Lectures 10: Modelling case studies and additional topics

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Overview

- Model decomposition
- Case studies
- Additional topics
  - Data acquisition & analysis
  - Process modelling for control & diagnosis
  - Modelling of discrete event systems
  - Modelling of hybrid systems

Model Decomposition

PSE for SPEED

General model-based problem definition

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

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

Process*/product model (2)

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

Process/product constraints (3)

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

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

“Other” (selection) constraints (4a) (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 model-based problem solution

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

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

$\underline{Y} = 0$ 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

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

Solution strategy:

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

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

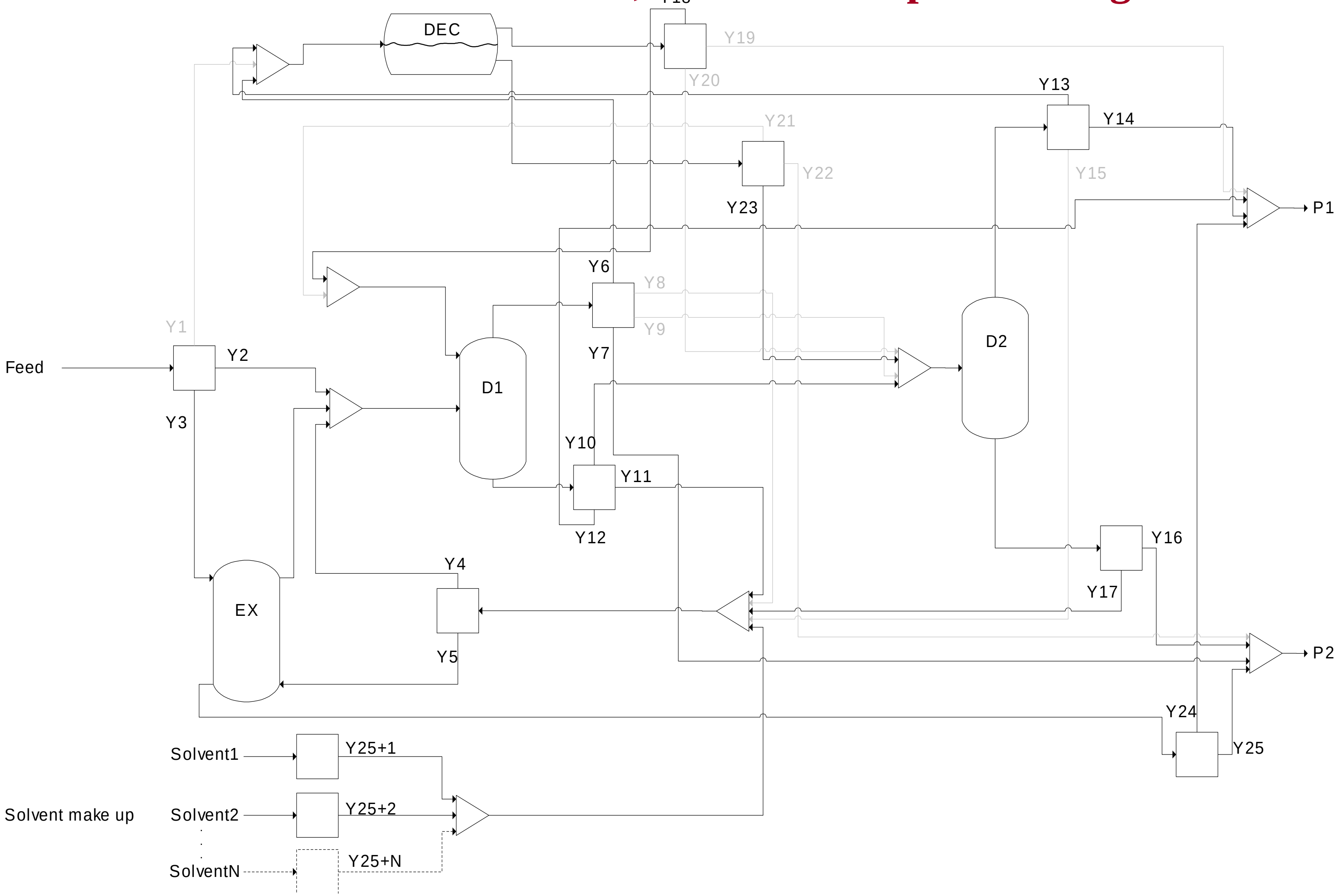
Solve III: Eq. 4 & Eq. 5 are satisfied for both sets of Y and the calculated values of X

