Additional Notes – Lecture 2

Rafiqul Gani

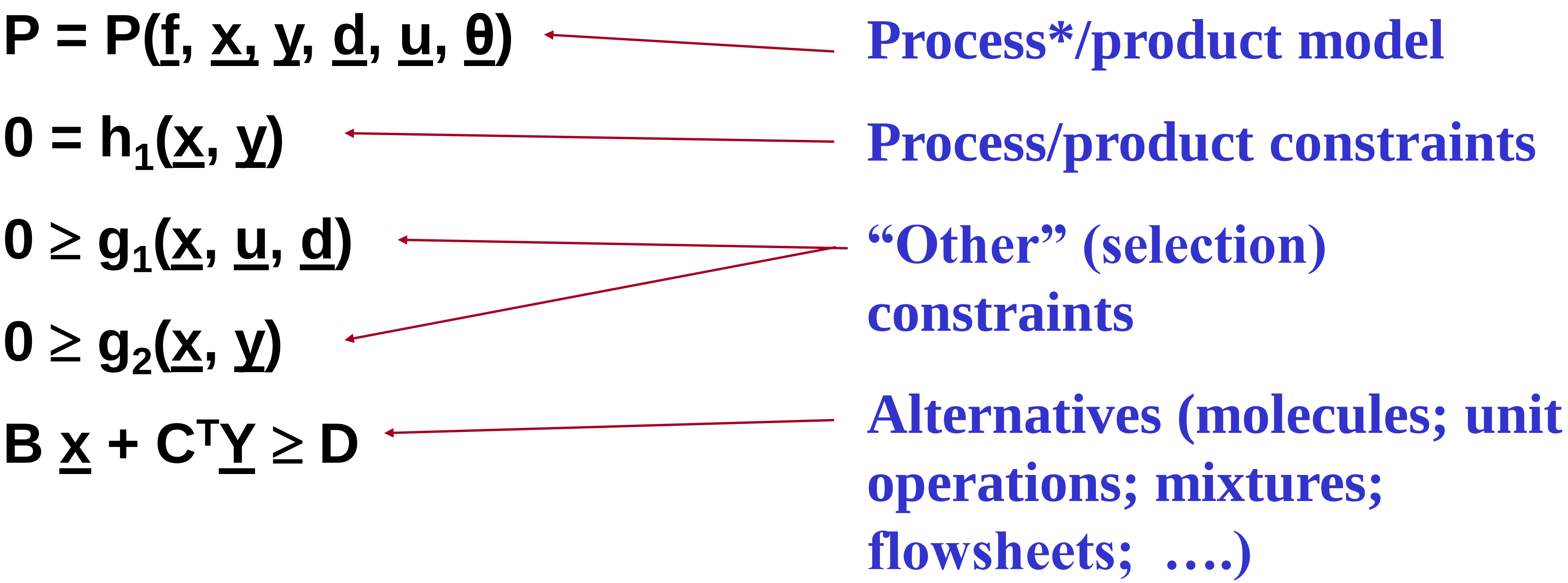
PSE for SPEED
Skyttemosen 6, DK-3450 Allerod, Denmark
rgani2018@gmail.com

www.pseforspped.com

General problem definition & solution

MINLP means Mixed Integer Non Linear Programming – optimization problems formulated as MINLP contains integer ($\underline{Y}$) and continuous variables ($\underline{x}$, $\underline{y}$) as optimization variables, and, at least the objective function and/or one of the constraints is non-linear.

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



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

Process*/product model

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

Process/product constraints

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

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

"Other" (selection) constraints

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

Alternatives (molecules; unit operations; mixtures; flowsheets; ….)

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General problem definition & solution

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

$P = P(\underline{f}, \underline{x}, \underline{y}, \underline{d}, \underline{u}, \underline{\theta})$ ← Process*/product model (2)

$0 = h_1(\underline{x}, \underline{y})$ ← Process/product constraints (3)

$0 \geq g_1(\underline{x}, \underline{u}, \underline{d})$ ← “Other” (selection) constraints (4a)

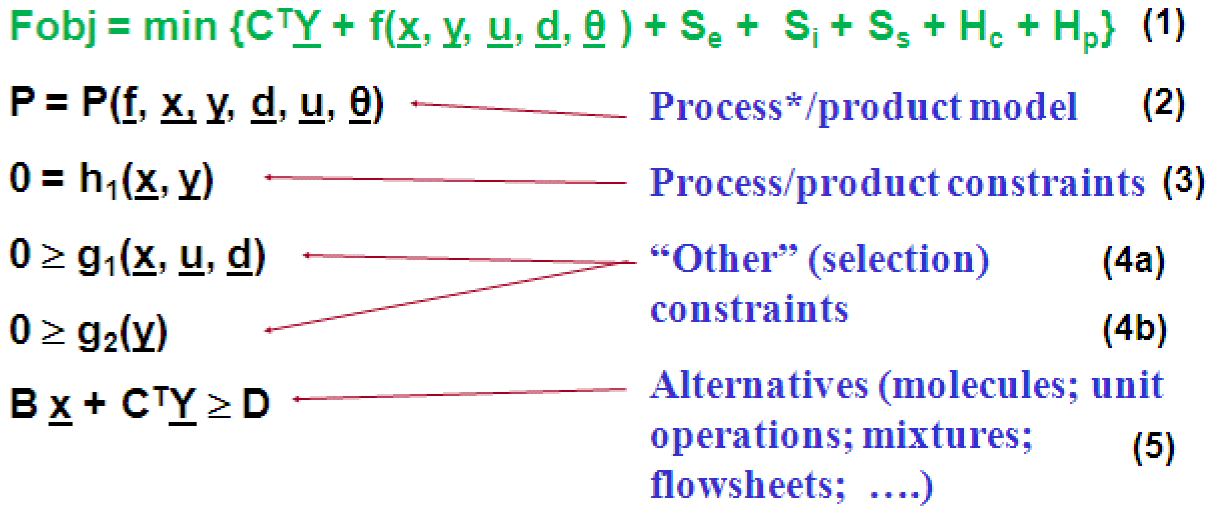
$0 \geq g_2(\underline{y})$ ← (4b)

$B\,\underline{x} + C^T\underline{Y} \geq D$ ← Alternatives (molecules; unit operations; mixtures; flowsheets; ….) (5)

Solution approaches

- Solve all Eqs. (1-5) simultaneously
- Solve 4b, 2, check 3, check 4a, check 5, calc. 1

General problem definition & solution



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

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$0 \geq g_1(\underline{x}, \underline{u}, \underline{d})$ ← "Other" (selection) constraints (4a)

$0 \geq g_2(\underline{y})$ (4b)

$B\,\underline{x} + C^T\underline{Y} \geq D$ ← Alternatives (molecules; unit operations; mixtures; flowsheets; ….) (5)

$\underline{Y}$ = 0 or 1

$\underline{x}$: process

$\underline{u}$: fixed

$\underline{d}$: equipment

$\underline{\theta}$: parameters

- Solve 4b, 2, check 3, check 4a, check 5, calc. 1
- Enumerate sets of $\underline{Y}$ that satisfy 4b
- Given $\underline{Y}$, $\underline{u}$, $\underline{d}$, $\underline{\theta}$, solve eq. 2 for $\underline{x}$ for all sets of $\underline{Y}$
- Given $\underline{x}$, $\underline{Y}$, check 3, then 4a, then 5 for remaining sets of $\underline{Y}$ to obtain the set of feasible solutions
- For each feasible solution, calc. FOBJ and find the optimal

