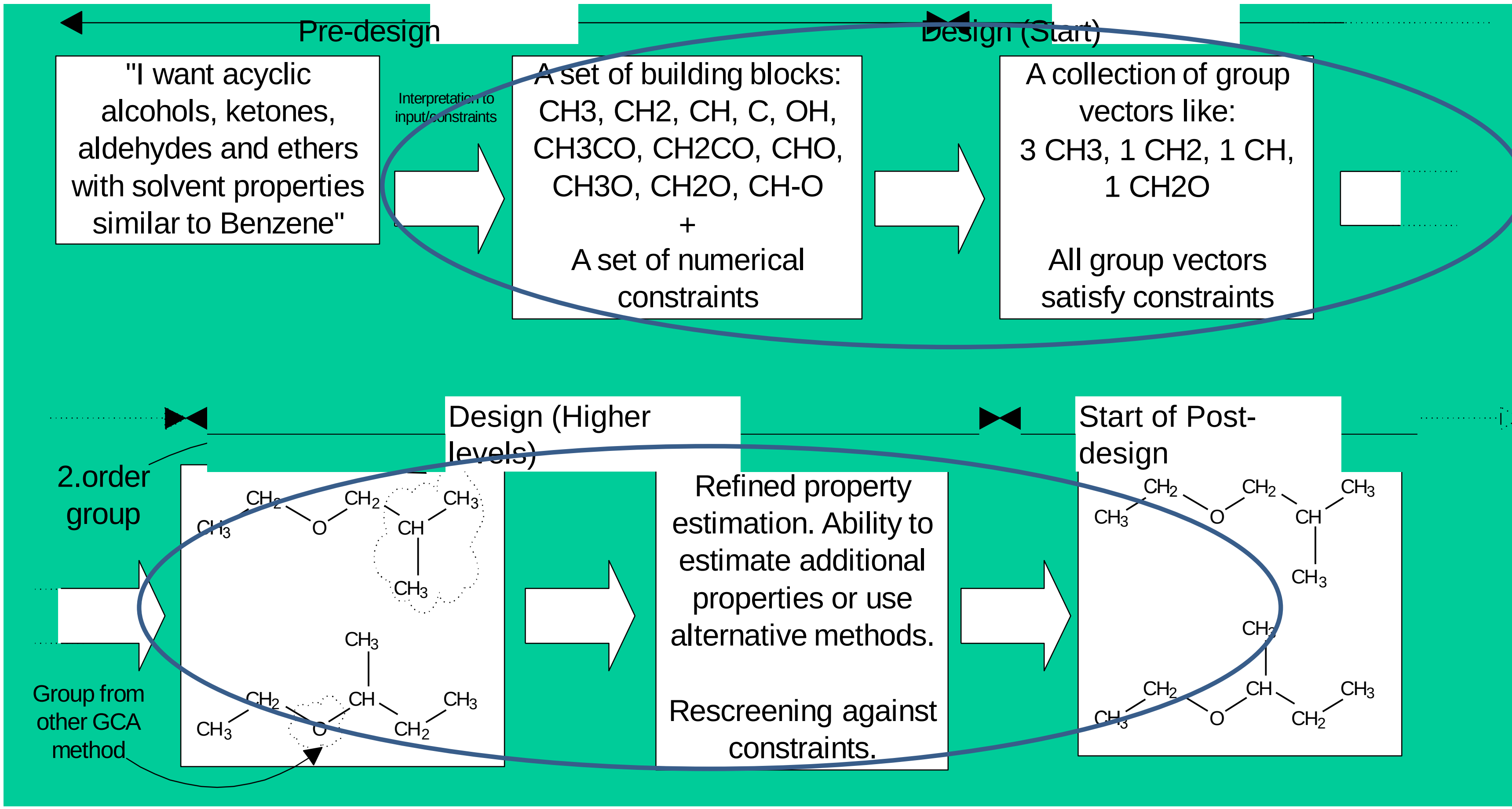
Chemical product classification

Product Type / Issues	Single species		Multiple species		Devices
	Small	Large	Formulated	Functional	
Examples	Solvents, refrigerants	APIs, surfactants, membranes	Blended fuels, solvents, lubricants	Detergents, personal care, healthcare, medicinal	Fuel-cells, microcapsules, hemodialysis device
Key factors in design	Cost of production		Cost and product functions	Product functions	
	N.A.	Time to market (speed)			
Basis of design	Process flowsheet (unit operations)	Synthesis routes (chemistry)	Blend properties and stability	Microstructure	Device form and constituent materials
Measure of performance	Closely related to process	Closely related to application	Closely related to application	Consumer satisfaction	Consumer satisfaction
Challenges in design	Translation of needs to molecular structure	Translation of needs to properties	Delivering product functions defined by needs		Translation of needs to product material properties and configuration
	Large number of product alternatives		Trial & error approach (non-optimal product)		
Risks	Feedstock availability			Absence of engineering science knowledge	
	Environmental impact and sustainability				

The concepts

Design of single species products

Find molecules with desired properties (also valid for mixtures)



Computer aided molecular design (generate & test)

Generation of Alternatives

Groups as building blocks: CH_3 -, - CH_2 -, - OH, CH_3CO -, … (a set of about 180 groups available)

Structural constraints (acyclic molecules)

$$\sum_{j=1}^{m}(2-u_j)n_j = 2q \qquad \sum_{i\neq j}^{m} n_i = n_j(u_j-2)+2 \quad \forall j$$

Size constraints

$$n_j^l \le n_j \le n_j^u \quad \forall j \qquad 2 \le \sum_{j=1}^{m} n_j \le n_{\max} \qquad n = \sum_{j=1}^{m} n_j$$

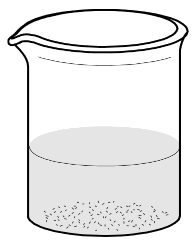
Example: $CH_3 - CH_2 - OH$: Ethanol (3 groups)

Evaluation of Generated Molecules: Models

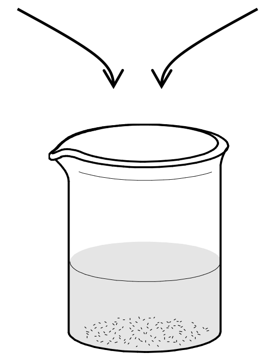
Group contribution (GC) methods for property prediction

GC MODELS

Pure compounds



Mixtures



Examples:

$$V_C = 17.5 + \sum_j n_j \Delta_j$$

Joback & Reid 1987

$$V_c - V_{c0} = \sum_i N_i Vc_{1i} + w \sum_j M_j Vc_{2j} + z \sum_k O_k Vc_{3k}$$

Gani, et al. 2001, 2007, 2012, 2013, 2014

Examples: UNIFAC (VLE, LLE, SLE)

$$\ln \gamma_i = \ln \gamma_i^{COM} + \ln \gamma_i^{RES}$$

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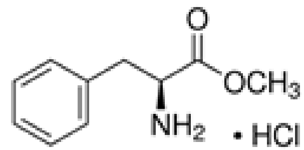
Amino acids property modelling

Compound:	**Molecular structure**
L-Phenylalanine methyl ester hydrochloride Molecula formula: C6H5CH2CH(NH2)COOCH3 · HCl	

First-order groups	**Occurrences**	**Group-contribution**
CH_3	1	0.7473
aCH	5	0.4297
aC-CH2	1	-0.2869
COO (except as above)	1	1.966
-HCl	1	0.4662
Second-order groups	**Occurrences**	**Group-contribution**
--	--	--
Third-order groups	**Occurrences**	**Group-contribution**
CH(NH3+Cl-)-(CH2)n-COO-(CH2)m n in (0,…2); m in (0,…,2)	1	-0.9282

$exp\left(\frac{Tm}{Tm0+a*MW}\right) = \sum_i NiCi + \sum_j MjDj + \sum_l EkOk$ => T_m ^{pred} = 430.9 (Note: Tmo = 237.0611 K; a = -0.0914 K mol g^{-1}). The experimental value of T_m is 433.2 K. Hence, absolute deviation = 2.2 K

Polymer Design: MINLP Applied to CAMD

$$Fobj = \Sigma\, [(P_i - P_i^*)/P_i^*]^2$$

s.t.

$$353\ K < T_g = [\Sigma\,(Y_k n_k)]/\,[\Sigma\,(M_k n_k)] < 393\ K$$

$$1.4 < \rho = [\Sigma\,(M_k n_k)]/\,[\Sigma\,(V_k n_k)] < 1.5\ \ g/cm^3$$

$0.0045 < W = [\Sigma\,(H_k n_k)]/\,[\Sigma\,(M_k n_k)] < 0.0055)$ g H_2O/g polymer)

$2 \leq \Sigma y_j \leq 3$; y_j : 0 or 1 for j=1,7

$$2 \leq \Sigma y_k n_k \leq 9$$

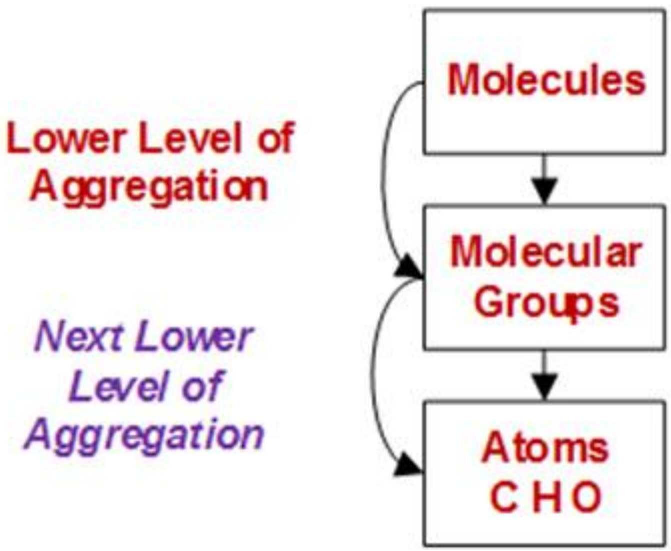
-CH2- ; -CO- ; -COO- ; -O- ; -CONH- ; -CHOH-; -CHCL-

Note: objective function and constraints are non linear; n_k, the optimization variables are integer (0-9)

Polymer repeat units designed for bottle-stops; synthetic fibers; coatings, etc (CACE 2009)