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

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

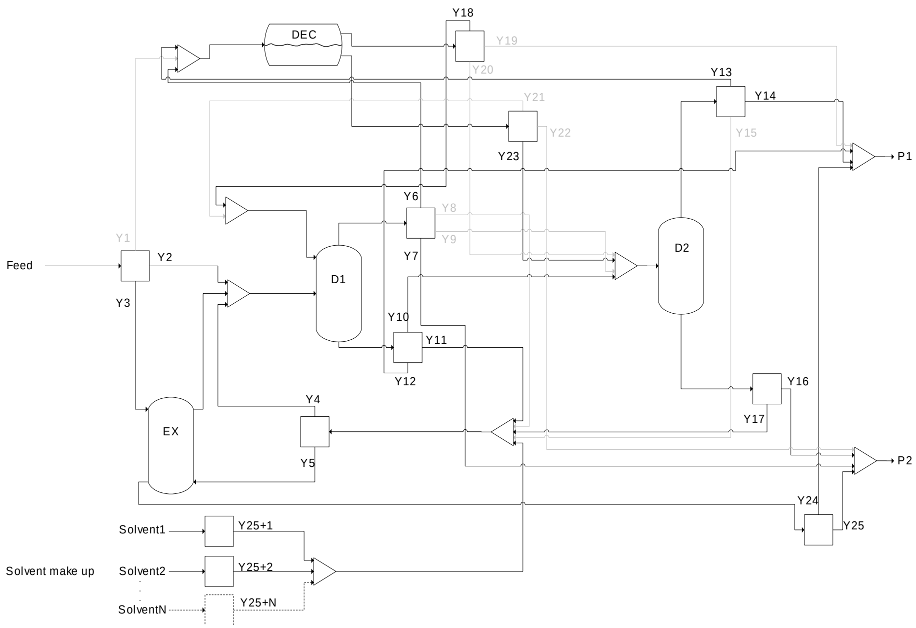
General model-based problem solution

Find solvent or membrane, flowsheet & optimal design

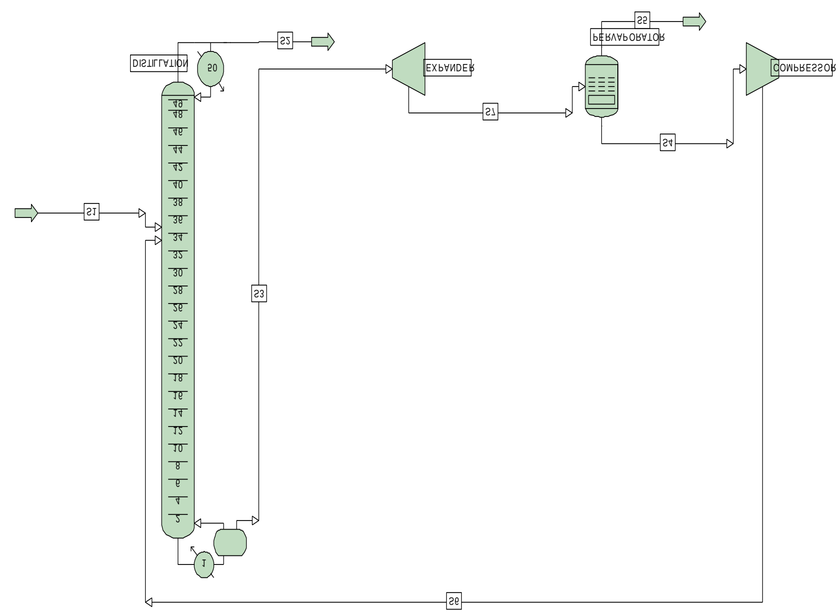


General model-based problem solution

Find solvent or membrane, flowsheet & optimal design



For fixed membrane and process flowsheet, find optmal design



General model-based problem solution

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

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

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

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

General model-based problem solution

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

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

Model analysis

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

Constitutive equations

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

Design constraints

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
C_1 and C_2	Known parameters

General model-based problem solution

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

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

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. 30-38 for specified $\underline{Z}$

Solve Eqs. 39-40 for $\underline{P}$

If 39-40 not satisfied, assume new $\underline{Z}$ 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				*					*	*	*

General model-based problem solution

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

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

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 = <u>P</u>

Solve Eqs. 39-40 for Y_1, Y_2

Solve Eqs. 30-36 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		*								*		*	*

Integrated Process Design and Control
Problem Definition

Integrated approach can be achieved by **identifying variables together with their target values** that have **roles in process-controller design**

$$\min_{\mathbf{x},\mathbf{y},\mathbf{u}} \quad F(\mathbf{x},\mathbf{y},\mathbf{u}) = \begin{bmatrix} F_1(\mathbf{x},\mathbf{y},\mathbf{u}) \\ F_2(\mathbf{x},\mathbf{y},\mathbf{u}) \end{bmatrix}$$

subject to:

$$\dot{\mathbf{x}}(t) = f(\mathbf{x},\mathbf{y},\mathbf{u},t)$$

$$0 = h(\mathbf{x},\mathbf{y},\mathbf{u})$$

$$0 \le g(\mathbf{x},\mathbf{y},\mathbf{u})$$

$$\mathbf{x}(t_0) = \mathbf{x}_0$$

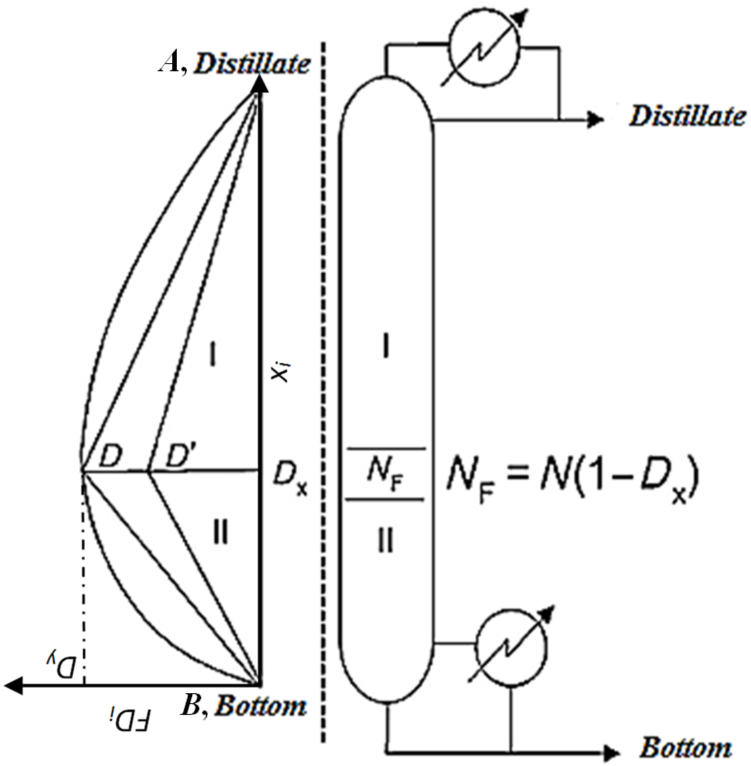
$$\mathbf{u}(t_0) = \mathbf{u}_0$$

The solution to this optimization problem must address the **trade-offs between conflicting design and control objectives** for the chemical processes

Identifying optimal design together with design-manipulated variables **u**, process-controlled variables **y**, their target set points, and their pairing.

Concept of Driving Force: Application to distillation columns

Driving Force: $D_{ij} = y_i - x_i = x_i\, \alpha_{ij} / [x_i (\alpha_{ij} - 1) + 1] - x_i$



A design method of distillation separation system based on **identification of the largest driving force.**

At the maximum driving force, separation becomes easier and **energy required is at the minimum**.