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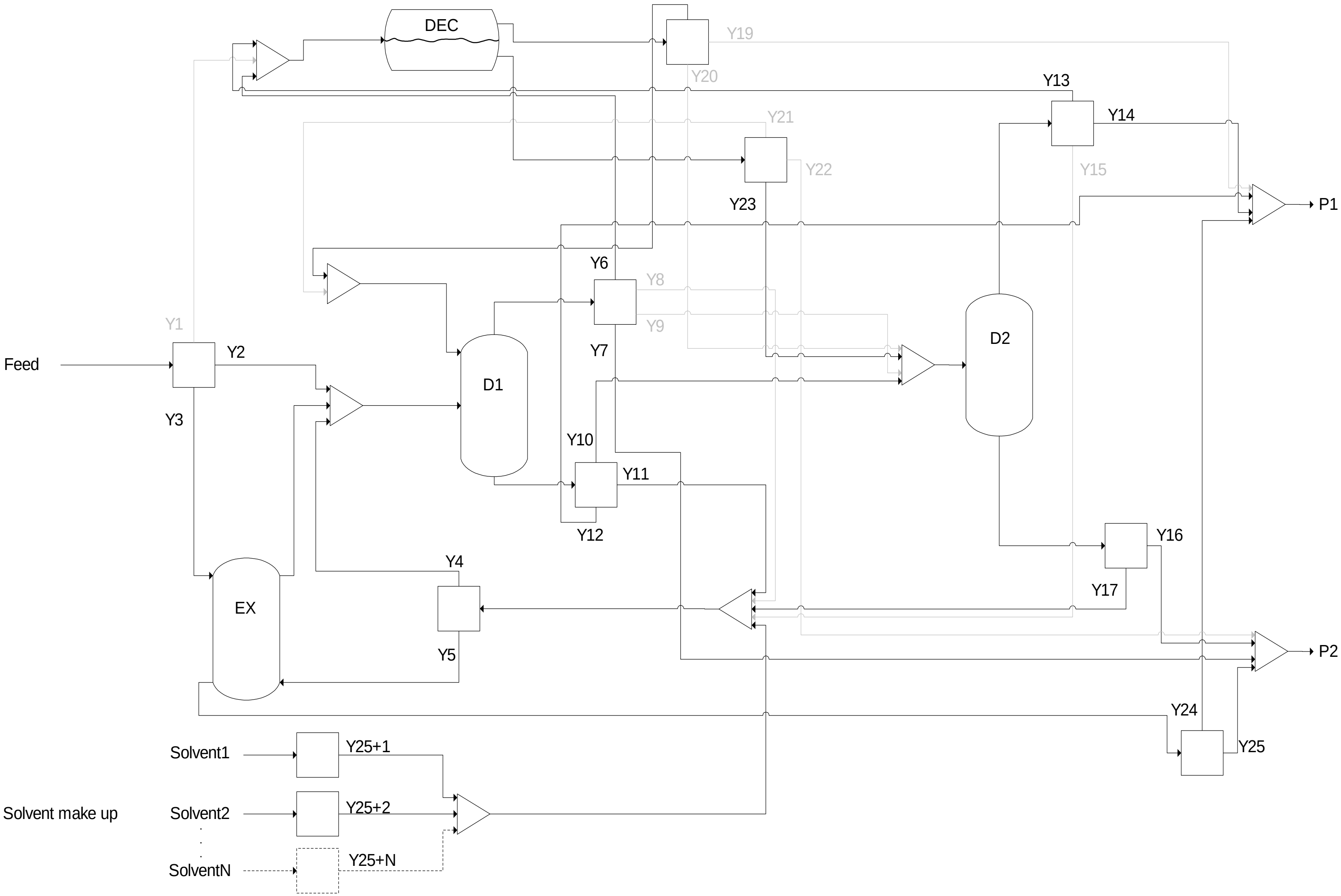
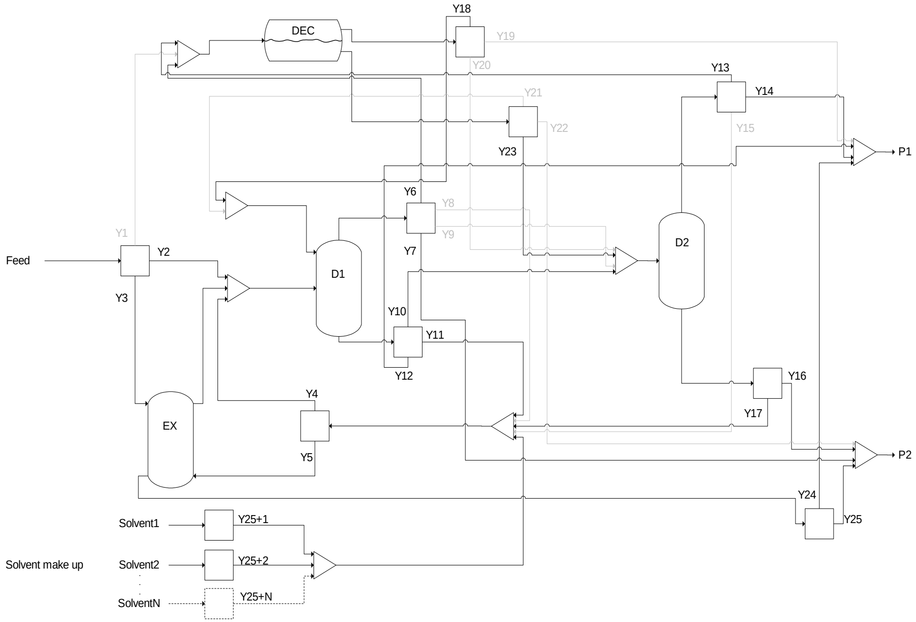
Example : Simultaneous product-process design

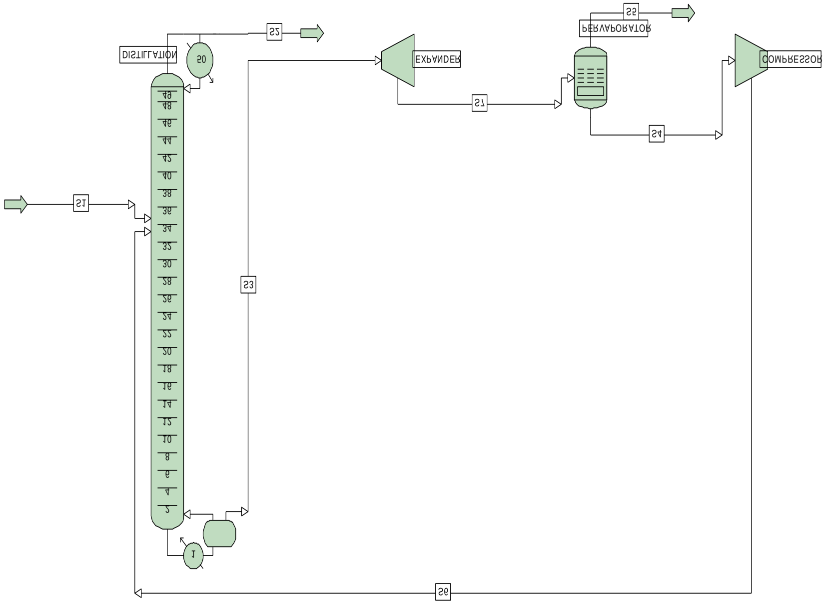
Find solvent or membrane, flowsheet & optimal design



SPEED Example – Simultaneous product-process design

Find solvent or membrane, flowsheet & optimal design





For fixed membrane and process flowsheet, find optmal design

Example – Simultaneous product-process design

Find solvent or membrane, flowsheet & optimal design

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

$P = P(\underline{f}, \underline{x}, \underline{y}, \underline{d}, \underline{u}, \underline{\theta})$ ← Process*/product model (2)

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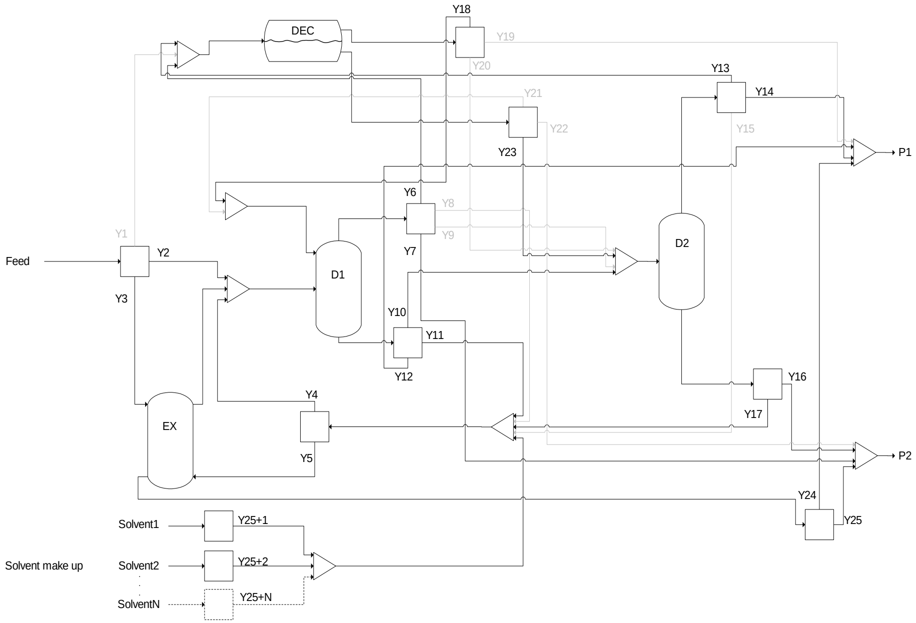
$0 \geq g_2(\underline{y})$ (4b)