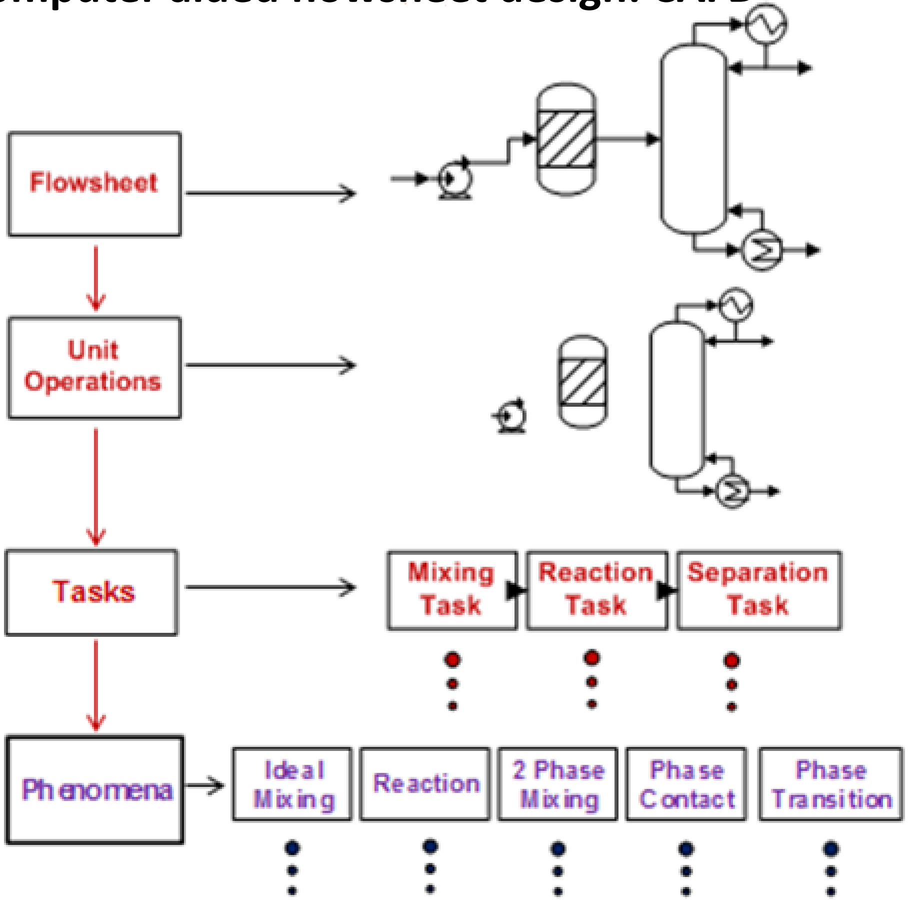
CAMD versus CAFD

Computer aided molecular design: CAMD



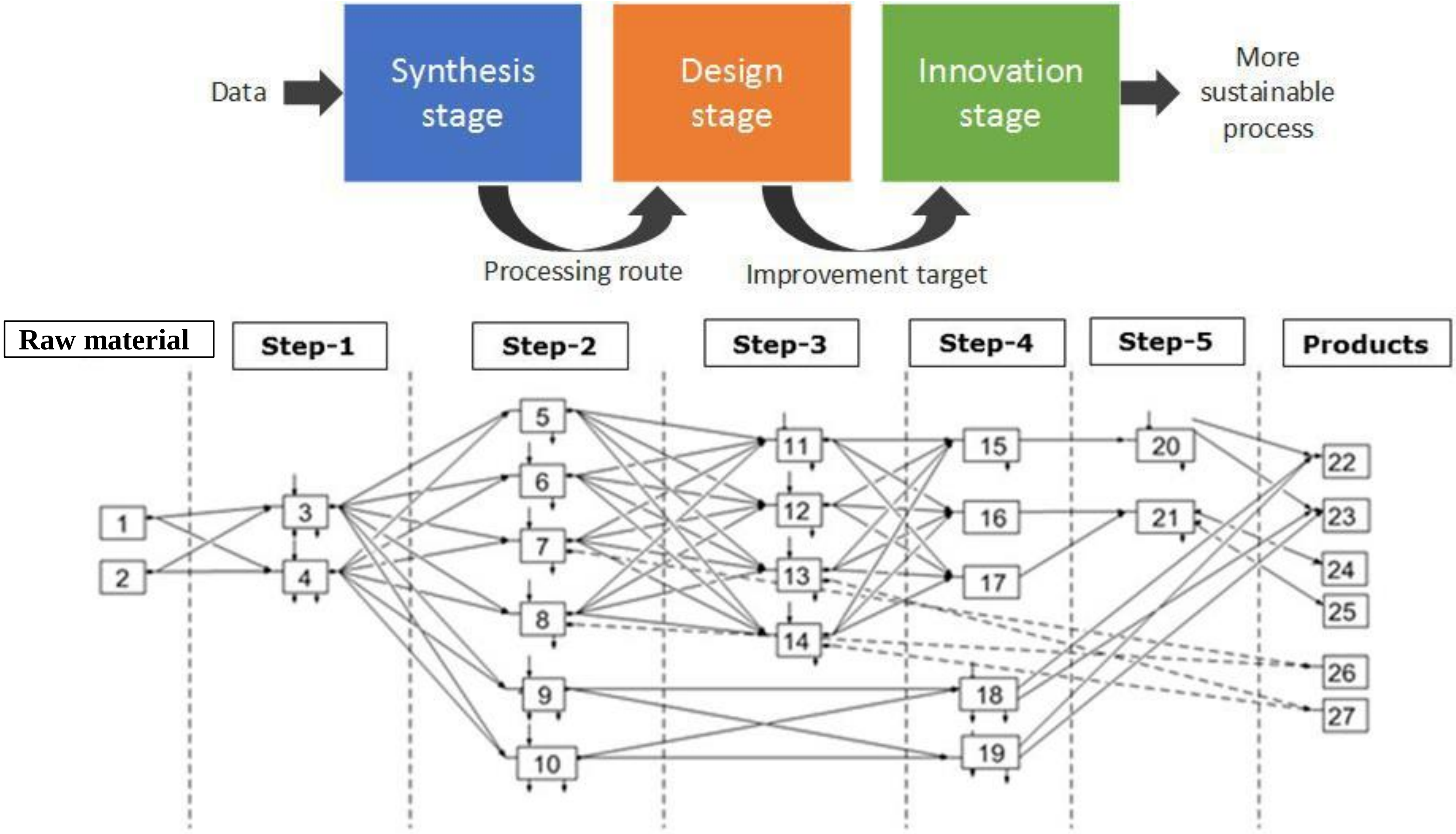
Gani et al. (1994)

Computer aided flowsheet design: CAFD



Babi et al. (2014)

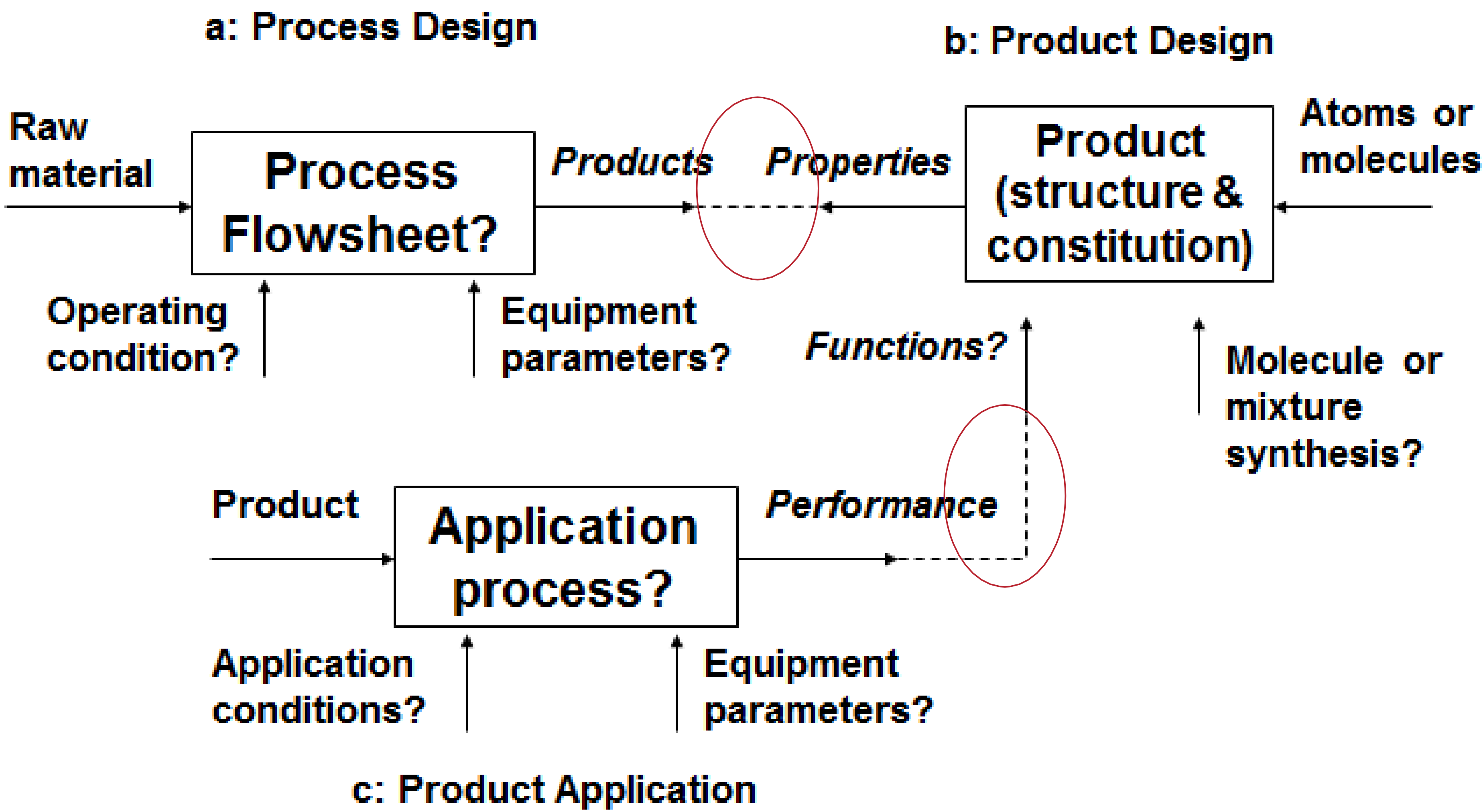
Sustainable Product-Process Development



Applications: Biorefinery; CCU; CAMD; Waste-water treatment; …..

The problem definitions

Product-process & product-application relations



Problems may have multiscale & multidiscipline features

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Mathematical generic problem formulation

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

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

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

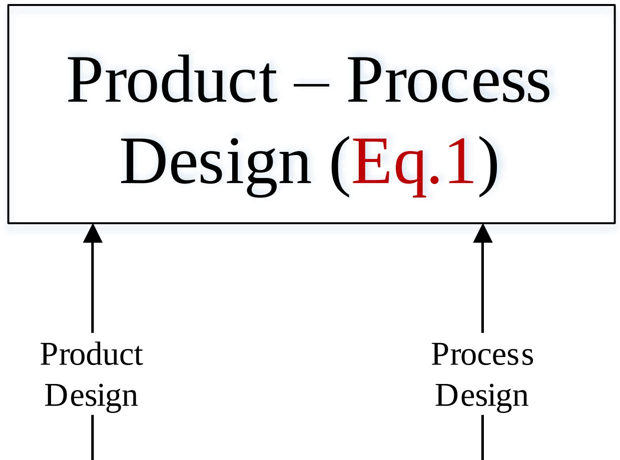
$l_2 \leq g_2(\underline{x}, \underline{y}) \leq u_2$ **molecular structure constraints (Eq. 6)**

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

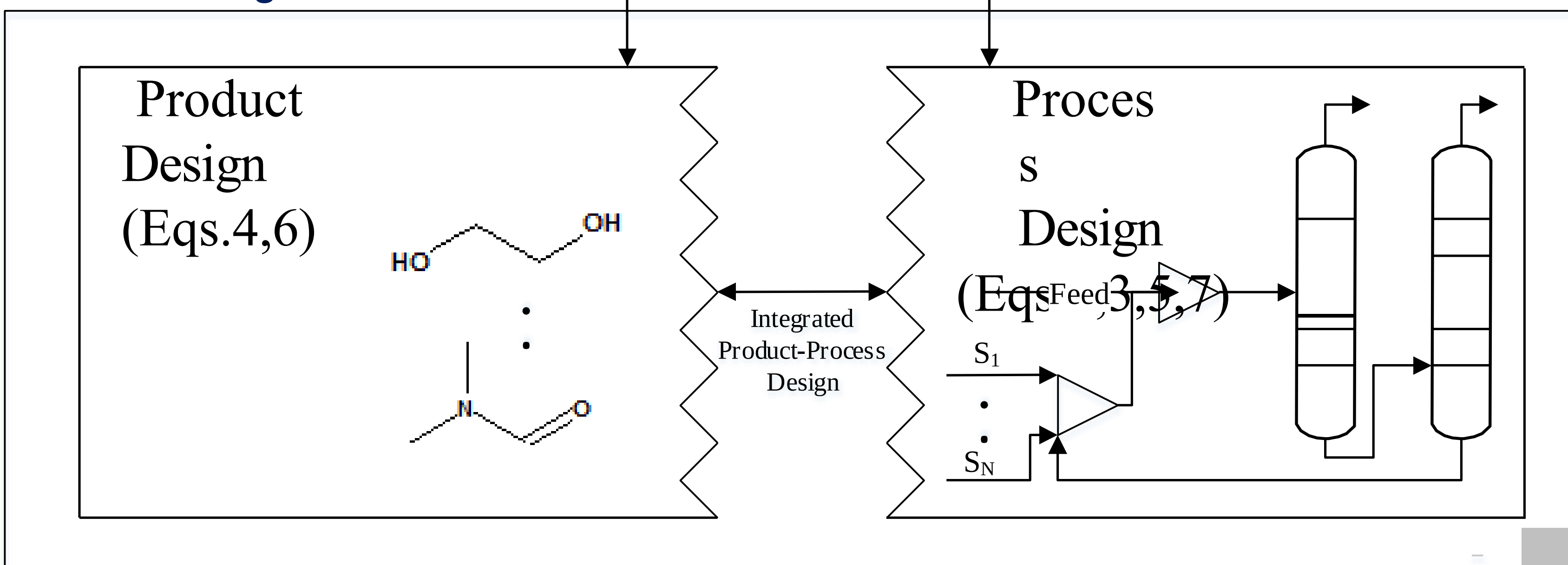
$\underline{x}$: real-process variables; $\underline{y}$ integer-decision variables;
u: process design variables; d: process input variables;
θ: property; B, C, D coefficient matrices

SPEED 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 constrainst
Eq. 7: Processing networks



- Process simulation
- Process optimization
- Product evaluation
- Optimal product
- Product + implicit application
- Product-process-application
- ……….