Bek-Pedersen, E., Gani, R. (2004). Design and synthesis of distillation systems using a driving-force-based approach, Chem. Eng. Process., 43, 251–262

A Conceptual Example: Design & Control

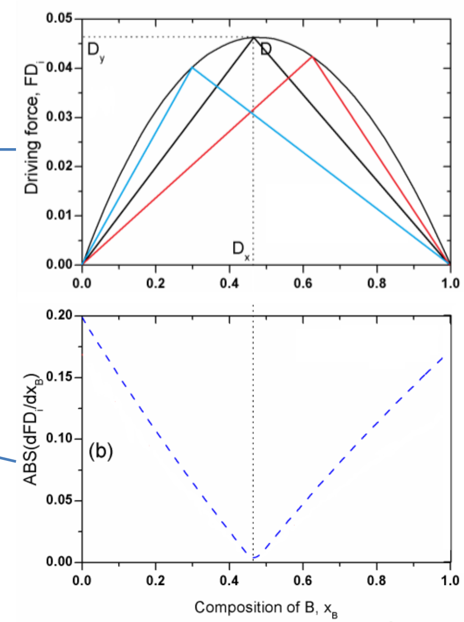
Binary non-Reactive Distillation Column

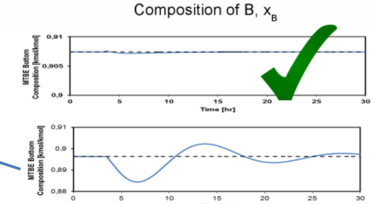
Step 1: Process Design:
N Design alternatives that
match design targets to separate A from B

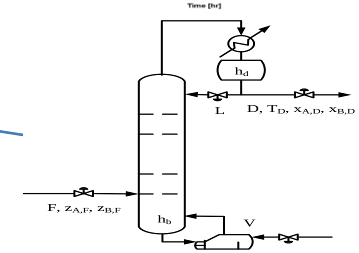
Step 2: Optimal Design-Control Solution
N – M Design alternatives that
match design and control objectives

Step 3: Final Selection and Verification
N – M – L Design alternatives that *have matched all the constraints are compared*

Optimal solution





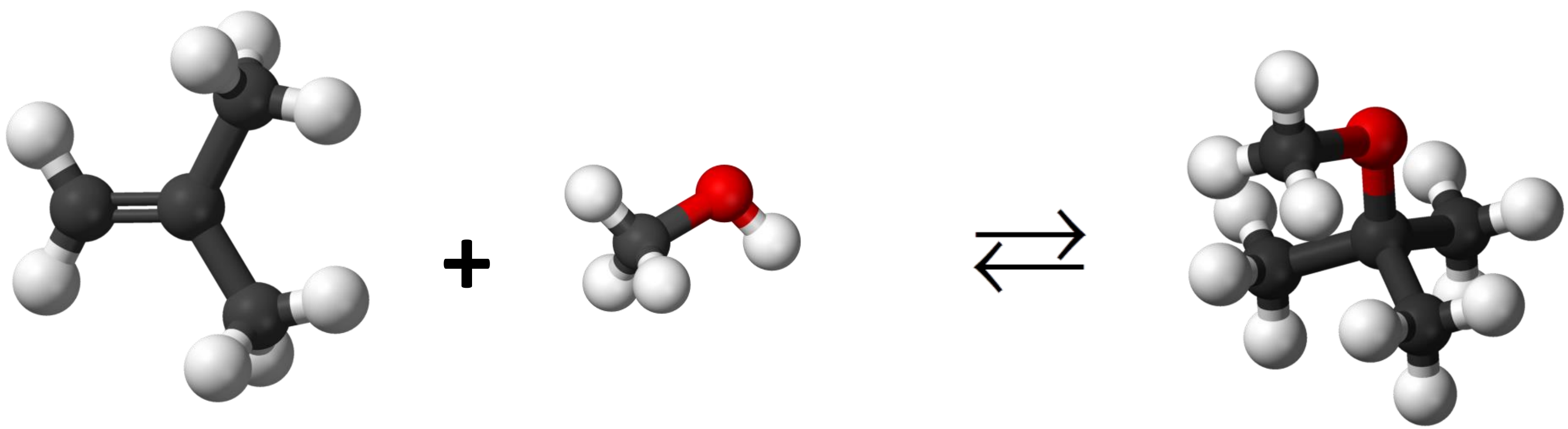


Will the same method work for PI?

For example, a reactive distillation column?

$$Isobutene\left(C_4H_8\right) + Methanol\left(CH_4O\right) \rightarrow MTBE\left(C_5H_{12}O\right)$$

Number of Compounds – Number of Reactions = 2



Element A **Element B** **Element AB**

With respect to ”elements”, this is a binary element system

Pérez Cisneros, E.S., Gani, R., Michelsen, M.L. (1997). Reactive separation systems—I. Computation of physical and chemical equilibrium, Chem. Eng. Sci., 52, 527–543.

Case Study: Reactive Distillation

Step 1 – Process Design

- **Reactive distillation column design**

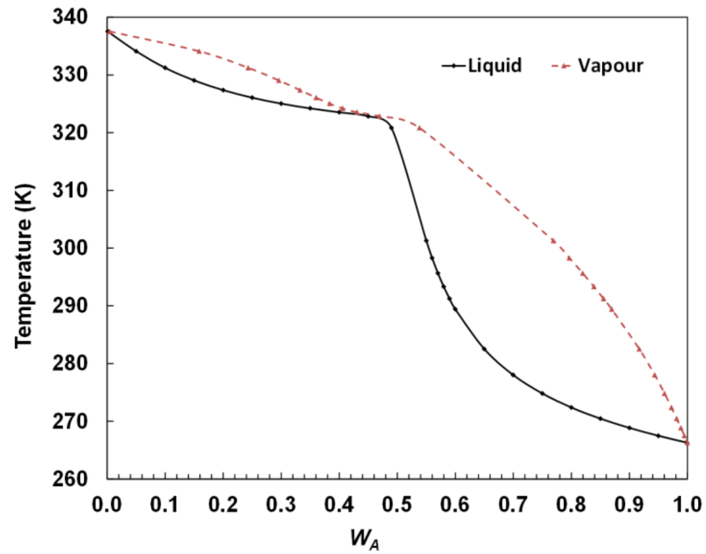
Reactive VLE data is obtained by consecutive calculation of reactive bubble points*.