$B\,\underline{x} + C^T\underline{Y} \geq D$ ← Alternatives (molecules; unit operations flowsheets

For fixed membrane and process flowsheet, find optmal design



SPEED Conceptual product process design problem

$$0 = C_1 \left(Y_1 \cdot A_1 + \theta_1 / X_2\right)$$
$$0 = C_2 \left(Y_2 \cdot A_2 - \theta_2 \cdot X_1\right)$$
$$0 = C_1 \cdot X_2 + \theta_1 \cdot Y_3 - A_1$$

Balance equations

$$A_1 = h_1 \cdot X_1 + Y_1 \cdot (X_2)^2$$
$$A_2 = \theta_2 / X_2 + Y_2 \, (X_1)^2$$
$$X_1 = (A_1 \cdot Y_1 \cdot t) \, / \, (A_1 + A_2)$$
$$X_2 = (A_2 + Y_2) \, / \, t$$

Conditional/ constraint equations

$$\theta_1 = Z_1 Z_2 Y_1 \, / \, (Z_1 + Z_2)$$
$$\theta_2 = [(Z_1)^2 + (Z_2)^2] / Y_2$$

Constitutive equations

$$P_1 - P_1(\underline{Y}, \underline{P}) = 0$$
$$P_2 - P_2(\underline{Y}, \underline{P}) = 0$$

Design constraints

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Model analysis

$$0 = C_1 (Y_1 \cdot A_1 + \theta_1/X_2)$$
$$0 = C_2 (Y_2 \cdot A_2 - \theta_2 \cdot X_1)$$
$$0 = C_1 \cdot X_2 + \theta_1 \cdot Y_3 - A_1$$

Balance equations

$$A_1 = h_1 \cdot X_1 + Y_1 \cdot (X_2)^2$$
$$A_2 = \theta_2/X_2 + Y_2 (X_1)^2$$
$$X_1 = (A_1 \cdot Y_1 \cdot t) / (A_1 + A_2)$$
$$X_2 = (A_2 + Y_2) / t$$

Conditional/ constraint equations

$$\theta_1 = \mathrm{Z_1 Z_2 Y_1} / (\mathrm{Z_1} + \mathrm{Z_2})$$
$$\theta_2 = [(\mathrm{Z_1})^2 + (\mathrm{Z_2})^2]/\mathrm{Y_2}$$

Constitutive equations

$$P_1 - P_1(\underline{Y}, \underline{P}) = 0$$
$$P_2 - P_2(\underline{Y}, \underline{P}) = 0$$

Design constraints

Variable	Type
Y_1 , Y_2 and Y_3	Dependent (differential or state) variables
Z_1 and Z_2	Design (decision) variables
θ_1 and θ_2	Property parameters (constitutive variables)
A_1, A_2, X_1, X_2	Intermediate variables (unknown)
P_1 and P_2	Performance criteria
$\mathrm{C_1}$ and C_2	Known parameters

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Iterative design process

30 $0 = C_1 (Y_1 \cdot A_1 + \theta_1/X_2)$

31 $0 = C_2 (Y_2 \cdot A_2 - \theta_2 \cdot X_1)$

32 $0 = C_1 \cdot X_2 + \theta_1 \cdot Y_3 - A_1$

Balance equations

33 $A_1 = h_1 \cdot X_1 + Y_1 \cdot (X_2)^2$

34 $A_2 = \theta_2/X_2 + Y_2 (X_1)^2$

35 $X_1 = (A_1 \cdot Y_1 \cdot t) / (A_1 + A_2)$

36 $X_2 = (A_2 + Y_2) / t$

Conditional/ constraint equations

38 $\theta_1 = Z_1 Z_2 Y_1 / (Z_1 + Z_2)$

39 $\theta_2 = [(Z_1)^2 + (Z_2)^2]/Y_2$

Constitutive equations

39 $P_1 - P_1(\underline{Y}, \underline{P}) = 0$

40 $P_2 - P_2(\underline{Y}, \underline{P}) = 0$

Design constraints

Number of eqs = 11

Number of variables = 13

Degrees of freedom = 2

Variables to specify = Z_1, Z_2

Solve Eqs. 30-39 for specified Z

Solve Eqs. 39-40 for P

If 39-40 not satisfied, assume new Z and repeat

Eqs.	X_1	X_2	Y_1	Y_2	Y_3	A_1	A_2	θ_1	θ_2	Z_1	Z_2
31	*			*			*		*		
30		*	*			*		*			
33	*	*	*			*					
34	*	*		*					*		
32		*			*	*		*			
35	*		*			*	*				
36	*			*			*				
37			*					*		*	*
38				*					*	*	*

Non-iterative product-process design

Balance equations

30 $0 = C_1\,(Y_1 \cdot A_1 + \theta_1/X_2)$
31 $0 = C_2\,(Y_2 \cdot A_2 - \theta_2 \cdot X_1)$
32 $0 = C_1 \cdot X_2 + \theta_1 \cdot Y_3 - A_1$

Conditional/ constraint equations

33 $A_1 = h_1 \cdot X_1 + Y_1 \cdot (X_2)^2$
34 $A_2 = \theta_2/X_2 + Y_2\,(X_1)^2$
35 $X_1 = (A_1 \cdot Y_1 \cdot t) / (A_1 + A_2)$
36 $X_2 = (A_2 + Y_2) / t$

Constitutive equations

37 $\theta_1 = Z_1 Z_2 Y_1 / (Z_1 + Z_2)$
38 $\theta_2 = [(Z_1)^2 + (Z_2)^2]/Y_2$

Design constraints

39 $P_1 - P_1(\underline{Y}, \underline{P}) = 0$
40 $P_2 - P_2(\underline{Y}, \underline{P}) = 0$

Number of eqs = 11

Number of variables = 13

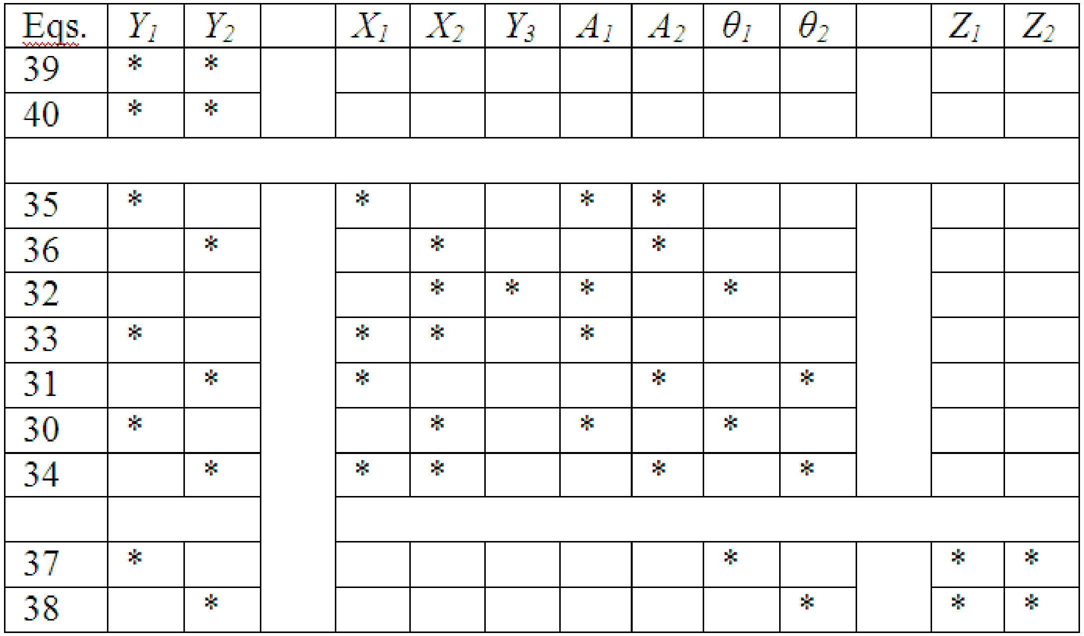
Degrees of freedom = 2

Variables to specify = $\underline{Z}$

Solve Eqs. 39-40 for Y_1, Y_2

Solve Eqs. 31-36 for X_1, X_2, Y_3, A_1, A_2, θ_1, θ_2

Match θ_1, θ_2 (target) with Z_1, Z_2 (product or material or chemical design)