Simultaneous Product – Process Design (multiscale & multidiscipline)

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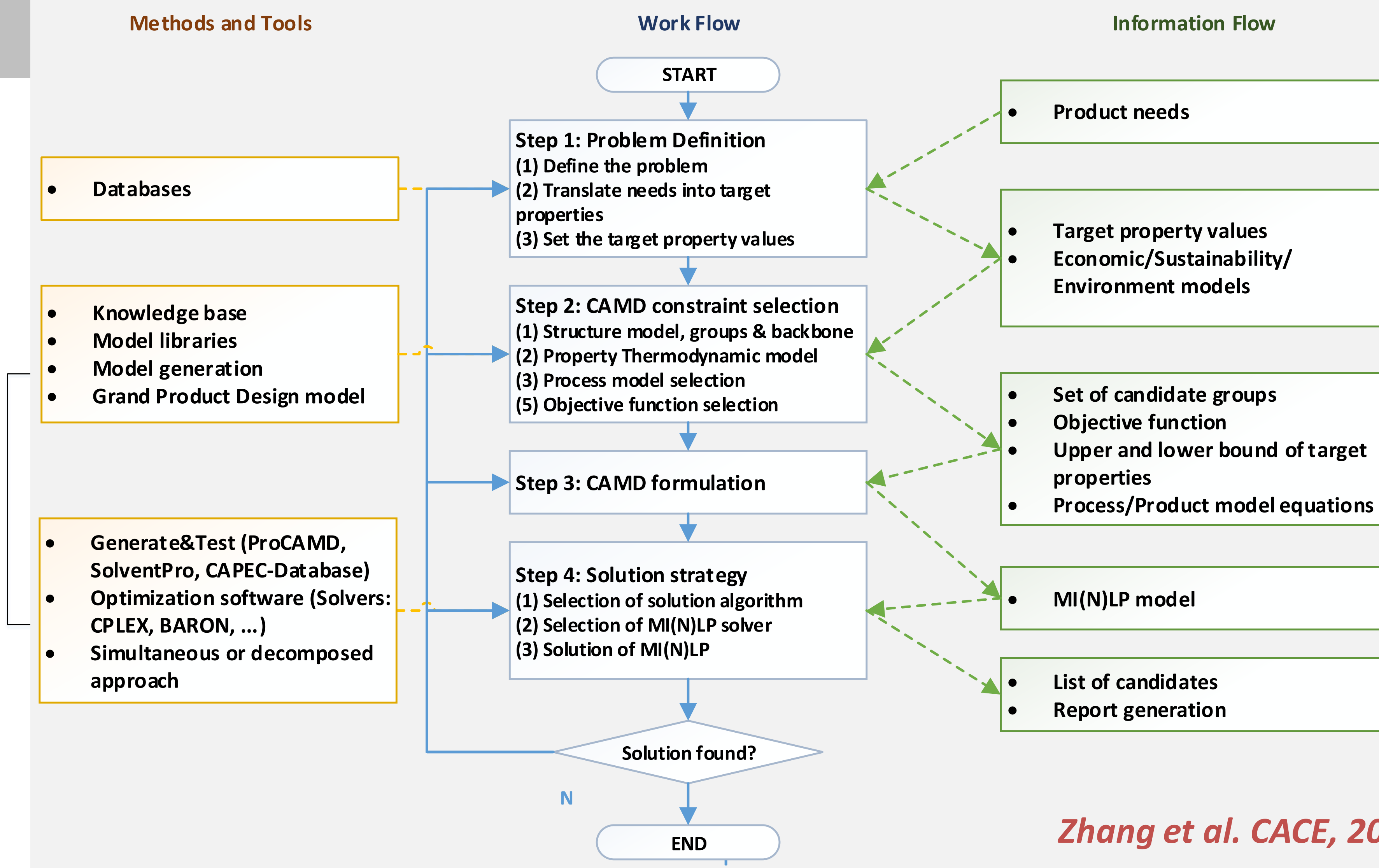
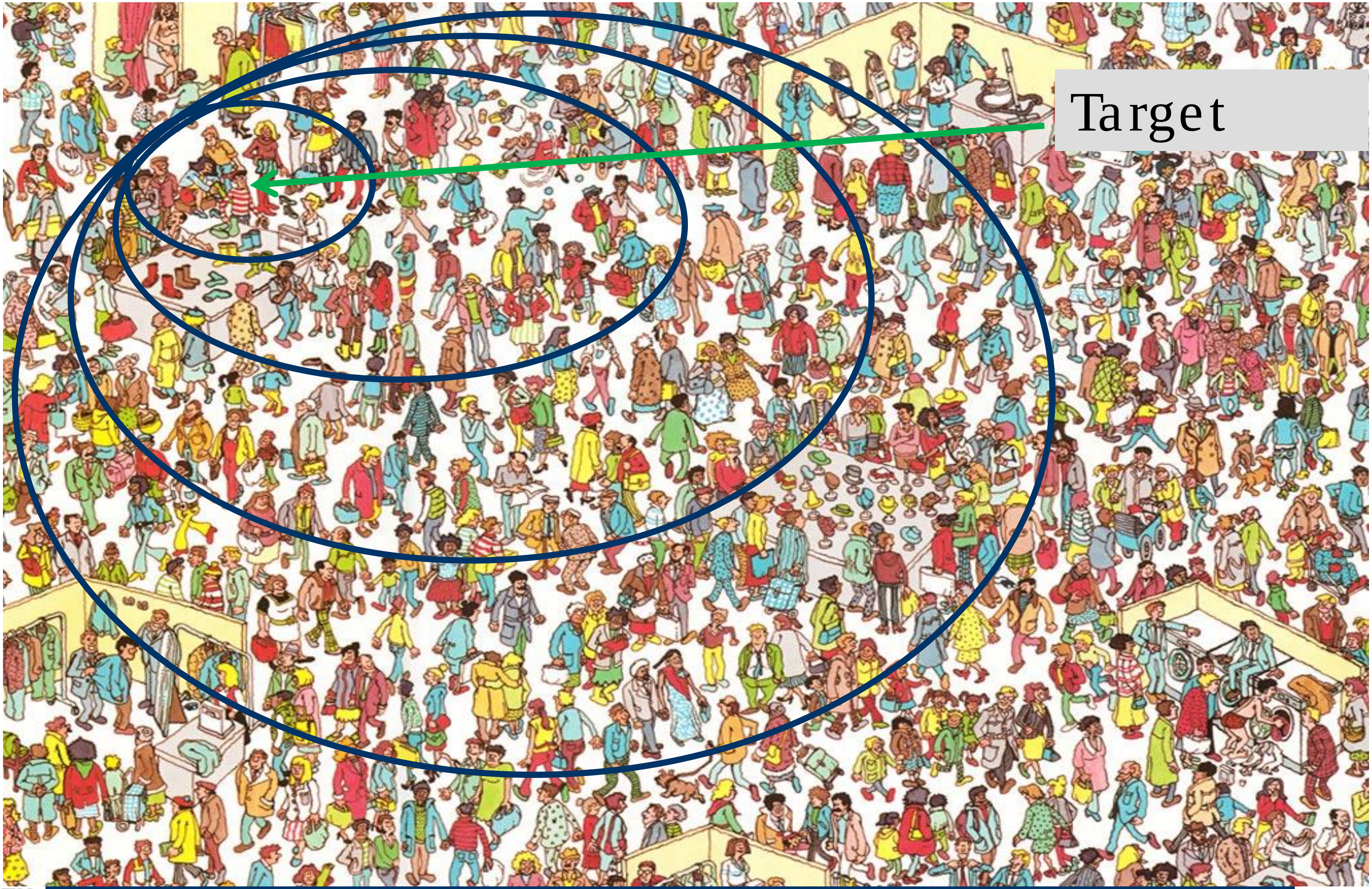
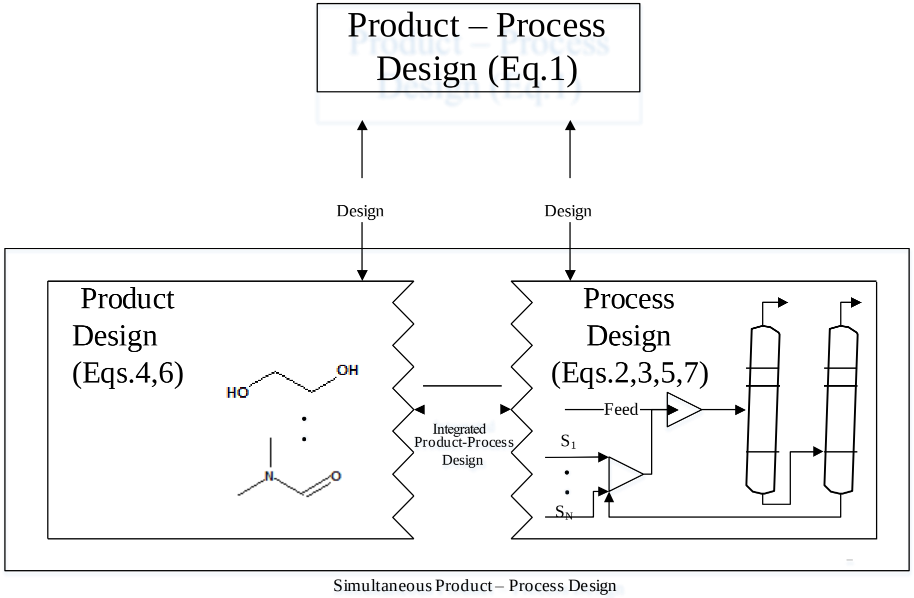
Concept of model based framework



Zhang et al. CACE, 2015

Mathematical Problem Solution

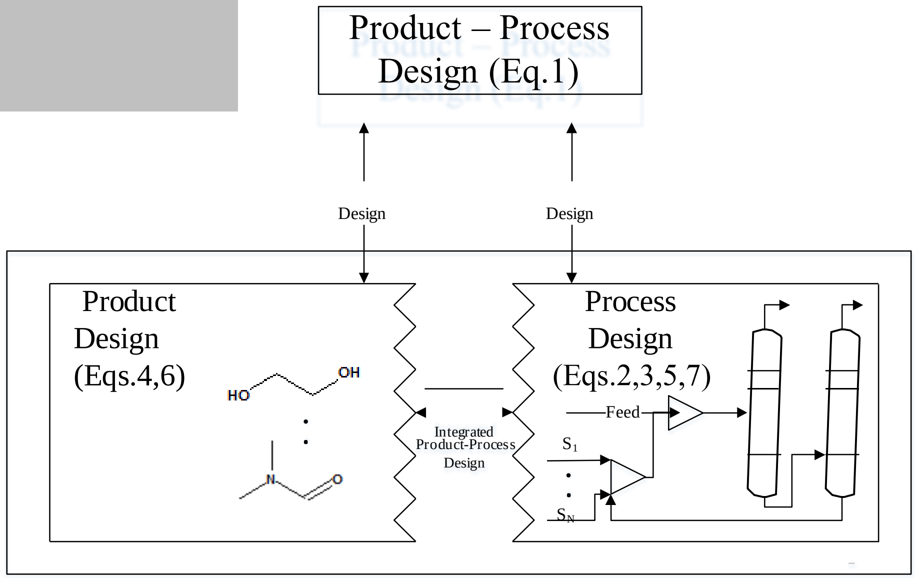




Eqs. 4, 6 with or without Eq. 1 (product design and implicit performance verification)

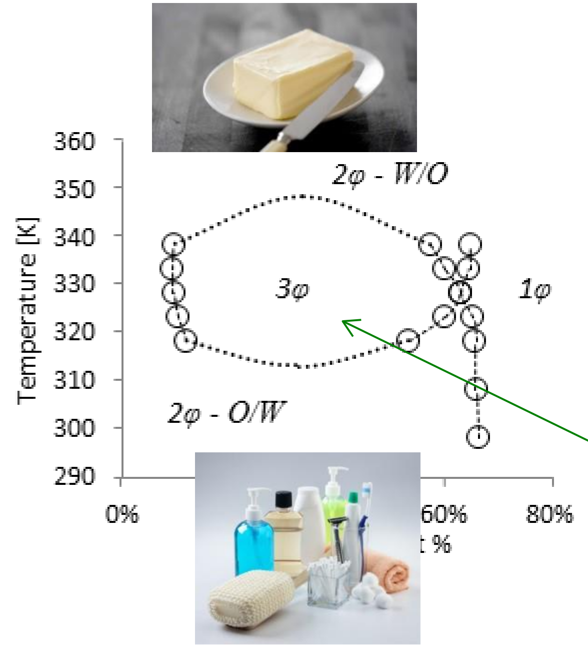
Examples: Molecular design (single species products)

- **Solvents**
- **Process fluids**
- **Surfactants**
- **Active ingredients**
- **Polymer repeat units**
- **…..**



Simultaneous Product – Process Design

Examples: Molecular design (single molecular products) -Surfactants

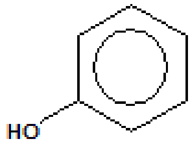


Homogeneous reactions

Eqs. 4, 6 with or without Eq. 1 (product design and implicit performance verification)

Surfactant Design - Product Design (1/3)

- **Step 1:** Design of a UV sunscreen, in the emulsified form, with a high sun protection factor. The phenol ring is fixed as backbone structure in this case study.
- **Step 2: Convert needs-functions to properties**
  - **Objective:** Toxicity should be minimized, but higher than a lower bound
  - **Group selection:** CH_3 , CH_2 , CH , C , aCH , aC-OH , CH_2COO , CH_3O , CH_2O , aC-O , OCH_2CH_2OH from 220 groups (Marrero and Gani, (2001)).
  - **Backbone selection:** $-C_6H_4OH$



  - **Structural and property constraints:**

Need	Lower bound	Upper bound
N_G	10	15
N_F	0	8
$lc50$	3.16log(mol/L)	-
Sp	-	25MPa$^{0.5}$
clp	343.15K	-
Fp	343.15K	-
Vm	0.1cc/mol	0.3cc/mol

LC_{50}: Fathead Minnow 96-hr exposure; *Sp*: Hildebrand solubility parameter; *clp*: cloud point; *Fp*: Flash point; *Vm*: Liquid molar volume at 298K.