i-Butene (W_A)	Temperature (K)	Component vapor composition			Component liquid composition		
		y(1)	y(2)	y (3)	x(1)	x(2)	x(3)
0.01	337.53	4.37E-04	0.99547	0.00408	6.43E-06	0.99899	0.00099
0.05	334.11	0.0169	0.81473	0.16836	0.00032	0.94738	0.05229
0.1	331.23	0.02759	0.68755	0.28484	0.00067	0.88896	0.11036
0.15	329.05	0.03538	0.59459	0.37001	0.00108	0.82372	0.17519
0.2	327.37	0.04187	0.52273	0.43539	0.00161	0.7504	0.24798
0.25	326.06	0.04803	0.46383	0.48812	0.00230	0.66743	0.33026
0.3	325.03	0.05475	0.41189	0.53334	0.00326	0.57282	0.4239
0.35	324.21	0.06341	0.36097	0.57561	0.00470	0.46407	0.53122
0.4	323.53	0.07759	0.30208	0.62031	0.00716	0.33811	0.65473
0.45	322.84	0.11239	0.21477	0.67283	0.01290	0.19238	0.7947
0.5	320.83	0.22288	0.09427	0.68284	0.03122	0.06921	0.89955
0.55	301.29	0.70051	0.00265	0.29683	0.1845	0.00328	0.81221
0.6	289.41	0.85004	0.00037	0.14958	0.33378	0.00067	0.66553
0.65	282.52	0.90949	0.00011	0.09039	0.46166	0.00022	0.53811
0.7	278.02	0.94019	4.46E-05	0.05976	0.57146	9.63E-05	0.42943
0.75	274.82	0.95888	2.16E-05	0.04109	0.66668	4.47E-05	0.33327
0.8	272.39	0.97161	1.14E-05	0.02837	0.75001	2.16E-05	0.24997
0.85	270.46	0.98103	6.16E-06	0.01895	0.82353	1.03E-05	0.17645
0.9	268.86	0.98846	3.13E-06	0.01152	0.88888	4.52E-06	0.1111
0.95	267.49	0.99464	1.20E-06	0.00532	0.94736	1.52E-06	0.05262
0.99	266.31	0.99989	2.04E-08	0.0001	0.99899	2.08E-08	0.001

*(1), (2) and (3) denote to i-Butene, methanol and MTBE, respectively.

$$W_A^l = \frac{x_1 + x_3}{x_1 + x_2 + 2 \cdot x_3}$$

$$W_B^l = \frac{x_2 + x_3}{x_1 + x_2 + 2 \cdot x_3}$$

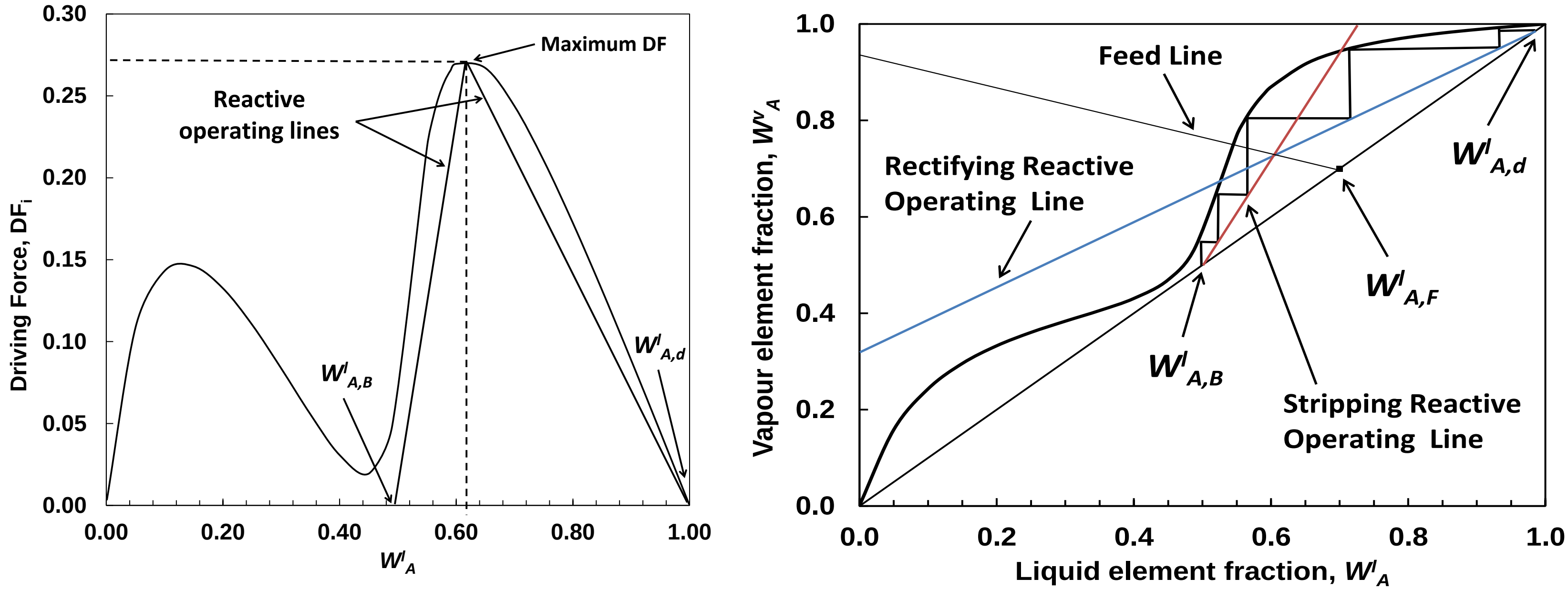


*Tool: ICAS-Process Design Studio

Case Study: Reactive Distillation

Step 1 – Process Design

- **Reactive Distillation Design**



Reflux ratio: 2

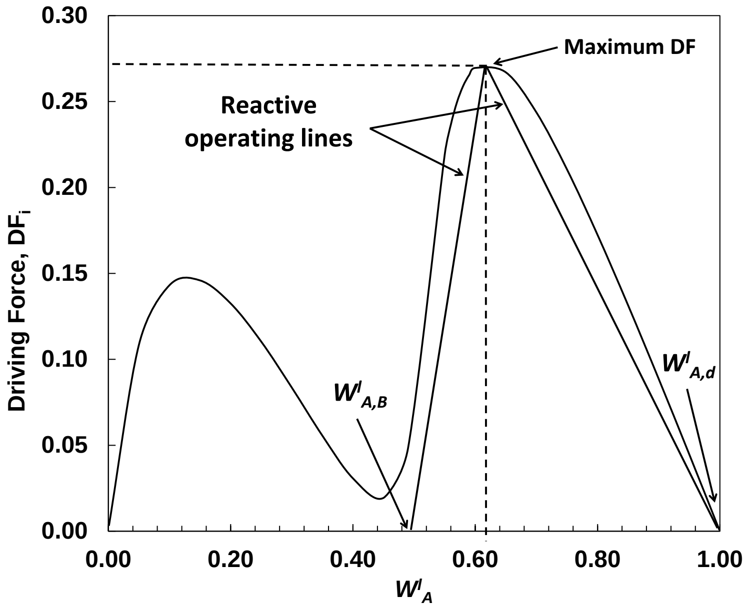
Theoretical number of trays: 5 plus non-reactive reboiler and condenser