Eqs.	Y_1	Y_2		X_1	X_2	Y_3	A_1	A_2	θ_1	θ_2		Z_1	Z_2
39	*	*											
40	*	*											
35	*			*			*	*					
36		*			*			*					
32					*	*	*		*				
33	*			*	*		*						
31		*		*				*		*			
30	*				*		*		*				
34		*		*	*			*		*			
37	*								*			*	*
38		*								*		*	*

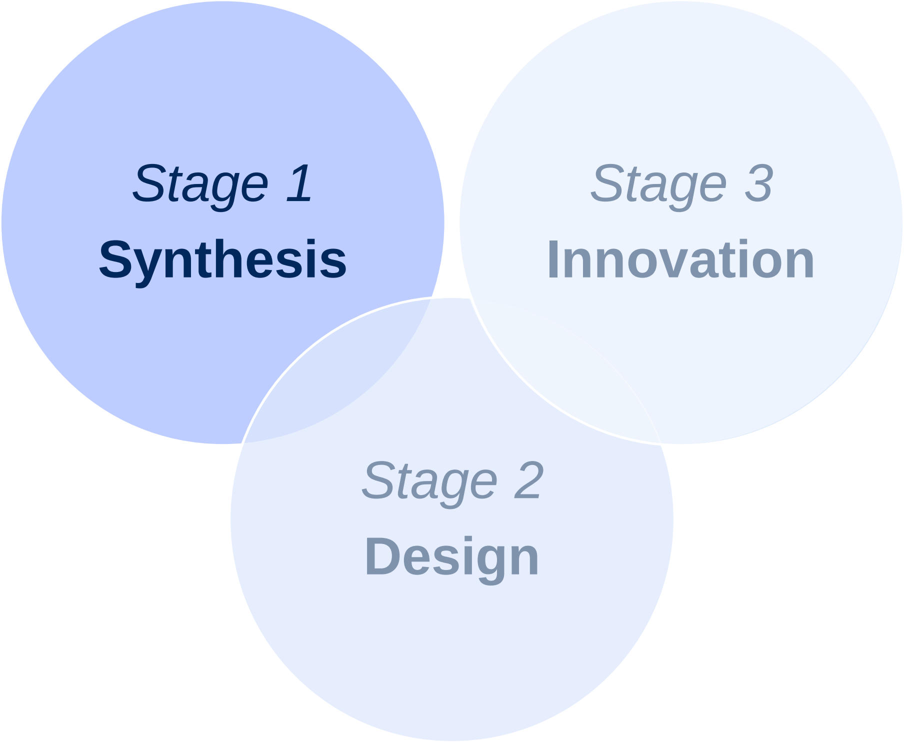
Superstructure based optimization to find optimal processing routes

A 3-Stage approach to sustainable process design

Focus on Stage 1

Given: set of feedstock & products
Find: processing route

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



Stage 1
Synthesis

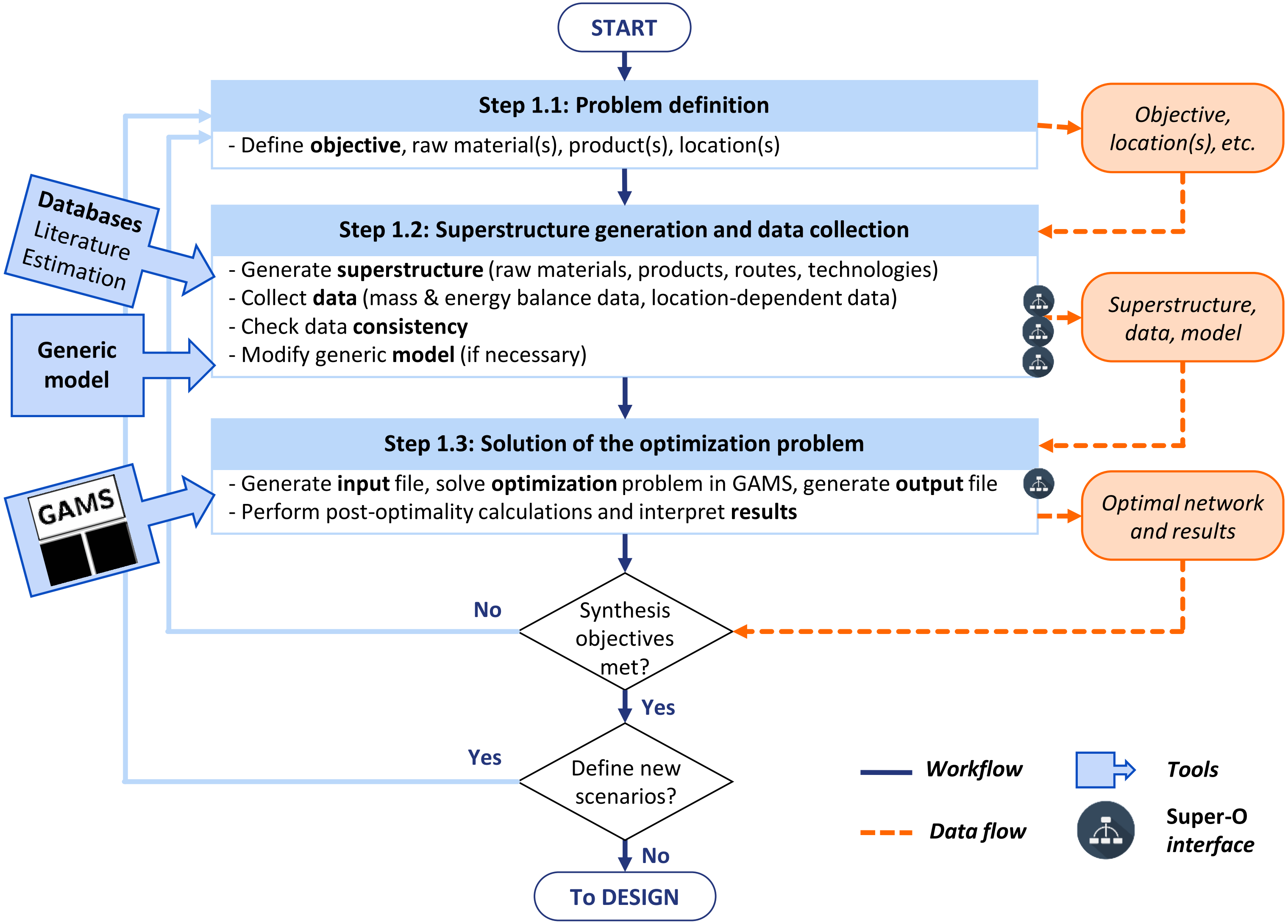
Stage 3
Innovation

Stage 2
Design

Given: processing route
Find: feasible design

Stage 1: Synthesis

The objective of Stage 1 is to obtain the processing route (including feedstock and products)



START

Step 1.1: Problem definition

- Define **objective**, raw material(s), product(s), location(s)

Step 1.2: Superstructure generation and data collection

- Generate **superstructure** (raw materials, products, routes, technologies)
- Collect **data** (mass & energy balance data, location-dependent data)
- Check data **consistency**
- Modify generic **model** (if necessary)

Step 1.3: Solution of the optimization problem

- Generate **input** file, solve **optimization** problem in GAMS, generate **output** file
- Perform post-optimality calculations and interpret **results**

Source: Bertran, M., Frauzem, R., Zhang, L., Gani, R. (2016). A generic methodology for superstructure optimization of different processing networks. Computer Aided Chemical Engineering (26th European Symposium on Computer Aided Process Engineering, ESCAPE26).