Surfactant Design (2/3)

- **Step 3: Formulate the mathematical problem**

$$\max lc50 = lco + \sum_{i_1} n_{i_1}^{(1)} lc50_{i_1}^{(1)} + \sum_{i_2} n_{i_2}^{(2)} lc50_{i_2}^{(2)}$$

1. Structural constraints:

1.1 Octet rule and group number constraints:

$$\sum_{i} (2 - \nu_{i_1}) n_{i_1}^{(1)} = 0$$

$$\sum_{i_1, i_1 \neq i_1'} n_{i_1}^{(1)} \geq n_{i_1'}^{(1)} \left(\nu_{i_1'} - 2\right) + 2 \quad \forall i_1'$$

$$1 \leq n_{i_1}^{(1)} \leq 5 \quad \forall i$$

$$10 \leq \sum_{i_1} n_{i_1}^{(1)} \leq 15$$

1.2 Adjacency matrix constraints.

1.3 Second-order group constraints.

2. Pure component property constraints:

$$lco + \sum_{i_1} n_{i_1}^{(1)} lc50_{i_1}^{(1)} + \sum_{i_2} n_{i_2}^{(2)} lc50_{i_2}^{(2)} \geq 3.16$$

$$Spo + \sum_{i_1} n_{i_1}^{(1)} Sp_{i_1}^{(1)} + \sum_{i_2} n_{i_2}^{(2)} Sp_{i_2}^{(2)} \leq 25$$

$$\sum_{i_1} n_{i_1}^{(1)} clp_{i_1}^{(1)} \geq 343.15$$

$$Fpo + \sum_{i_1} ni_1^{(1)} Fp_{i_1}^{(1)} + \sum_{i_2} n_{i_2}^{(2)} Fp_{i_2}^{(2)} \geq 343.15$$

$$0.1 \leq Vmo + \sum_{i_1} ni_1^{(1)} Vm_{i_1}^{(1)} + \sum_{i_2} n_{i_2}^{(2)} Vm_{i_2}^{(2)} \leq 0.3$$

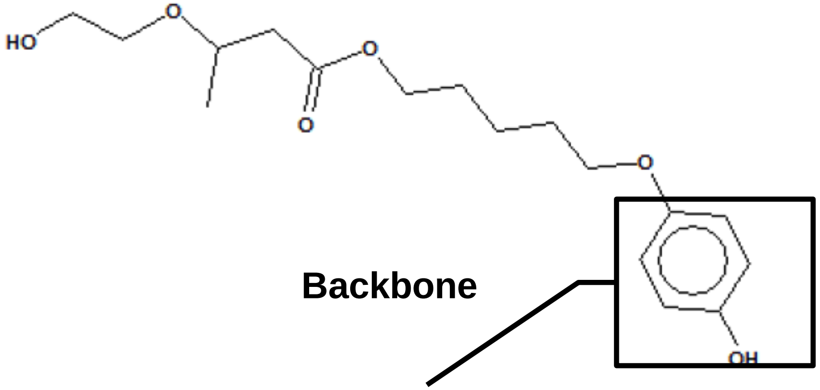
#Equations: 1,324,764; #Variables: 1,286,278 (1,286,266 Integer variables).

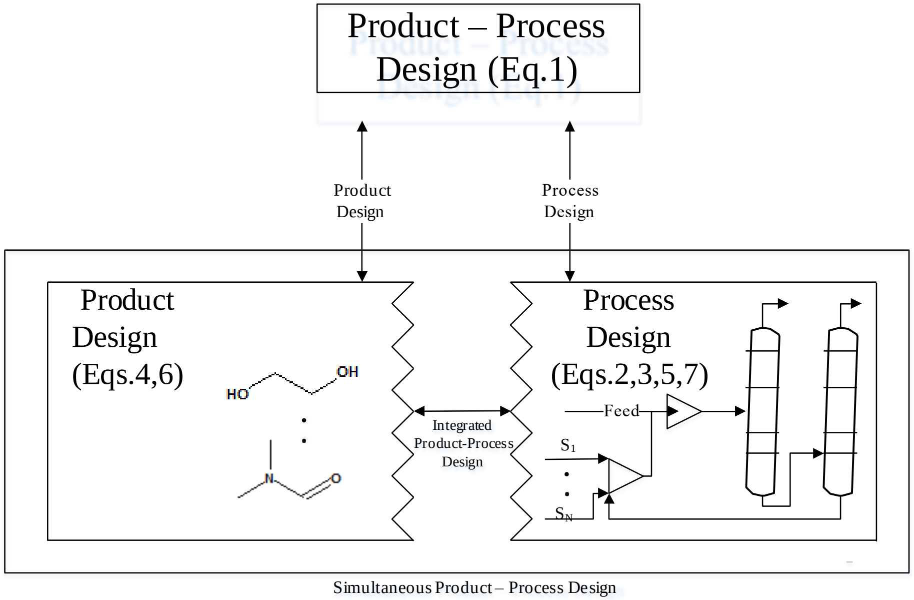
- **Step 4:** This design problem can also be solved directly using the GAMS CPLEX solver.

Surfactant Design (3/3)

Table: Optimization results of surfactant design problem

n_1	1 CH_3, 5 CH_2, 1 CH, 4 aCH, 1 aC–OH, 1 CH_2COO, 1 aC–O, 1 OCH_2CH_2OH
n_2	1 AROMRINGs1s4
$lc50$	4.124log(mol/L)
Sp	24.732MPa$^{0.5}$
clp	300.016K
Fp	552.383K
Vm	0.281cc/mol



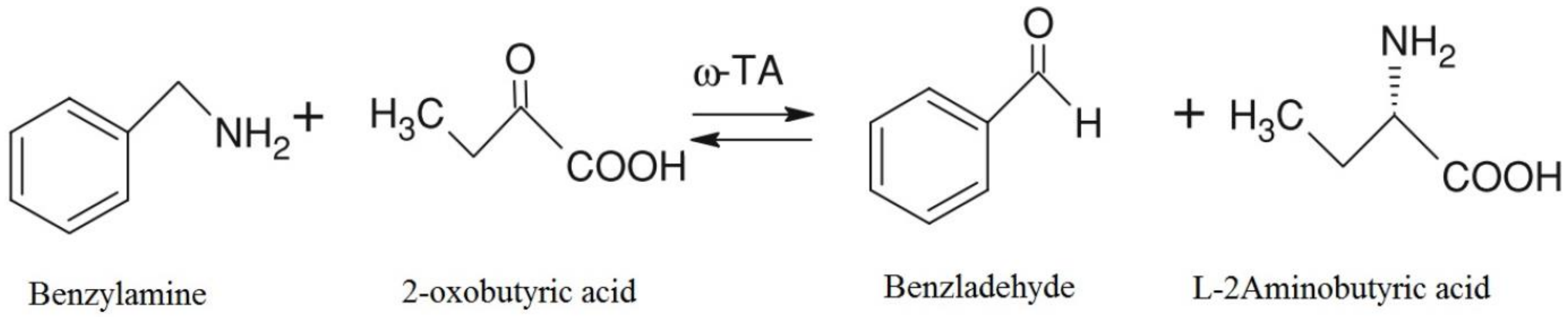


Eqs. 2, 3, 4, 5, 6 with or without Eq. 1 (product-process development; solvent design-verification)

Examples: Molecular and/or mixture design with process application

- **Solvents for separations and/or product recovery**
- **Process fluids for specific operations**
- **Reactive agents**
- **…..**

Generation of alternatives for the production of L-2-aminobutyric acid



Objective of the study: Identify possible process hotspots to improve the process in terms of:

- Conversion to continuous manufacturing
- Solvent selection to improve productivity
  - Reaction improvement
  - Separation improvement

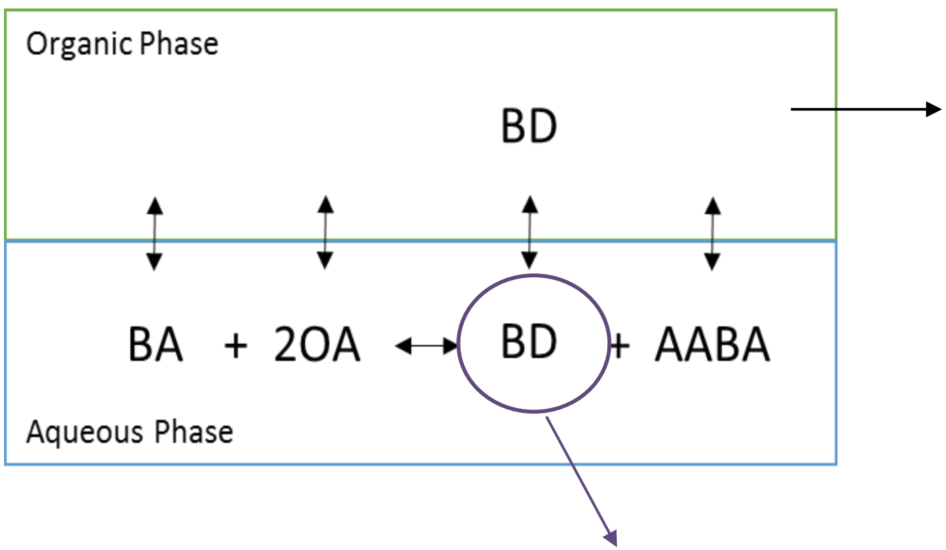
SPEED Solvent based reaction-separation processes

Generation of alternatives for the production of L-2-aminobutyric acid

Reaction type Database

A. Single phase system
B. Biphasic system

Experimental data available
Kinetic model is not available



Solvent selection:

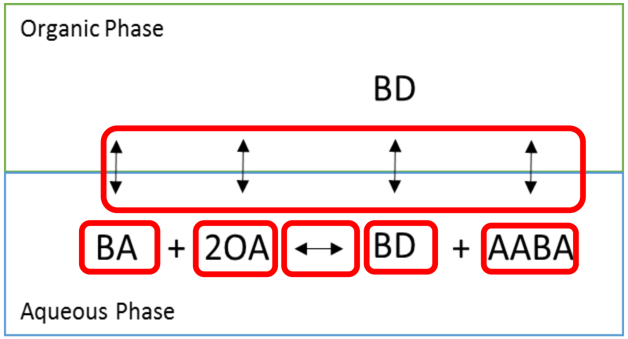
Organic solvent that is,

- Immiscible with the aqueous phase
- Higher by-product selectivity

Inhibits the enzyme

Solvent based reaction-separation processes

Generation of alternatives for the production of L-2-aminobutyric acid

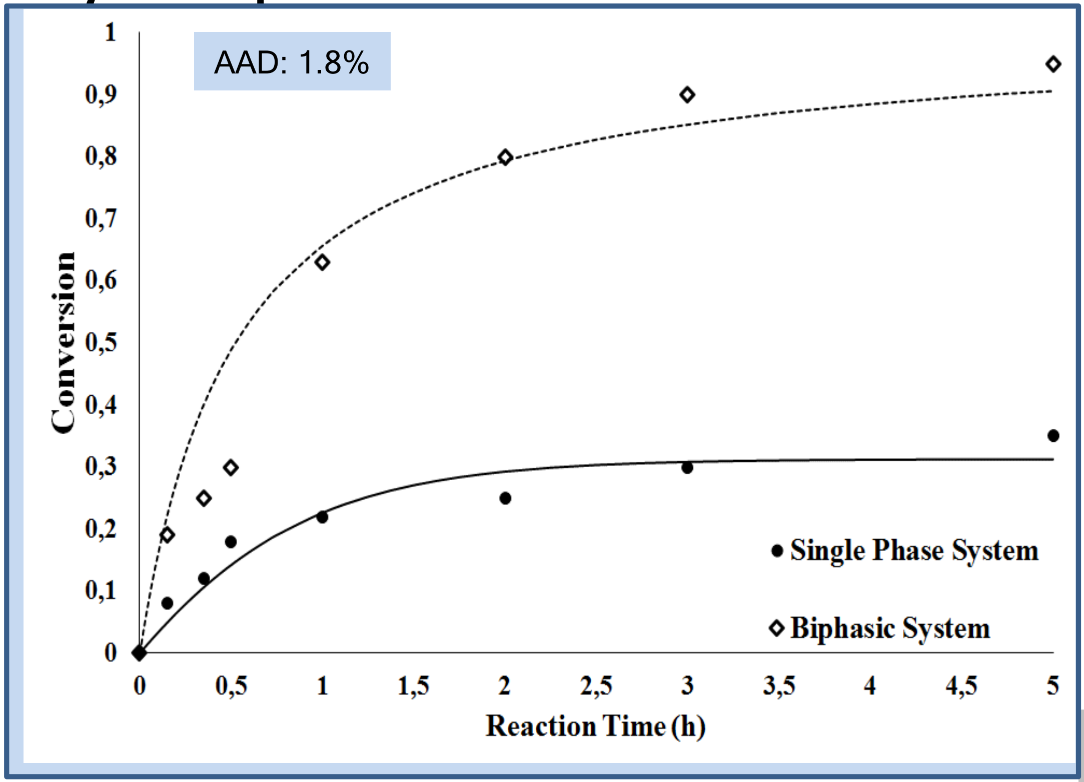


Model development method: Multiphase reaction modeling (Anantpinijwatna et al. 2016)

Physical Equilibrium **Mass Balance**

Reaction type Database:

Experimental data



Generation of alternatives for the production of L-2-aminobutyric acid

Extractive solvent selection:

Partition $\left(\frac{\gamma_i^\alpha}{\gamma_i^\beta}\right)$	Benzylamine	2OA	AABA	Benzaldehyde
Hexane	0.986	8.33E-06	4.50E-06	8.06E+03
Heptane	1.178	5.41E-06	3.56E-06	8.33E+03
Isooctane	3.096	8.33E-06	6.85E-06	1.59E+04
Octane	2.959	3.73E-04	1.19E-04	1.30E+04

Batch to continuous :

Batch to continuous database

Enzyme membrane reactor

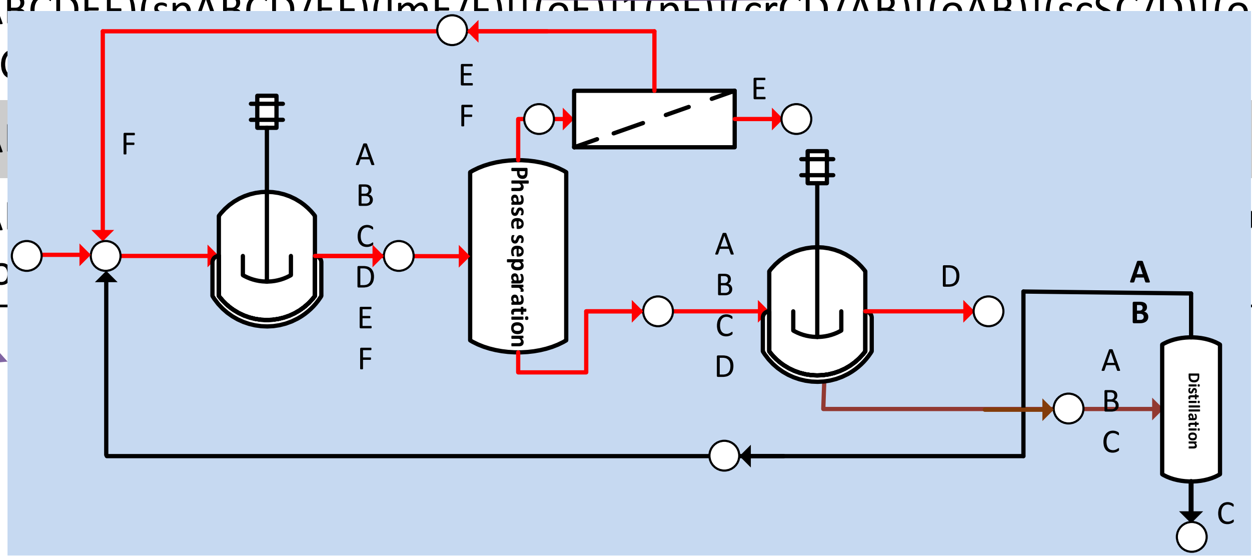
Facilitates enzyme stability and avoid the enzyme contact with the organic solvent in a continuous operation

Generation of alternatives for the production of L-2-aminobutyric acid

Objectives:

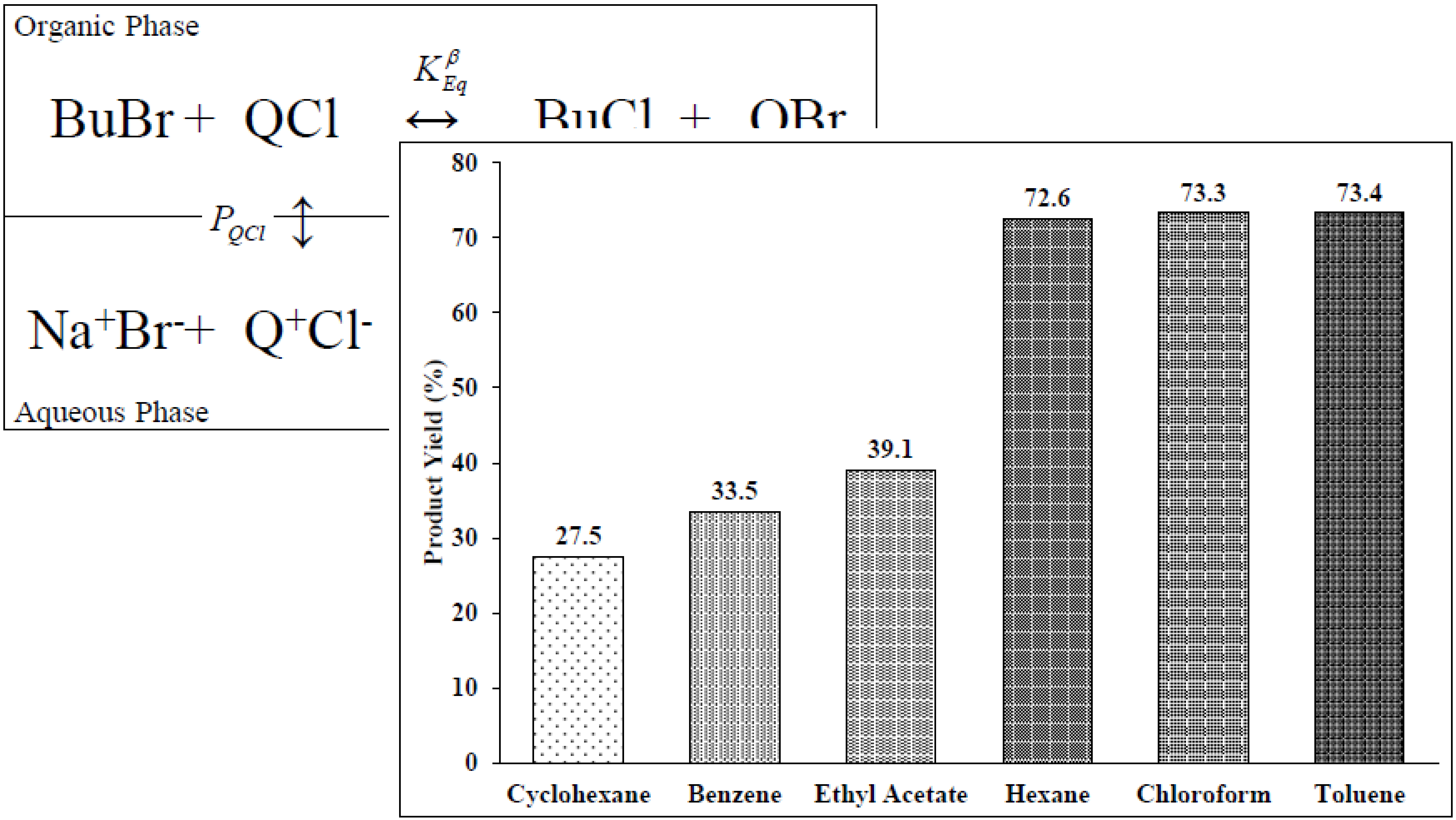
- Recover the main product
- Recover and recycle the extraction solvent (Hexane) and the reaction solvent (water)
- Recycle unreacted Benzamine

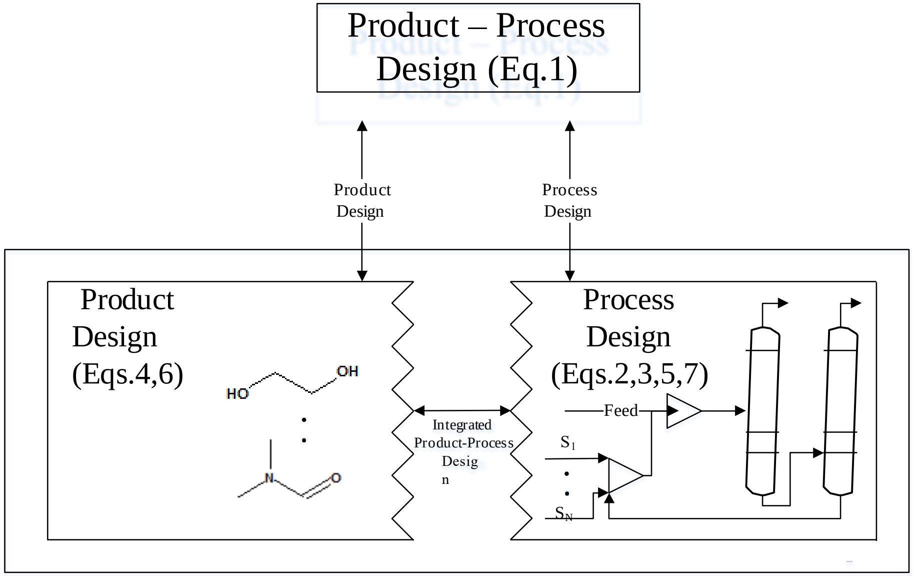
Rank	Process alternatives [SFILES]
1	(rABCDEF)(spABCD/EF)(lmE/F)[[(oE)]1(pF)](crD/ABC)[(oD)](dsAB/C)[(oAB)] (oC)
2	(rABCDEF)(spABCD/EF)(lmE/F)[[(oE)]1(pF)](crCD/AB)[(oAB)](scSC/D)[(oD)](scS/C)[2(oS)](o
3	(rA … oS)](oABC)
4	(rA … D))] …)](c



A: water
B: BA
C: 2OA
D: AABA
E: BD
F: Hexane

Other biphasic reaction-separation systems





Simultaneous Product – Process Design

Eqs. 1-7: simultaneous product design & process application

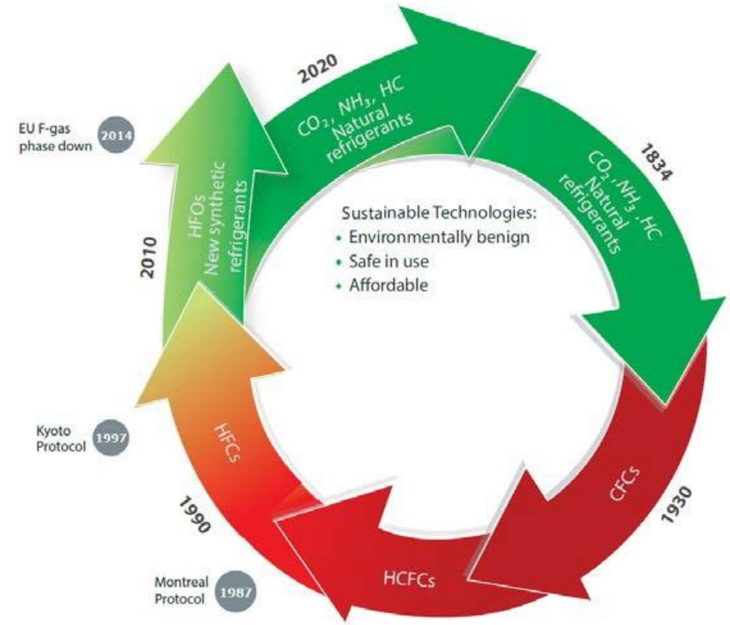
Examples: Molecular design (single molecular products) with process constraints

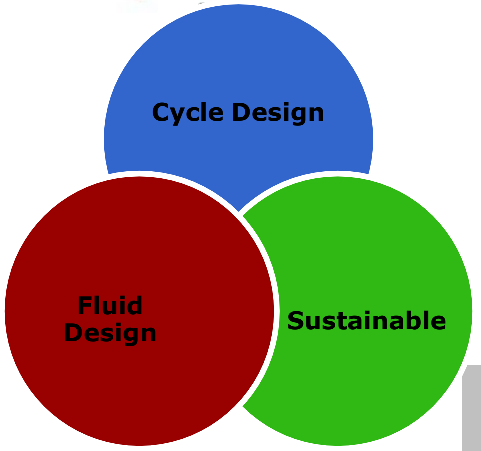
- Solvents for separations and/or product recovery
- **Process fluids for specific operations**
- Reactive agents
- …..

Refrigerant and cycle design-1

- **Refrigeration cycle and fluid affect each other. Therefore, product and process application considered.**
- Objective is to determine novel working fluids and mixtures that comply with current and upcoming regulations.
- **Requirements for substitution of existing fluids:**
  - New fluid should have same or improved cycle efficiency.
  - New fluid should have similar operational behavior.
  - New fluid should improve sustainability.

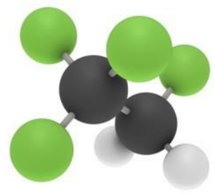
➢Relate process with product properties.
➢Find optimal product-cycle design.