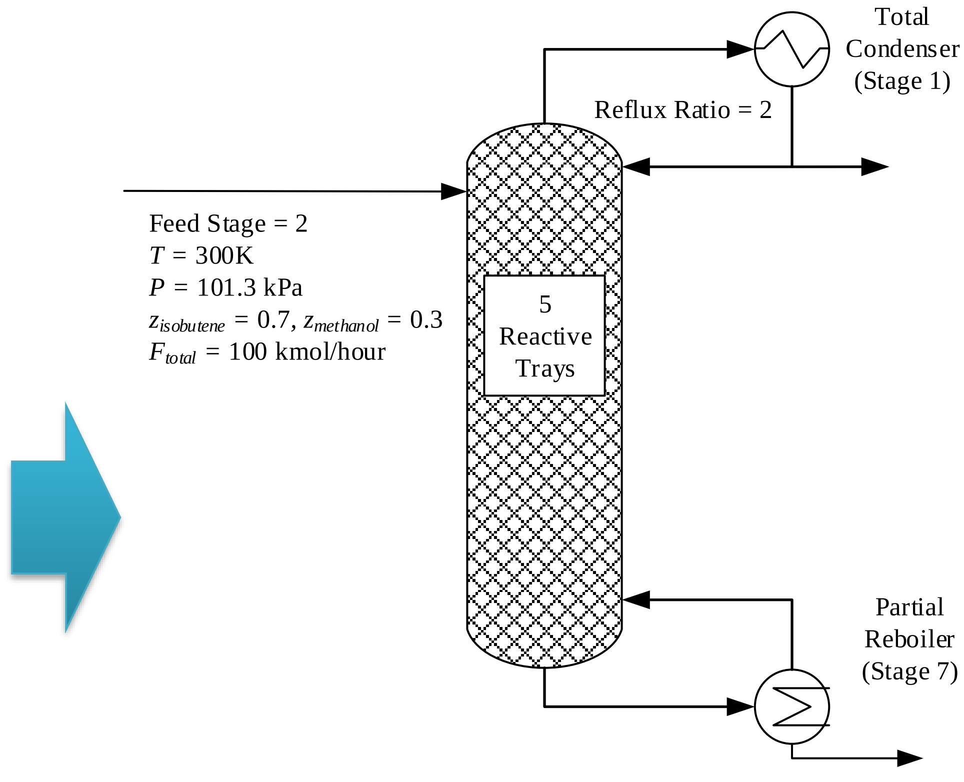
Assumptions: Total condenser, Partial reboiler, Chemically saturated liquid reflux

Case Study: Reactive Distillation

Step 1 – Process Design

- **Reactive Distillation Design**



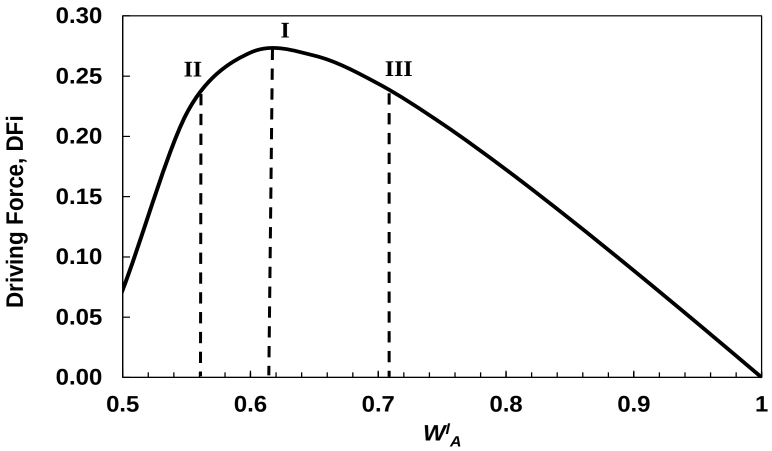


Case Study: Reactive Distillation

Step 2 – Optimal Design-Control Solution

- **Selection of controlled variables**

- $W_{A,max}$ – primary controlled variable (uncontrolled output)
- W_A^d or W_A^B – secondary controlled variable (desired output)



- **Set-points value for controlled and manipulated variables**

- The calculated value of **y** and **u** at Point (I) are the optimal set-points.

Case Study: Reactive Distillation

Step 2 – Optimal Design-Control Solution

- **Sensitivity of controlled variables with respect to disturbances in the feed**

- It is verified that disturbance rejection in the feed is the best at the maximum driving force (Point I) than other points.

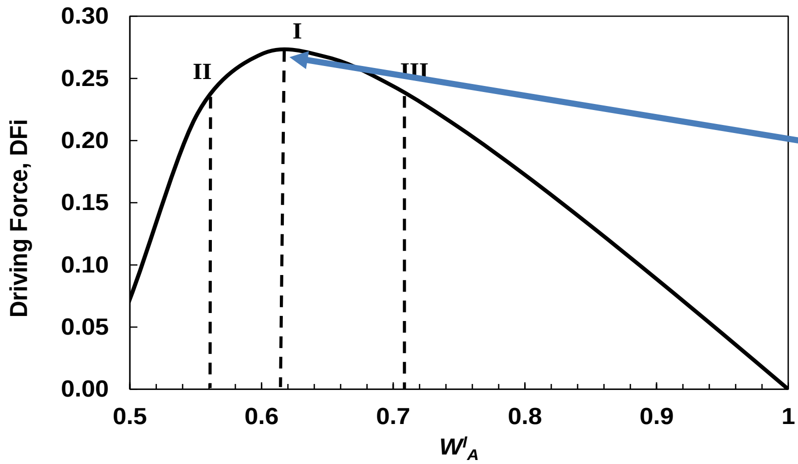
$$\frac{dy}{dd} = \begin{bmatrix} \frac{dW_A^d}{dF_f} & \frac{dW_A^d}{dz_{W_{Af}}} \\ \frac{dW_A^B}{dF_f} & \frac{dW_A^B}{dz_{W_{Af}}} \end{bmatrix} = \begin{bmatrix} \left(\frac{dW_A^d}{dDF_i}\right)\left(\frac{dDF_i}{dW_A^l}\right)\left(\frac{dW_A^l}{dF_f}\right) & \left(\frac{dW_A^d}{dDF_i}\right)\left(\frac{dDF_i}{dW_A^l}\right)\left(\frac{dW_A^l}{dz_{W_{Af}}}\right) \\ \left(\frac{dW_A^B}{dDF_i}\right)\left(\frac{dDF_i}{dW_A^l}\right)\left(\frac{dW_A^l}{dF_f}\right) & \left(\frac{dW_A^B}{dDF_i}\right)\left(\frac{dDF_i}{dW_A^l}\right)\left(\frac{dW_A^l}{dz_{W_{Af}}}\right) \end{bmatrix}$$