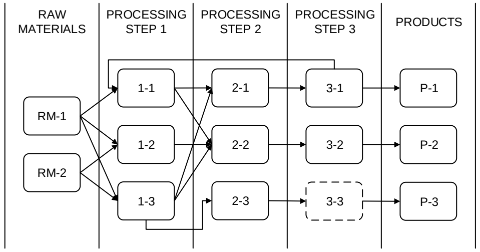
Overview of the Synthesis stage

The key elements of the framework require methods & tools

Problem →

Superstructure of alternatives

Need: Superstructure representation

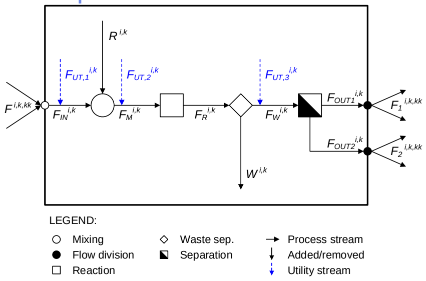


Need: Knowledge management

Database

Model

Need: Generic process model



Solution ←

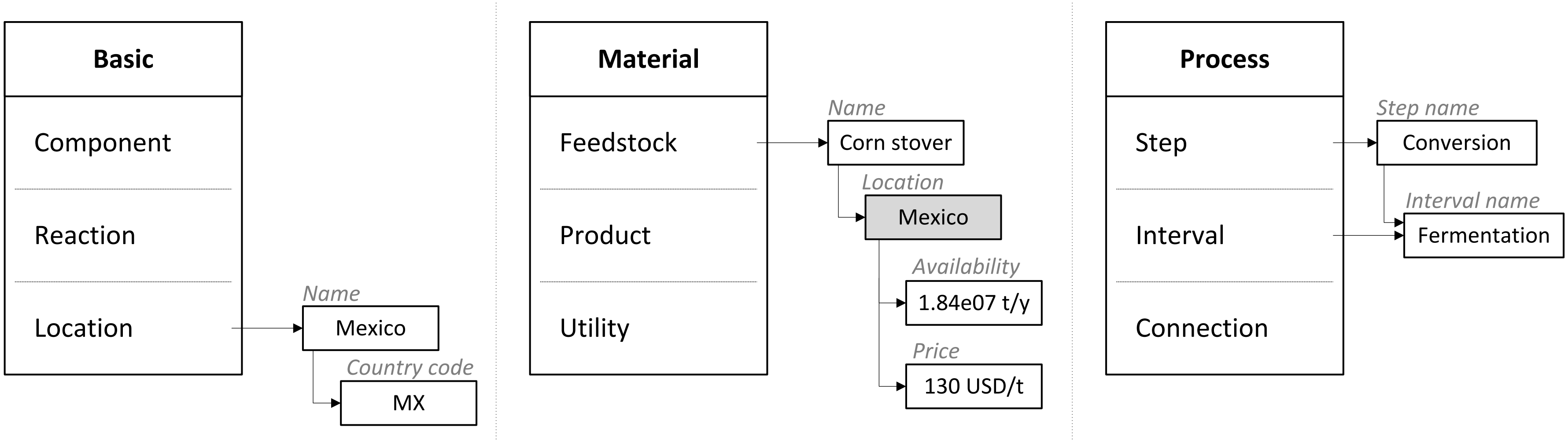
Solution strategy

Need: Integration with optimization environment

Source: Bertran, M., Frauzem, R., Sanchez-Arcilla, A., Zhang, L., Woodley, J.M., Gani, R. (submitted). A generic methodology for processing route synthesis and design based on superstructure optimization. Computers and Chemical Engineering (Special Issue ESCAPE26).

Data management through databases

Specific databases are built on a common data structure that fits the problem requirements



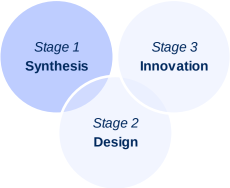
Basic
- Component
- Reaction
- Location
  - *Name*: Mexico
    - *Country code*: MX

Material
- Feedstock
  - *Name*: Corn stover
    - *Location*: Mexico
      - *Availability*: 1.84e07 t/y
      - *Price*: 130 USD/t
- Product
- Utility

Process
- Step
  - *Step name*: Conversion
    - *Interval name*: Fermentation
- Interval
- Connection

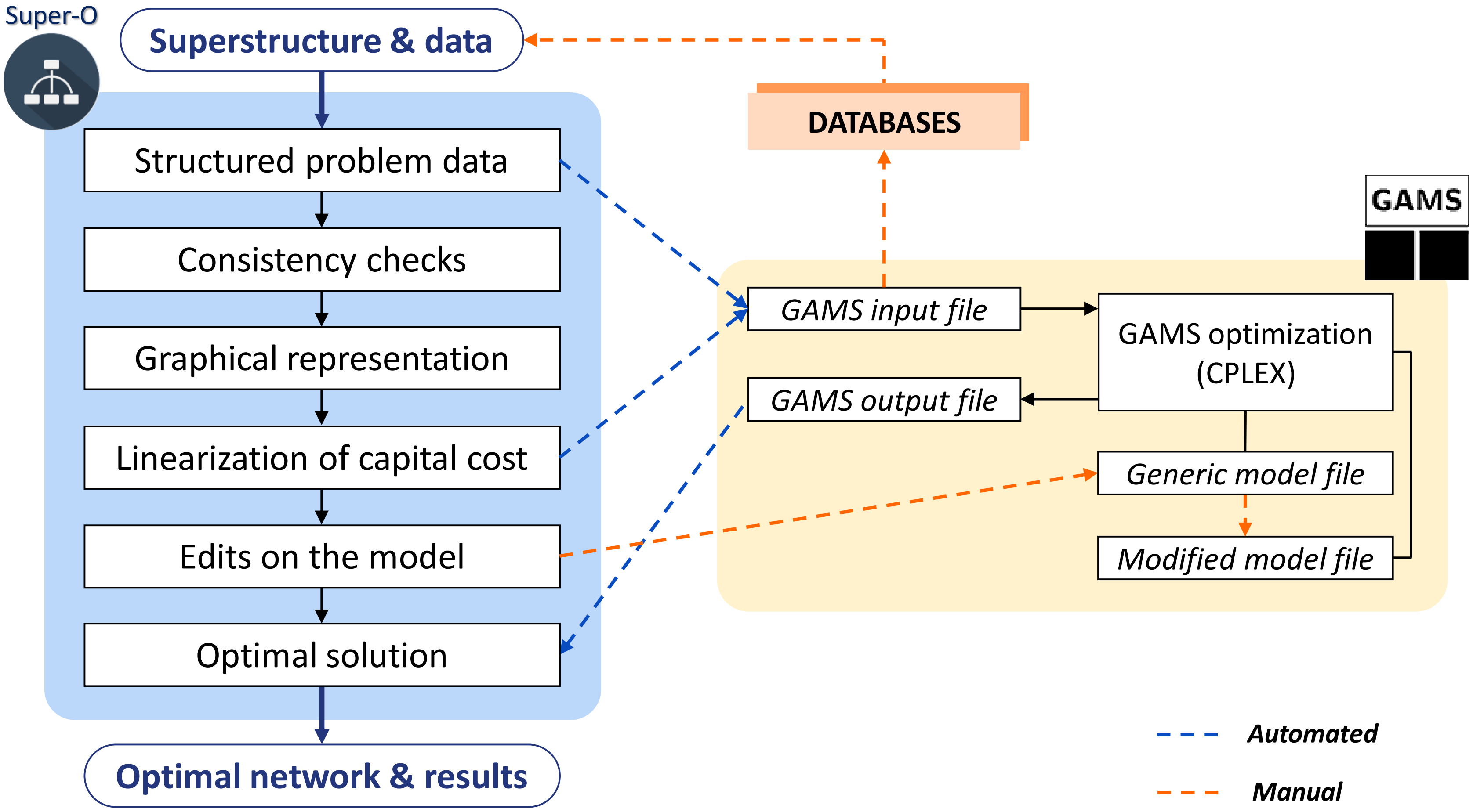
Data	CO_2 Database	Biorefinery Database
Components	22	71
Utilities	4	4
Processing steps	5	21
Processing intervals	30	102
Feedstocks	2	11
Products	11	9
Reactions	21	63
Locations	-	10

Source: Bertran, M., Frauzem, R., Sanchez-Arcilla, A., Zhang, L., Woodley, J.M., Gani, R. (submitted). A generic methodology for processing route synthesis and design based on superstructure optimization. Computers and Chemical Engineering (Special Issue ESCAPE26).