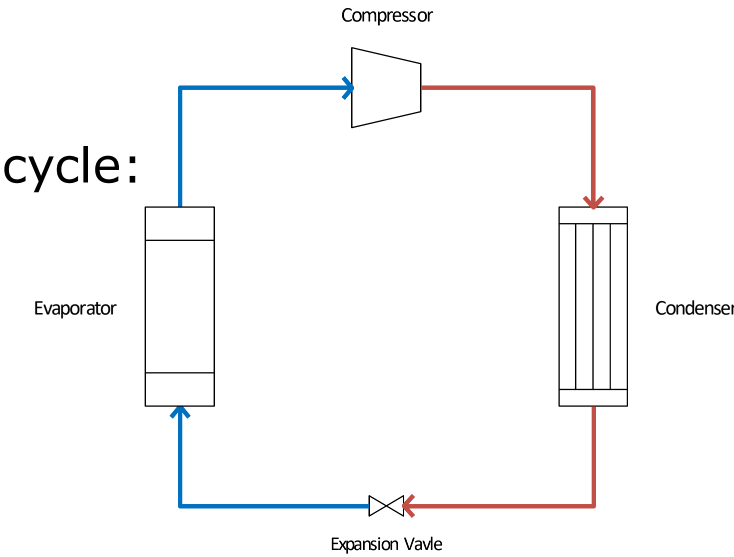


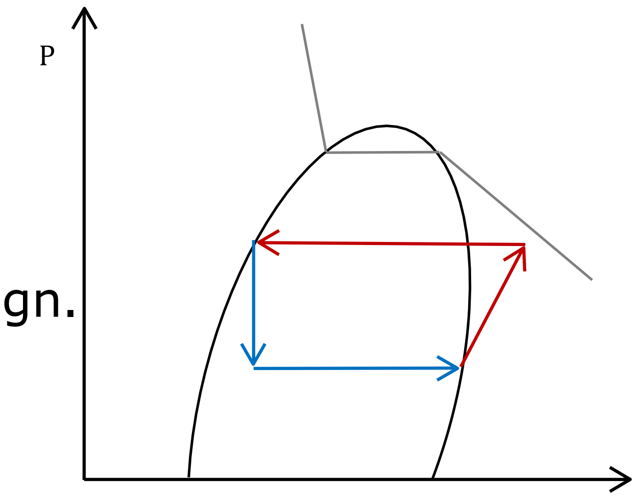


Refrigerant-cycle design: Step 1

- R134a is a commonly used refrigerant that is being phased out.
- Product properties that affect the process cycle:
  - Critical properties;
  - Heat capacity;
  - Compressibility;
  - Accentric factor;
  - Vapor pressure;
  - Heat of vaporization…
- These product properties influence the process cycle and its efficiency.
- Also, other properties (enthalpy, entropy, fugacity) are needed for process cycle design.
- Equation of state and for estimation of PVT relationship.







Simultaneous product and application process design

- Look for novel fluids that can contain C, H, F and Cl (up to 10 groups).
- 30 molecular groups are selected from M-G method.
- Target properties are chosen for product and process:

Step 2

Target Property	Lower bound	Upper bound
Molecular mass		110 g/mol
Normal boiling point		250 K
Critical temperature	350 K	400 K
Critical pressure	30 bar	50 bar
Thermal conductivity (liquid, Tb)	0.08 W/m.K	
Enthalpy of Vaporization at Tb	200 kJ/kg	
ODP		0
GWP		1400
Atmospheric Lifetime *		14 years
Number of groups	1	5
Number of functional groups	1	3

Process needs	Lower bound	Upper bound
Evaporation temperature	313.15 K	333.15
Condensation temperature	265.65 K	280.15

Refrigerant-cycle design: Step-3 (complete model-1)

- Molecular constraints

$$\sum_i n_i (2 - v_i) = 2$$

$$1 \le \sum_i n_i \le 10$$

$$0 \le \sum_i n_i \le 3$$

- Property constraints

$$\sum_i n_i Mw_i \ge 110 g/mol$$

$$T_{b0} \ln\left(\sum_i n_i T_{b_i}\right) \ge 250K$$

$$350K \le T_{c0} \ln\left(\sum_i n_i T_{ci}\right) \le 400K$$

$$30bar \le \frac{1}{\left(\sum_i n_i P_{ci} + P_{c02}\right)^2} + P_{c01} \le 50bar$$

$$\frac{1.11}{\left(\sum_i n_i Mw_i\right)^{1/2}} \times \frac{\left(3 + 20\left(1 - \frac{T}{T_c}\right)^{2/3}\right)}{\left(3 + 20\left(1 - \frac{T_b}{T_c}\right)^{2/3}\right)} \ge 0.1 W/m.K$$

$$\Delta H_v(T_0)\left(\frac{1 - \frac{T_1}{T_c}}{1 - \frac{T_0}{T_c}}\right)^{0.38} \ge 200 kJ/kg$$

- Process constraints

$$f(Z_{V1}) = 0 = Z_{V1}^3 - Z_{V1}^2 + Z_{V1}(-B^2 + A - B) - AB$$

$$f(Z_{V2}) = 0 = Z_{V2}^3 - Z_{V2}^2 + Z_{V2}(-B^2 + A - B) - AB$$

$$f(Z_{L3}) = 0 = Z_{L3}^3 - Z_{L3}^2 + Z_{L3}(-B^2 + A - B) - AB$$

Needed for efficient solution of cubic EoS [4]:

$$f(Z_{V1}) = 0 \qquad f'(Z_{V2}) \ge 0$$

$$f'(Z_{V1}) \ge 0 \qquad f''(Z_{V2}) \ge 0$$

$$f''(Z_{V1}) \ge 0 \qquad f(Z_{L3}) = 0$$

$$f(Z_{V2}) = 0 \qquad f'(Z_{L3}) \ge 0$$

$$f''(Z_{L3}) \le 0$$

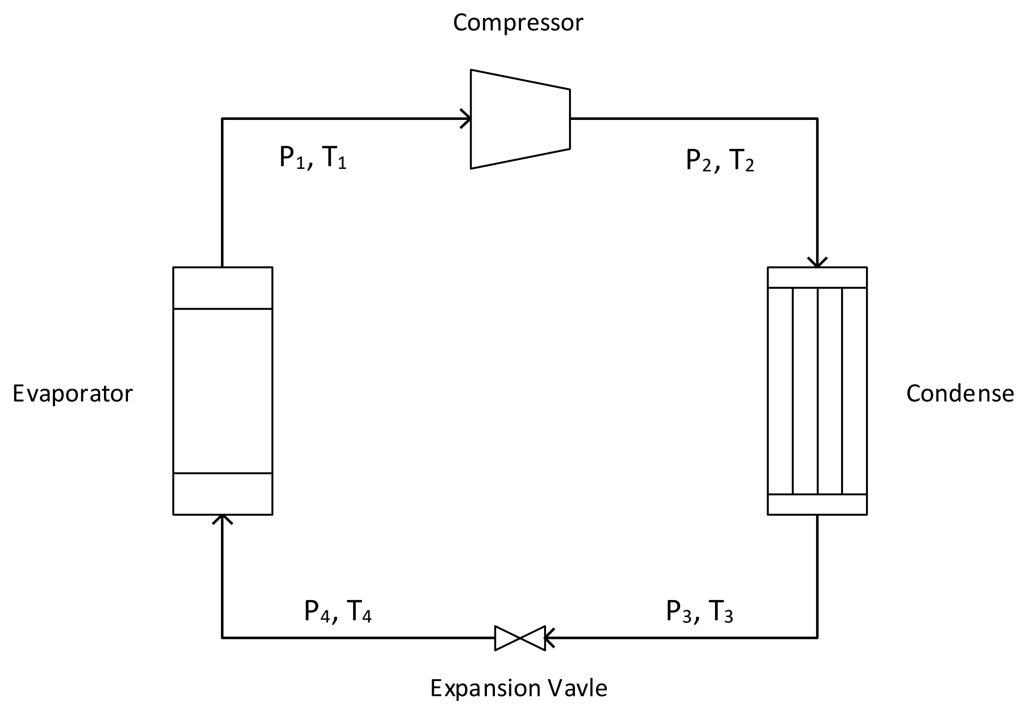
4] Kamath, R.S., Biegler, L.T., Grossmann, I.E., 2010, Comput. Chem. Eng. 34, 2085–2096.

Refrigerant-cycle design: Step-3 (complete model-2)

- Process constraints

$$\ln \varphi_{V1} = \ln \varphi_{L1}$$
$$\ln \varphi_{V2} = \ln \varphi_{L2}$$
$$H_{L3}(T_3, P_3) - H_{L4}(T_4, P_4) = 0$$
$$S_{V2}(T_2, P_2) - S_{V1}(T_1, P_1) = 0$$

$$P_1 = P_4$$
$$P_2 = P_3$$
$$T_1 = T_4$$
$$P_1 \geq P_0$$
$$P_2 \leq 0.8 P_c$$
$$T_2 \leq 0.8 T_c$$
$$265.65K \leq T_1 \leq 280.15K$$
$$313.15K \leq T_3 \leq 333.15K$$



- Objective function

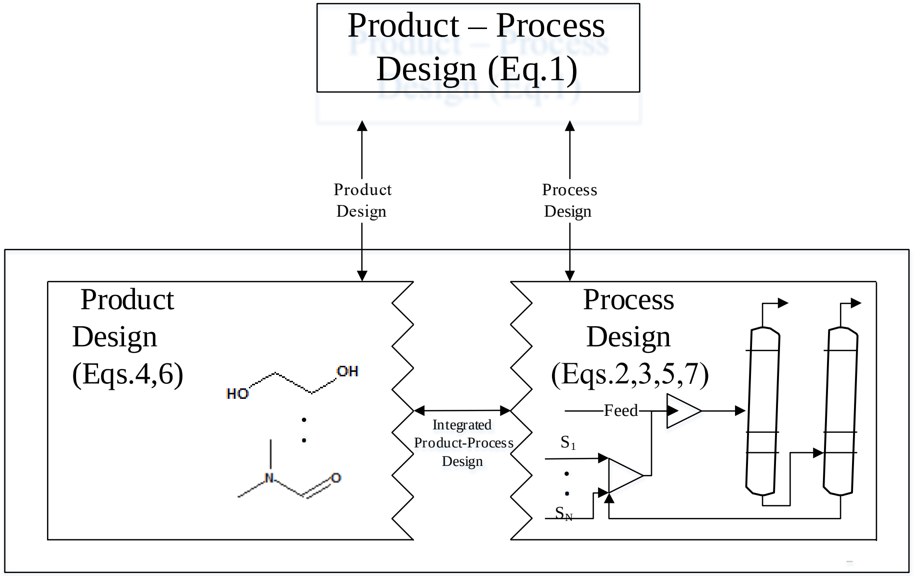
$$\max COP = \frac{H_1(Z_{V1}, T_1, P_1) - H_3(Z_{L3}, T_3, P_3)}{H_2(Z_{V2}, T_2, P_2) - H_1(Z_{V1}, T_1, P_1)}$$

Case study: Product-process design

Results

Cycle design for each molecules is given by Problem (II)

		r134a	r152a	3,3,3-triFluoro propyne	3,3-diFluoro butene	2,2-diFluoro butane
Problem I	Mw	102 g/mol	66 g/mol	94 g/mol	92 g/mol	94.1 g/mol
	Tb	236 K	230 K	242 K	246 K	252 K
	Tc	374 K	366 K	369 K	392 K	389 K
	Pc	37.32 bar	46.75 bar	38.13 bar	39.27 bar	37.8 bar
	ω	0.33	0.27	0.28	0.14	0.18
	k	0.082 W/m.k	0.097 W/m.k	0.086 W/m.K	0.093 W/m.K	0.092 W/m.K
	ΔH_v at T_b	26523 J/mol	28562 J/mol	18635 J/mol	21312 J/mol	26991 J/mol
	ODP	**0**	**0**	**0**	**0**	**0**
	GWP	**1370 (ASHRAE, 2005)**	**133 (ASHRAE, 2005)**	**134.6**	**2.4**	**0.9**
	Atmospheric lifetime	**13.4 years (ASHRAE, 2005)**	**1.5 years (ASHRAE, 2005)**	**-**	**-**	
Problem II	COP	10.1	12.8	9.5	11.0	11.1



Simultaneous Product – Process Design

Eqs. 1, 4 & 6: mixture-blend design

Examples: Formulated and/or blend design

- **Liquid formulated products**
- **Tailor-made blends**
- **Emulsified products**
- **………**

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Tailor-made fuel blends - 1

The main challenge involves how to identify the blends that satisfy the blend target properties with various types of additives

Problems solved: Tailor made design of gasoline blends, diesel blends, jet-fuel blends and lubricant blends.

Example: Blending gasoline with different **additives:**

✓impact of fuel consumption on the environment.

✓performances can be retained and improved.

Blend templates help to efficiently narrow down the search space of feasible chemicals to be added and obtain improved tailor-made blends in a faster, reliable and robut manner

* Collaboration with Texas A&M in Qatar.