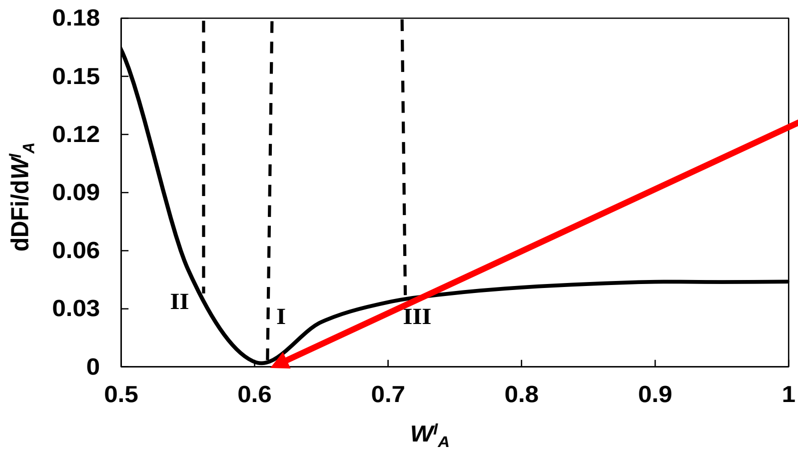
- At Point (I), $\left.\frac{dDF_i}{dW_A^l}\right|_{W_{A,\max}^d} = 0$

$$\frac{dy}{dd} = \begin{bmatrix} \frac{dW_A^d}{dF_f} & \frac{dW_A^d}{dz_{W_{Af}}} \\ \frac{dW_A^B}{dF_f} & \frac{dW_A^B}{dz_{W_{Af}}} \end{bmatrix} \approx \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

Case Study: Reactive Distillation

Step 2 – Optimal Design-Control Solution





Optimal process design: the lowest energy required [3]

Optimal controller design the lowest sensitivity of d**y**/d**d** and the highest sensitivity of d**y**/d**u**.[4]

[4] Bek-Pedersen, E., Gani, R. (2004). Design and synthesis of distillation systems using a driving-force-based approach, Chem. Eng. Process., 43, 251–262

[1] Hamid, M. K. A., Sin, G., and Gani, R. (2010). Integration of process design and controller design for chemical processes using model-based methodology. Comput. Chem. Eng., 34, 683-699.

Case Study: Reactive Distillation

Step 2 – Optimal Design-Control Solution

- **Selection of the controller structure (pairing between controlled-manipulated variables)**

- It is verified that at the maximum point of the driving force diagram, pair of secondary controlled variable or with manipulated variable is always the best controller structure.

$$\frac{dy}{du}=\begin{bmatrix}\frac{dW_A^d}{dRR} & \frac{dW_A^d}{dRB}\\ \frac{dW_A^B}{dRR} & \frac{dW_A^B}{dRB}\end{bmatrix}=\begin{bmatrix} DF_i+(RR+1)\left(\frac{dDF_i}{dW_{Ai}^l}\right)\left(\frac{dW_A^l}{dRR}\right)+\frac{dW_A^l}{dRR} & (RR+1)\left(\frac{dDF_D}{dW_A^l}\right)\left(\frac{dW_A^l}{dRB}\right)+\frac{dW_A^l}{dRB}\\ \frac{dW_A^l}{dRR}-\left(\frac{dDF_i}{dW_A^l}\right)\left(\frac{dW_A^l}{dRR}\right)RB & \frac{dW_A^l}{dRB}-DF_i\end{bmatrix}$$

- At Point (I), $\left.\frac{dDF_i}{dW_A^l}\right|_{W_{A,\max}^d}=0$

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

Case Study: Reactive Distillation

Step 3 – Final Selection and Verification

- **Rigorous dynamic simulation***

- A rigorous reactive distillation dynamic model based on elements is used.
- The chemical reactions occurring are fast enough to reach the equilibrium.
- Chemical equilibrium condition is implicitly incorporated into the element mass balances.
- Alternative designs are selected in addition to the optimal design for verification purposes.

**Tool*: ICAS-Process Simulation

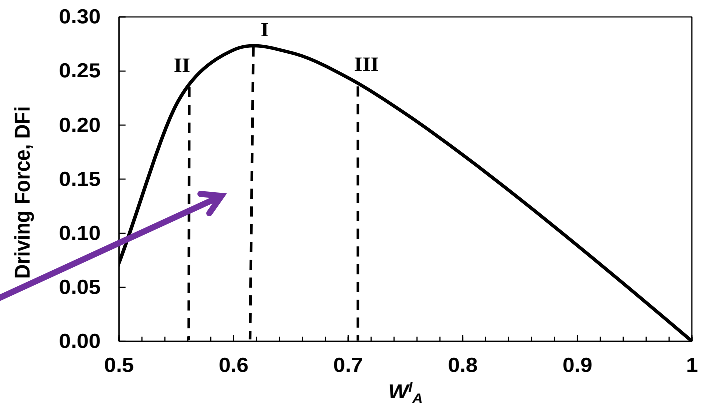
Case Study: Reactive Distillation

Step 3 – Final Selection and Verification

- **Controller structure verification**

- Controller structure at the maximum driving force:

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



- The relative gain array (RGA):

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

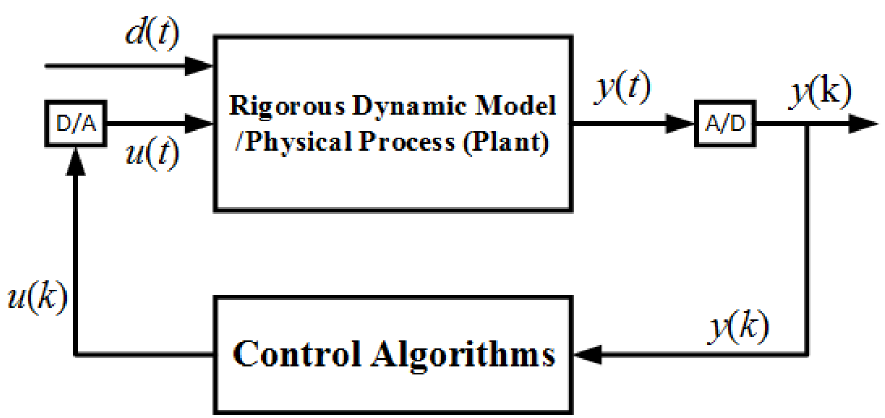
Candidate design alternatives
to the maximum driving force