Super-O

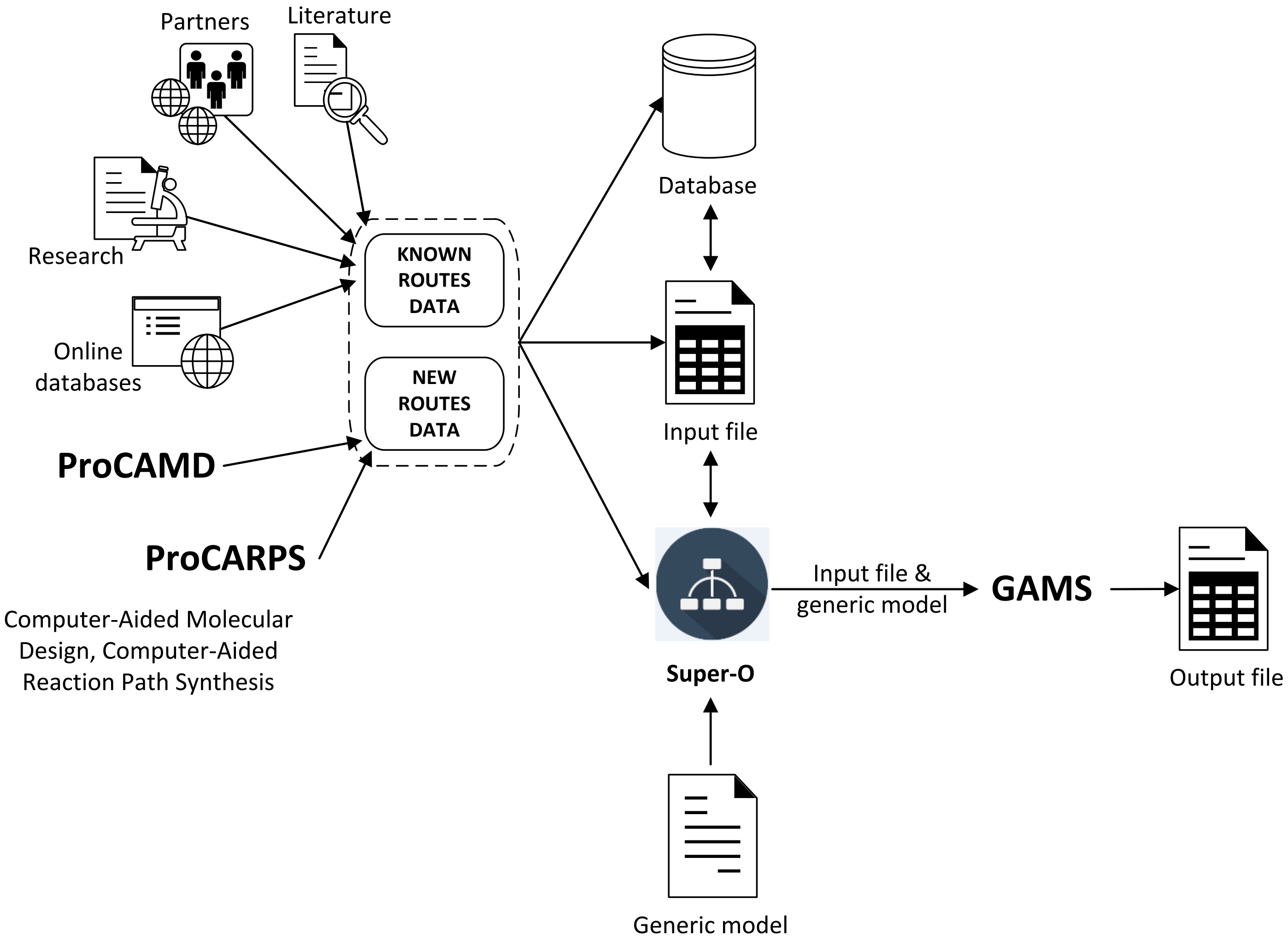
An interface for formulating and solving process synthesis problems using superstructure optimization



Source: Bertran, M., Frauzem, R., Zhang, L., Gani, R. (2016). A generic methodology for superstructure optimization of different processing networks. Computer Aided Chemical Engineering (26th European Symposium on Computer Aided Process Engineering, ESCAPE26).