**** To be presented at Session I-2, paper OL5, 16:40 by Sawitree Kalakul***

SPEED

Tailor-made fuels - 2

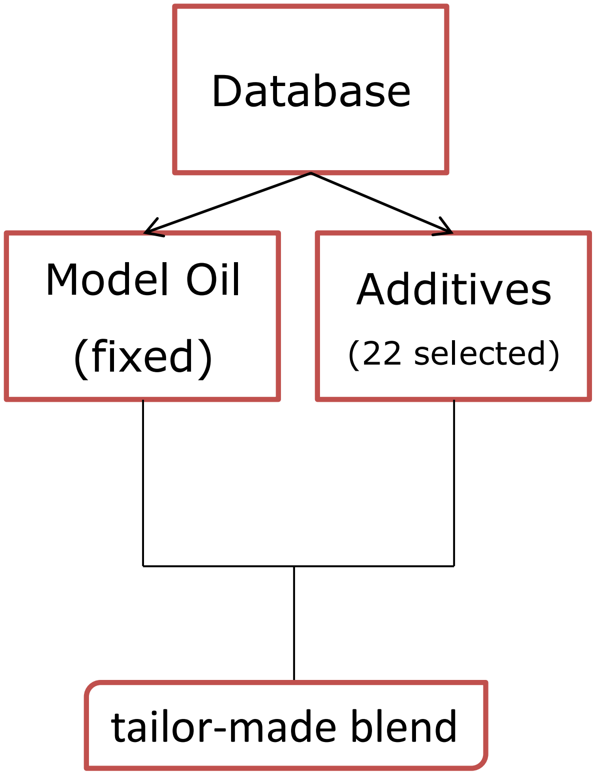
Task 1 Problem Defintion

1.1 Identify product needs

1.2 Translate needs into physico-chemical properties

1.3 Set target values

Need	Target property	Target value
Ability to be burned	RVP	$45 \leq RVP \leq 60$
Engine efficiency	RON	$RON \geq 92$
	HHV	$HHV \geq 40$
Consistency of fuel flow	η	$0.30 \leq \eta \leq 0.60$
	ρ	$0.720 \leq \rho \leq 0.775$
Flammability	T_f	$T_f \leq 300$
Toxicity	LC_{50}	$-logLC_{50} < 3.08$
Stability	ΔG^{mix}	$\Delta G^{mix} < 0$
Environmental aspect	Wt_{O2}	$2 \leq Wt_{O2} \leq 20$
Low oxidation	Choice of chemicals	



SPEED Tailor-made fuels

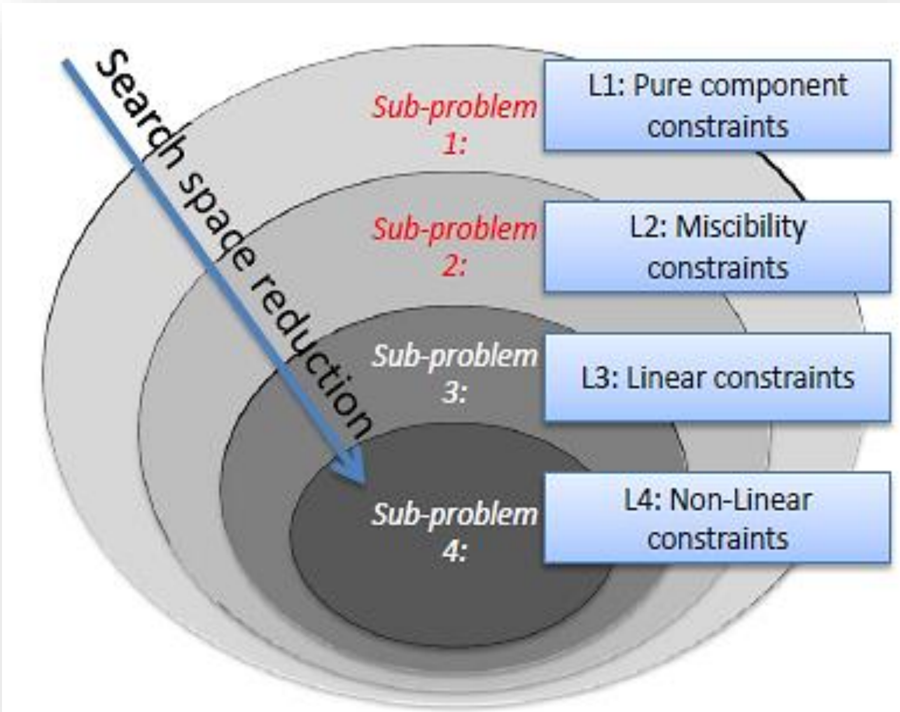
Task 2 Mixture/blend design

2.1 Pure component constraints (HHV, ρ, *η, LC50, WtO2*)

2.2 Miscibility constraint (ΔG^{mix})

2.3 Linear constraints (HHV, ρ, *η, LC50, WtO2*)

2.4 Non-linear constraints (RVP, Tf)



Miscibility test: $\Delta G^{Mix} < 0$

⇩

Linear Program

$$\text{min or max} \quad f_{obj}(x)$$

$s.t.$

$$\zeta_{LB}^{k} \leq \sum_{i}^{NC} x_i \zeta_i^k \leq \zeta_{UB}^{k}$$

(5 Eqs. One for each prop-erty)

$$\sum_{i=1}^{NC} x_i - 1 = 0$$

$$0 < x_i < 1$$

⇩

Nonlinear Program

$$\text{min or max} \quad f_{obj}(x)$$

$s.t.$

$$\sum_{i=1}^{NC} \frac{x_i \gamma_i P_i^{sat}(310.95\ \text{K})}{RVP_B} = 1$$

$$\sum_{i=1}^{NC} x_i \gamma_i T_{f,i} = T_{f,mix}$$

$$\sum_{i=1}^{NC} x_i - 1 = 0$$

$$x_{LB} < x_i < x_{UB}$$

Tailor-made fuels

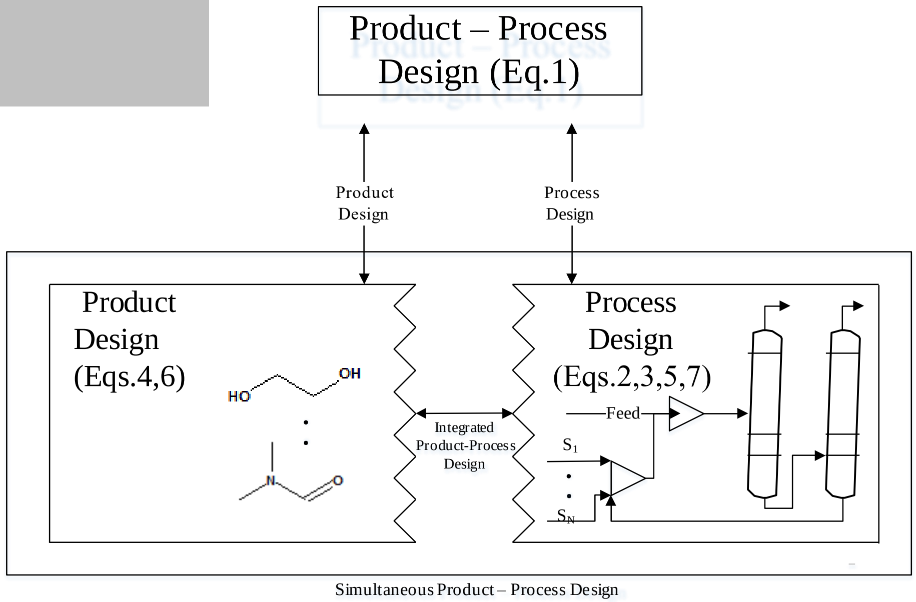
Task 3 Rank blend candidates according to a selection criterion

Blend	Composition (vol%)
Blend 1	MI (69), Tetrahydrofuran (11), 2-Methyl Tetrahydrofuran (20)
Blend 2	MI (67), Acetone (13), 2-Methyl Tetrahydrofuran (20)
Blend 3	MI (72), Acetone (10), 2-Butanone (18)
Blend 4	MI (75), 2-Butanone (13), 2-Methyl Tetrahydrofuran (12)
Blend 5	MI (77), Ethanol (12), 2-Methyl Tetrahydrofuran (11)

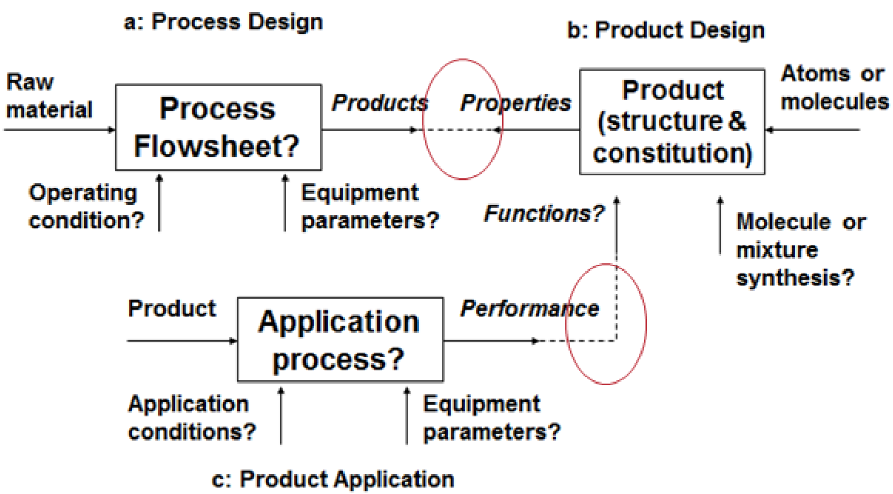
Task 4 Experimental verification

Sample	Density at 15^{o}C (g/〖cm〗^3)		Dynamic Viscosity(mPa.s)		Vapor Pressure at 37.8^{o}C (kPa)	
Target Values	0.720 – 0.775		0.3 – 0.6		45 - 60	
	Experimental	Model	Experimental	Model	Experimental	Model
Main Ingredient	0.71	0.73	0.50	0.51	51.0	54.0
Blend 1	0.76	0.76	0.54	0.46	46.2	50.8
Blend 2	0.75	0.74	0.46	0.43	60.4	64.5
Blend 3	0.73	0.74	0.45	0.43	58.9	63.7
Blend 4	0.74	0.73	0.46	0.45	50.1	53.5
Blend 5	0.74	0.74	0.61	0.58	55.1	58.9

What next?



Simultaneous Product – Process Design



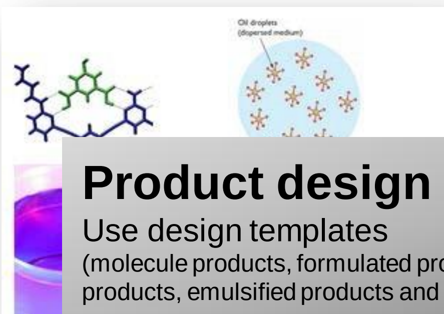
Some interesting developments:

- The chemical product simulator
- Product-process development
- .....

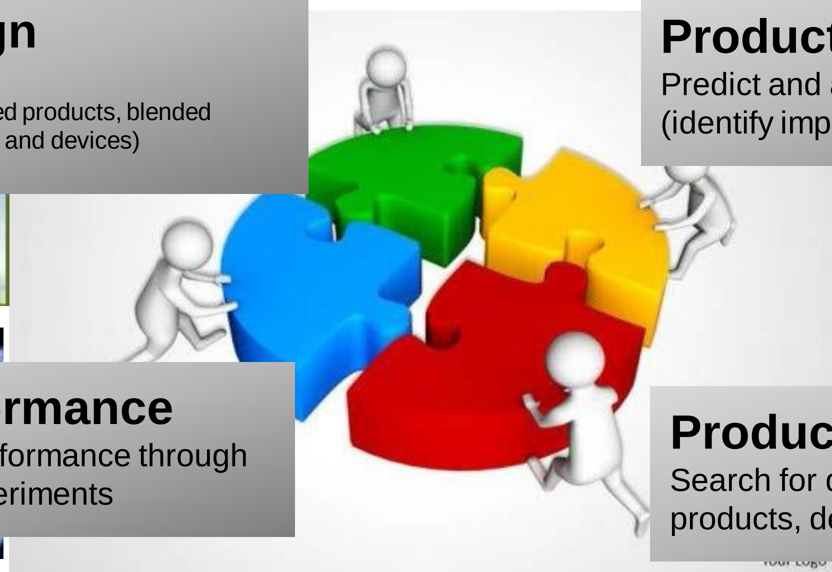
Chemical product design simulator

There is a need for a product simulator with similar 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***

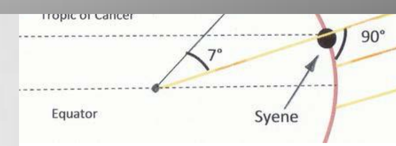
Kalakul et al, "VPPD-Lab: The Chemical Product Simulator", in "Methods and tools for chemical product design", Computer Aided Chemical Engineering, 39, 61-94 (chapter 3), 2017

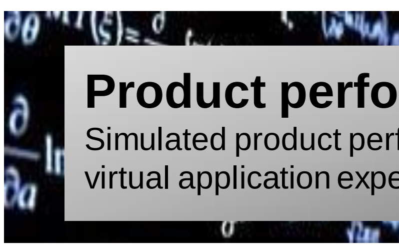


Product design
Use design templates
(molecule products, formulated products, blended products, emulsified products and devices)