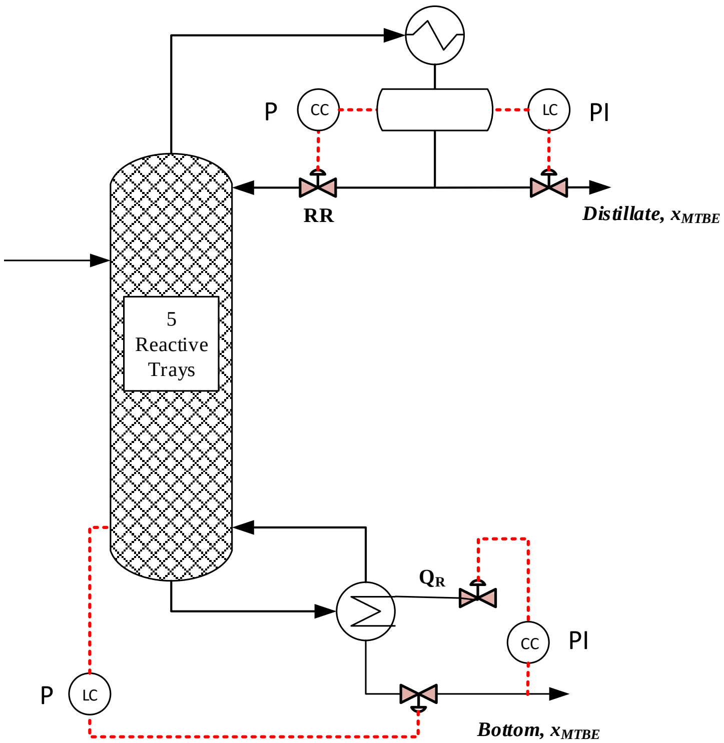
Case Study: Reactive Distillation

Step 3 – Final Selection and Verification

- **Rigorous dynamic simulation: Closed-loop**

- Controller structure implementation



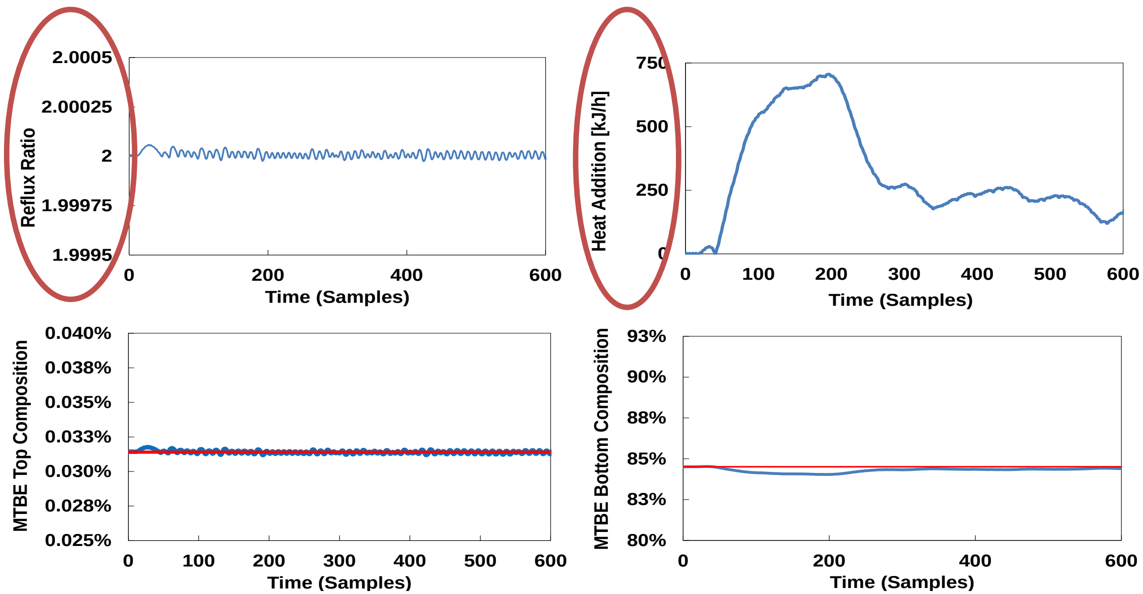


- Controller tuning : SIMC rules

Case Study: Reactive Distillation

Step 3 – Final Selection and Verification

- **Rigorous dynamic simulation: Closed-loop**



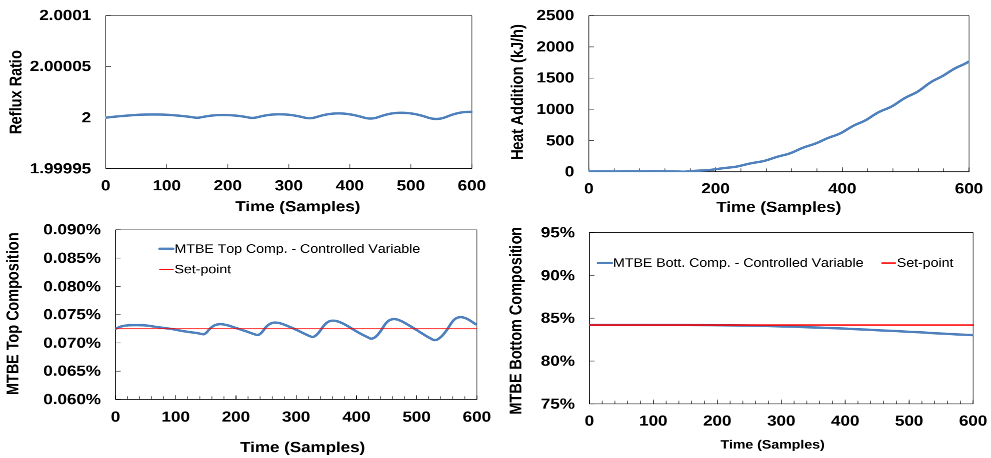
$$RGA_{(I)} = \begin{bmatrix} 0.93 & 0.07 \\ 0.07 & 0.93 \end{bmatrix}$$