Super-O

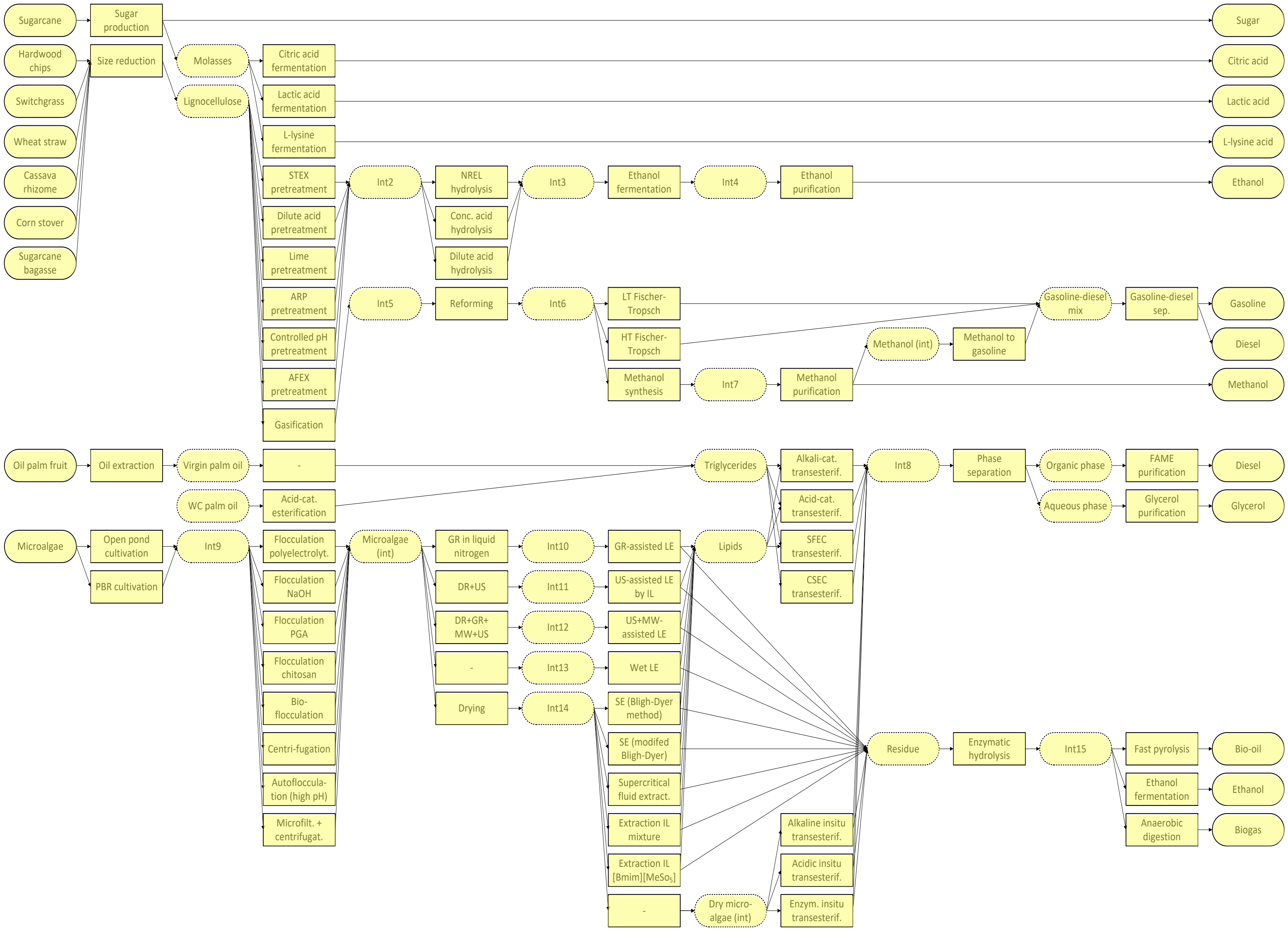
Tools integration



Computer-Aided Molecular Design, Computer-Aided Reaction Path Synthesis

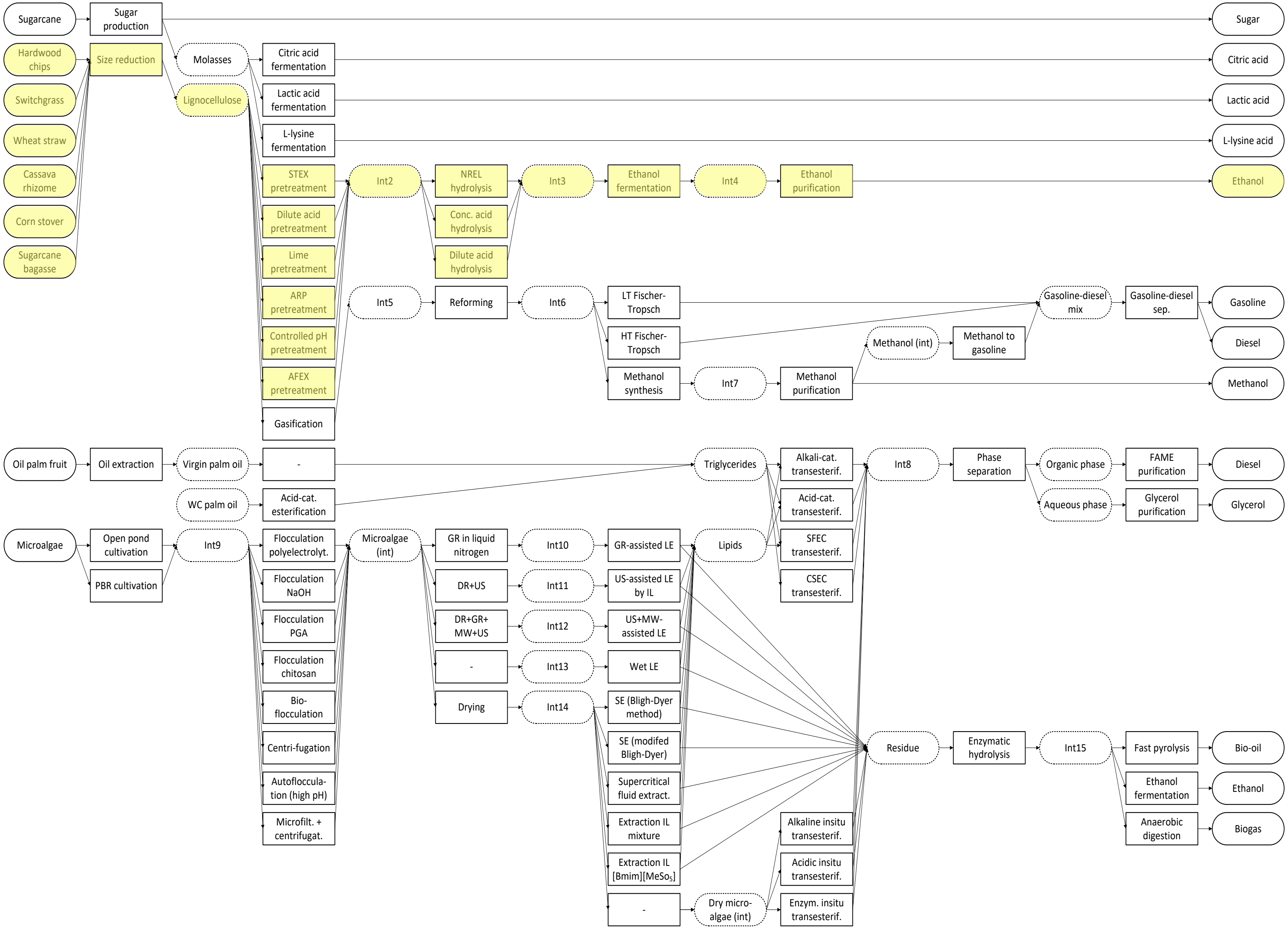
Source: Bertran, M., Frauzem, R., Sanchez-Arcilla, A., Zhang, L., Woodley, J.M., Gani, R. (submitted). A generic methodology for processing route synthesis and design based on superstructure optimization. Computers and Chemical Engineering (Special Issue ESCAPE26).

Biorefinery network



ARP: Ammonia Recycle Percolation, AFEX: Ammonia Fiber EXplosion, STEX: STeam EXplosion, LT: Low-Temperature, HT: High Temperature, WC: waste cooking, SFEC: Solvent-Free Enzyme-Catalyzed, CSEC: Co-Solvent Enzyme-Catalyzed, PBR: PhotoBioReactor, DR: DRying, US: UltraSound, GR: GRinding, MW: MicroWave, LE: Lipid Extraction, SE: Solvent Extraction, IL: Ionic Liquid

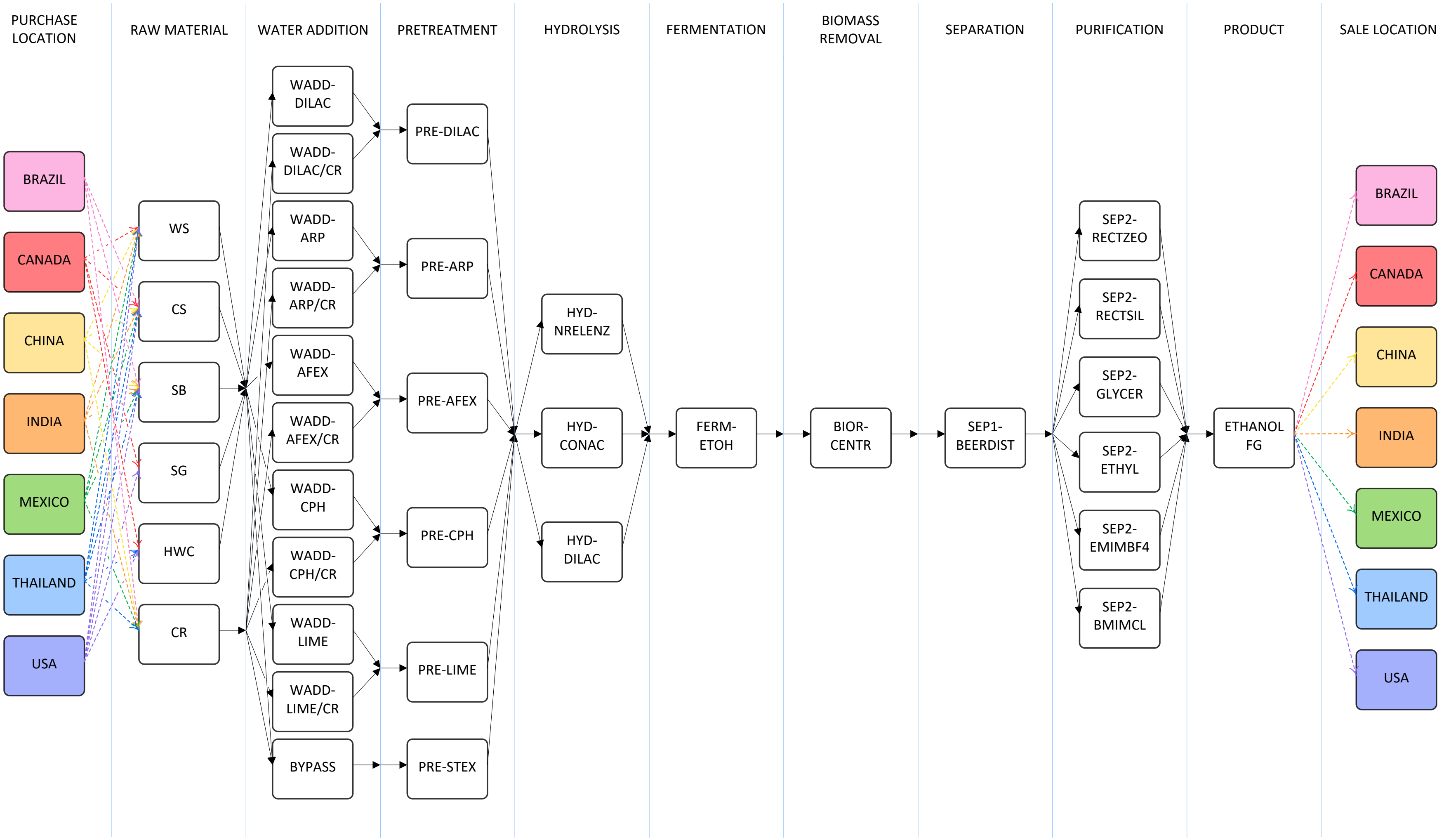
Application example



ARP: Ammonia Recycle Percolation, AFEX: Ammonia Fiber EXplosion, STEX: STeam EXplosion, LT: Low-Temperature, HT: High Temperature, WC: waste cooking, SFEC: Solvent-Free Enzyme-Catalyzed, CSEC: Co-Solvent Enzyme-Catalyzed, PBR: PhotoBioReactor, DR: DRying, US: UltraSound, GR: GRinding, MW: MicroWave, LE: Lipid Extraction, SE: Solvent Extraction, IL: Ionic Liquid