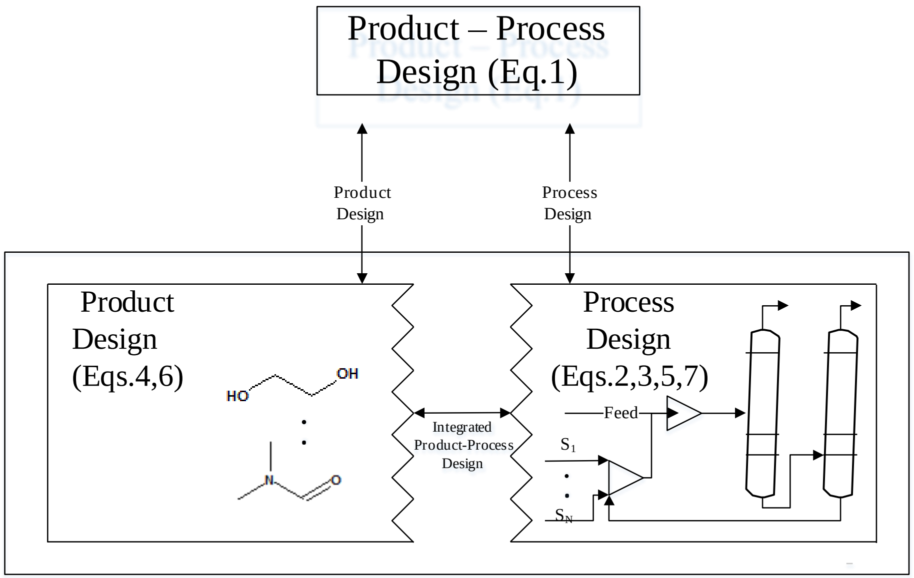
Product analysis
Predict and analyze product behavior (identify important product properties)





Product performance
Simulated product performance through virtual application experiments

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



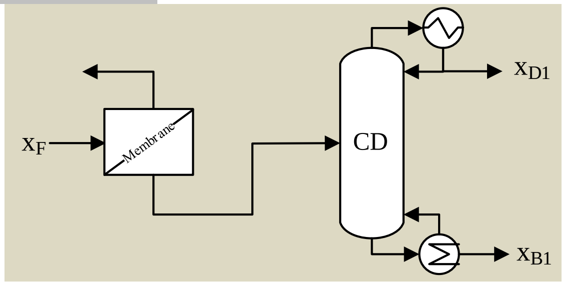
Simultaneous Product – Process Design

Eqs. 1-7: simultaneous product design & process application – decomposition-based solution approach

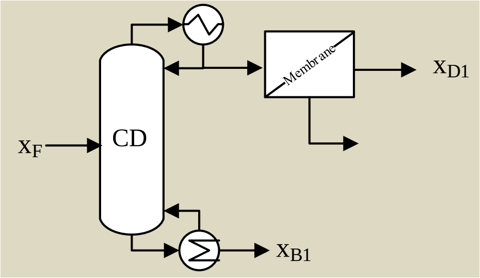
Examples: Molecular design (single molecular products) with process constraints

- Solvents for separations and/or product recovery
- Hybrid process design with membranes
- Process fluids for specific operations
- Reactive agents
- …..

Design of hybrid modules



1



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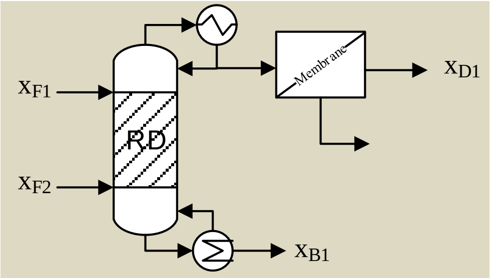

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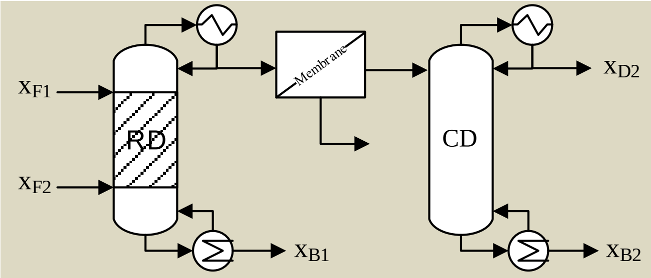
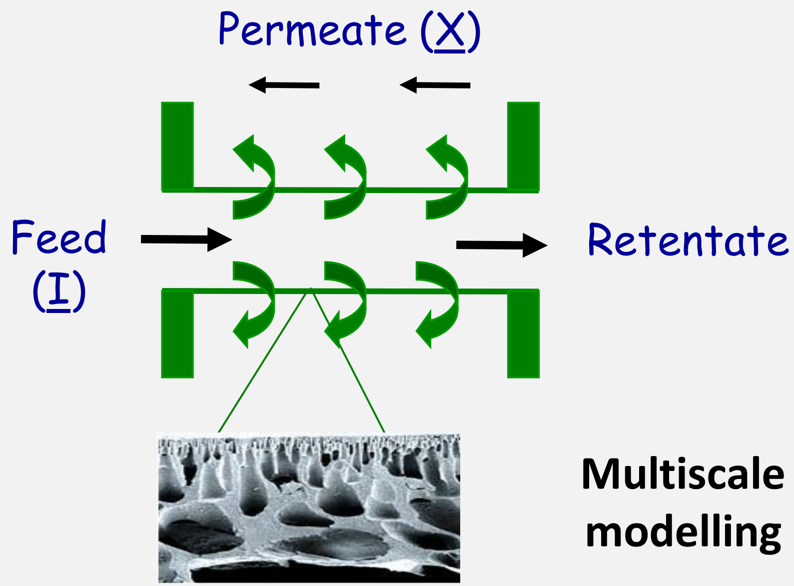


4

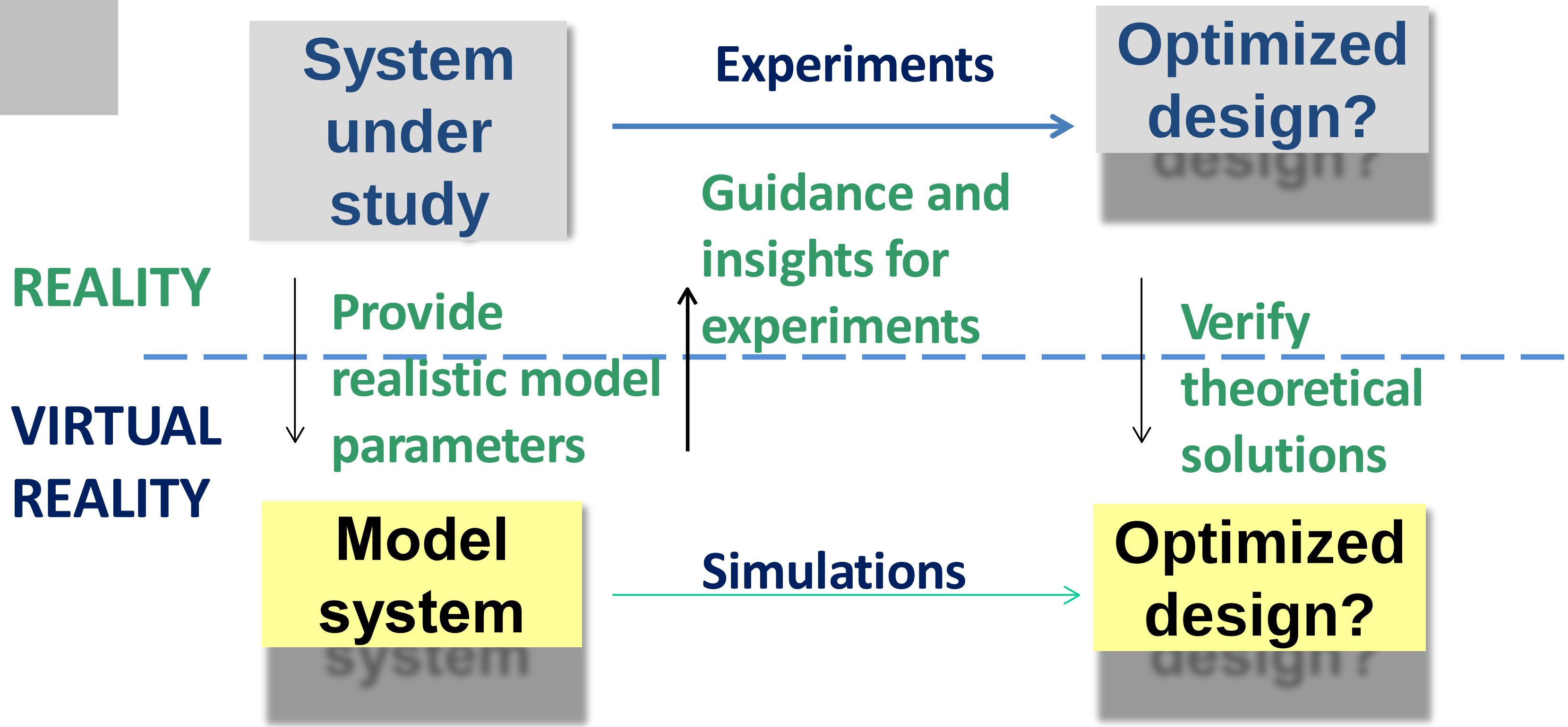
Which is the product design problem?



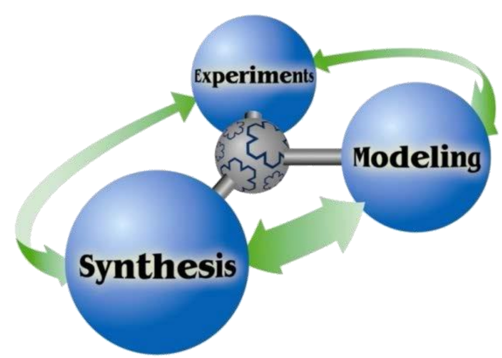
Multiscale modelling

Close to 50% or more energy reduction compared to original process achievable

Collaborative effort needed!



- Solution approaches
  - Integrated multiscale modeling, experiments and synthesis
  - Ability to find predictive-innovative solutions



Design Problem from 60 Years Ago

- **Non-scumming "soap bar" (world's best-selling soap bar) – Launched by Lever Bros (US division of Unilever) in 1955**
- **Attributes comparable to ordinary soap bars**
  - **Firmness**
  - **Lather**
  - **Rate of wear**
  - **Slipperiness**
  - **Mildness**
  - **No unpleasant odors**
  - **No "cracking" from wet/dry cycles**

Michael Hill
M Hill & Associates
Mahwah, NJ

- **Processable on ordinary soap bar line: model-based system yet to be developed**

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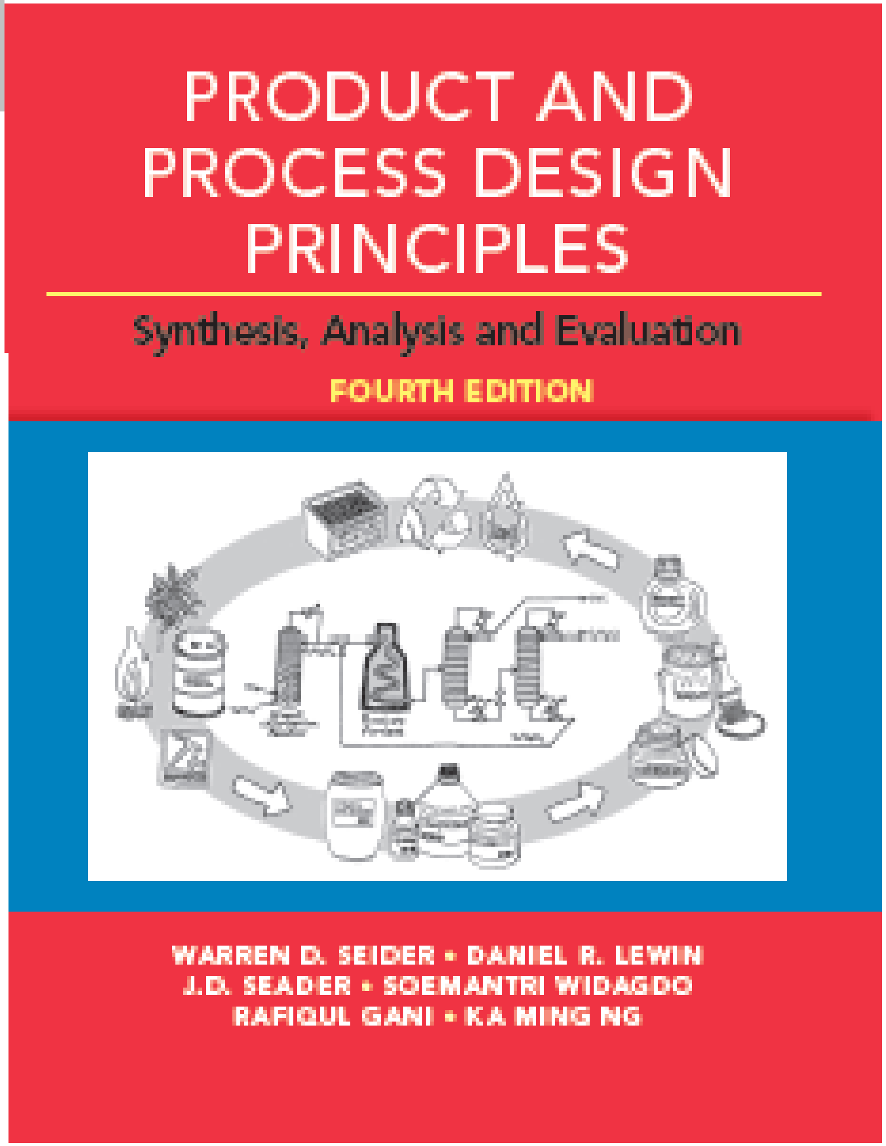
Textbook: Process-Product Design (4th edition)



Published by Wiley

Suitable for BSc, MSc level teaching of

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

The academic tree of Prof Rafiqul Gani