Application example

Ethanol from biomass: Superstructure



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Application example

Ethanol from biomass: Different locations yield different solutions

Location	RM	WADD	PRE	HYD	FERM	BIOR	SEP1	SEP2	PROD	Profit
BR	SCB	WADD-ARP	ARP	NREL	FERM	CENTR	BEER	BMIM	ETOH	**11.38**
CA	WS	-	STEX	NREL	FERM	CENTR	BEER	BMIM	ETOH	**-28.78**
CN	SCB	WADD-DA	DILAC	NREL	FERM	CENTR	BEER	BMIM	ETOH	**37.86**
IN	SCB	WADD-DA	DA	NREL	FERM	CENTR	BEER	BMIM	ETOH	**82.13**
MX	WS	-	STEX	NREL	FERM	CENTR	BEER	BMIM	ETOH	**-4.46**
TH	CR	-	STEX	DA	FERM	CENTR	BEER	BMIM	ETOH	**116.03**
US	HWC	-	STEX	CONCA	FERM	CENTR	BEER	BMIM	ETOH	**47.63**

↑

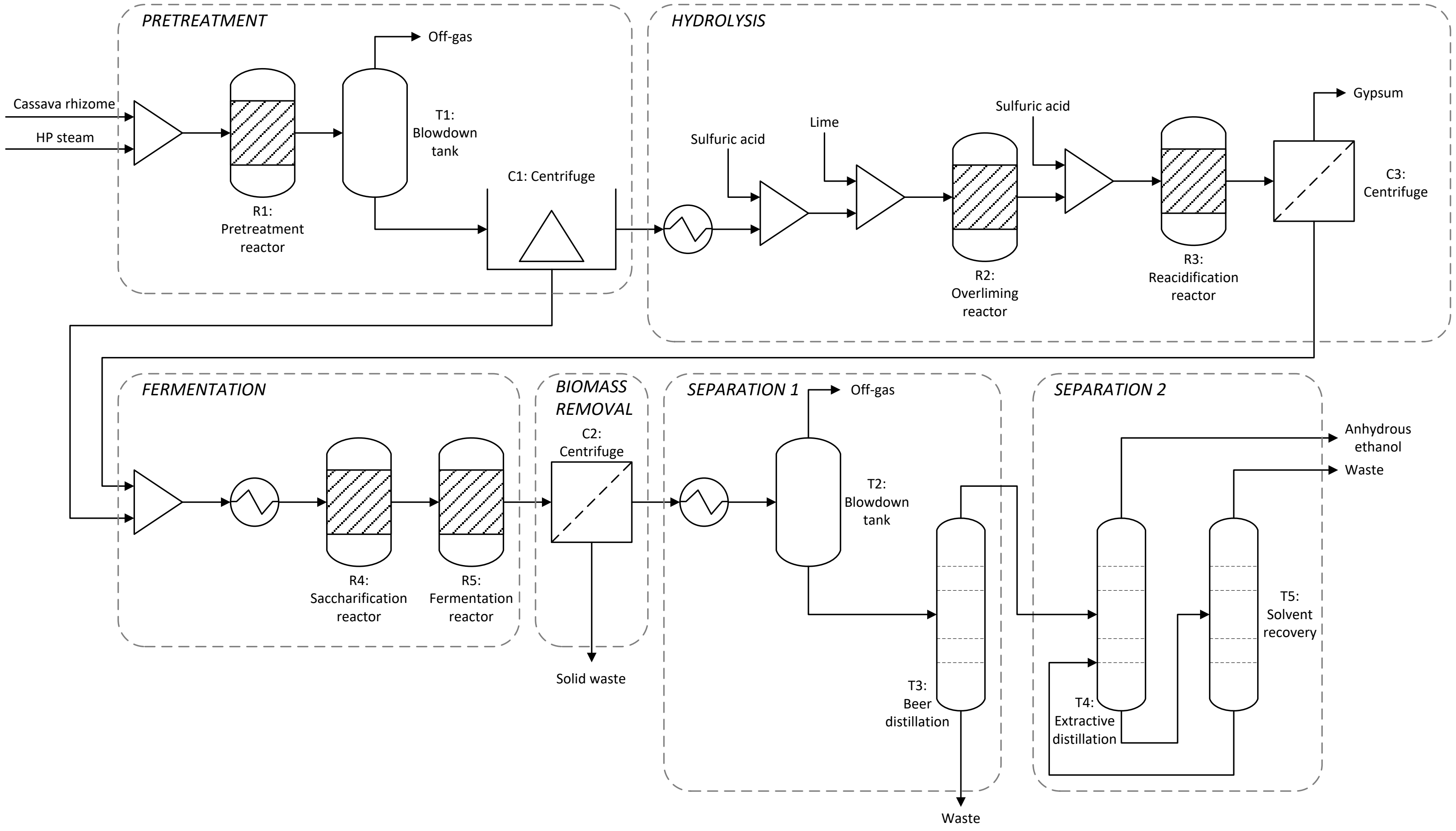
Given

RM	WADD	PRE	HYD	FERM	BIOR	SEP1	SEP2	PROD	Location	Profit
CR	-	STEX	DA	FERM	CENTR	BEER	BMIM	ETOH	**TH**	**116.03**

Source: Bertran, M., Frauzem, R., Sanchez-Arcilla, A., Zhang, L., Woodley, J.M., Gani, R. (submitted). A generic methodology for processing route synthesis and design based on superstructure optimization. Computers and Chemical Engineering (Special Issue ESCAPE26).

Application example

Ethanol from biomass: The output of Stage 1 is the processing route (flowsheet)



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Overview of problems & applications

- Synthesis of a new process
- Selection of potential products
- Residue revalorization
- Supply-chain management
- Process retrofitting
- Plant allocation
- …

Specialty chemicals

Chemical processes

Water management

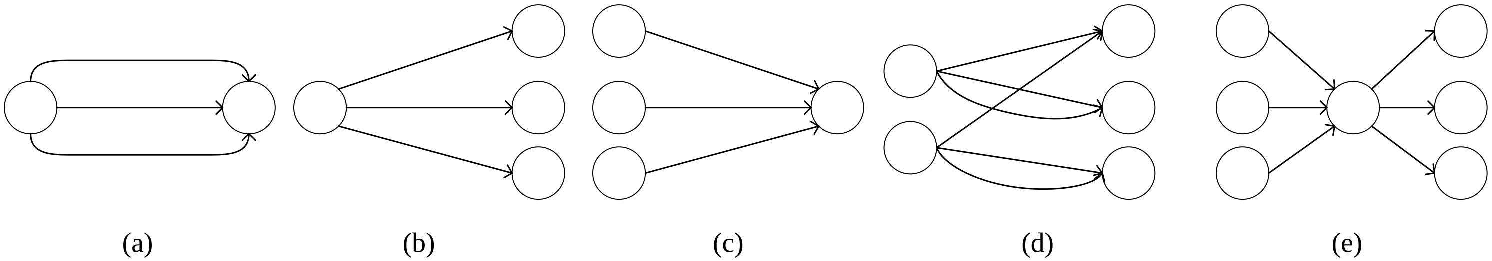
CO_2 utilization

Biorefinery

Overview of problems & applications

Synthesis problems in various fields have been solved using Super-O

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	985,666	951,826 (287)	Bertran et al. (submitted)



NF: number feedstocks, NP: number products, NI: number intervals, NC: number components, NU: number utilities, NR: number reactions, NL: number locations, NEQ: number equations, NV: number variables, NDV: number discrete variables