Optimal Design-Control Solution

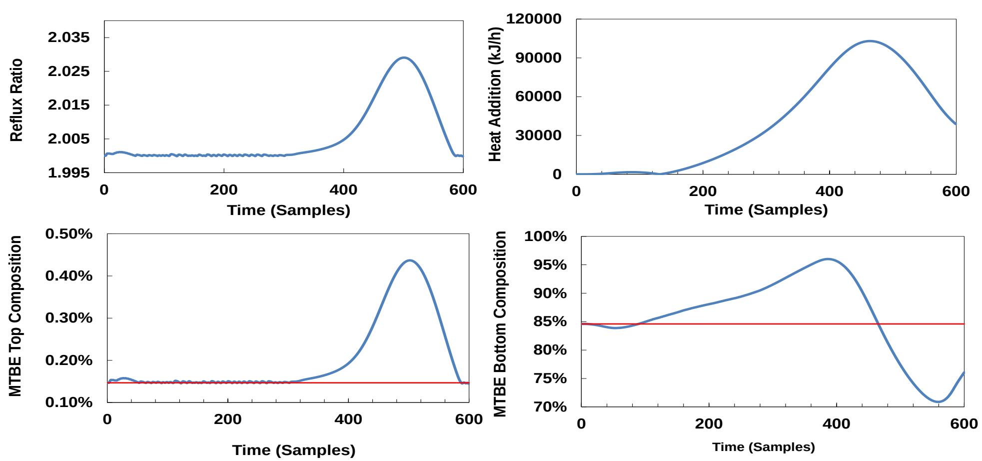
- Least sensitivity to the disturbances
- Least control loop interaction and effort in manipulation

Case Study: Reactive Distillation

Step 3 – Final Selection and Verification

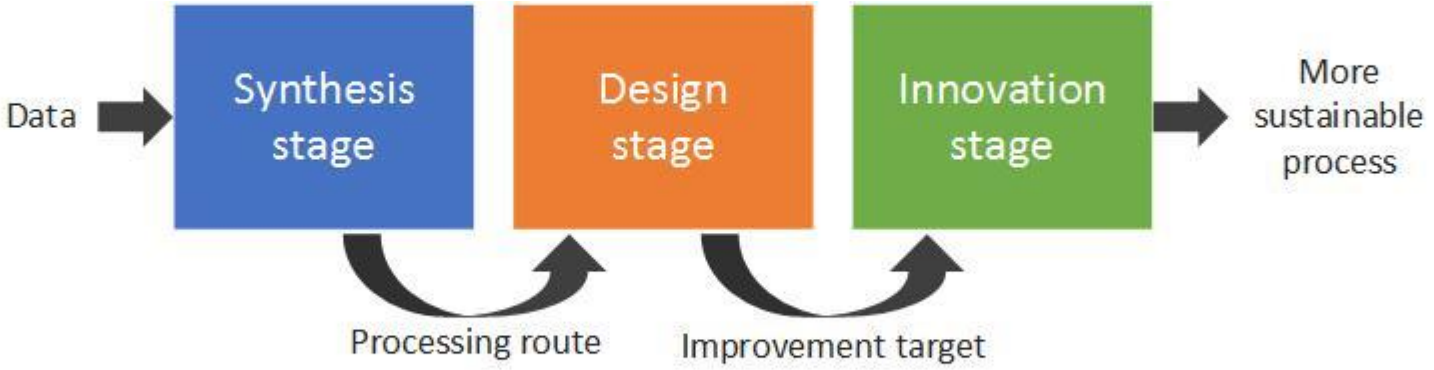


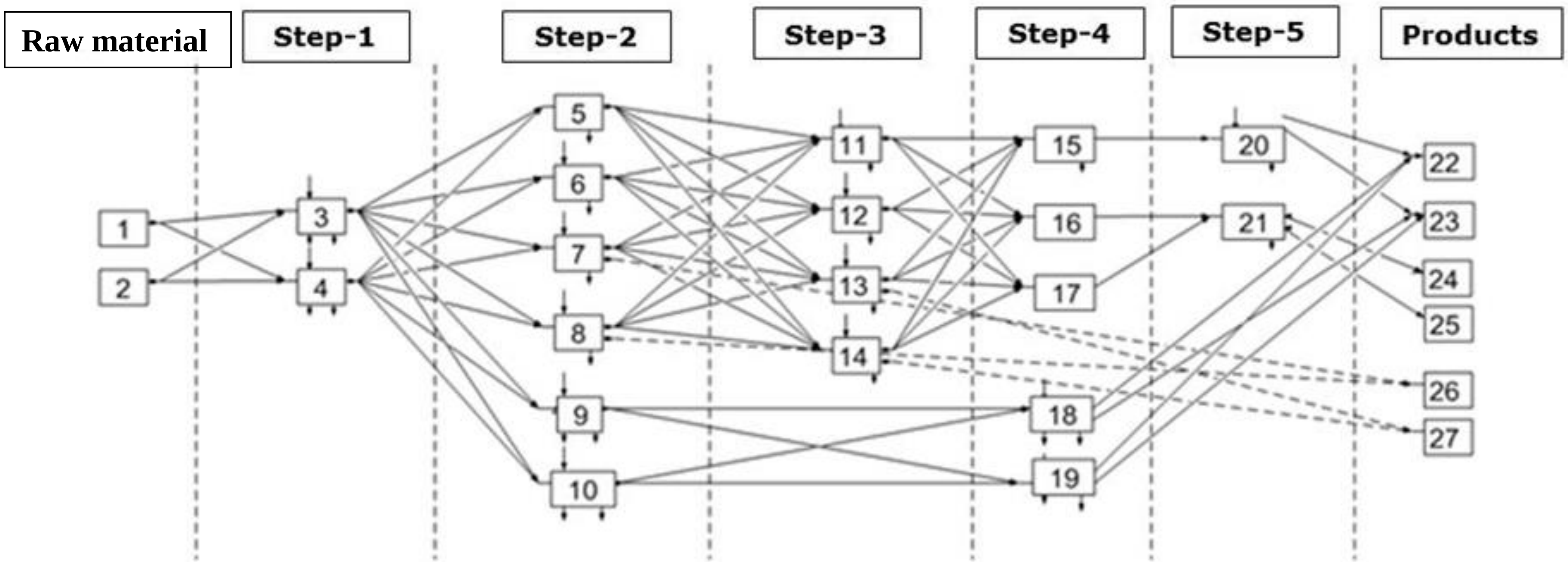
$$RGA_{(II)} = \begin{bmatrix} 9.06 & -8.06 \\ -8.06 & 9.06 \end{bmatrix}$$



$$RGA_{(III)} = \begin{bmatrix} -0.28 & 1.28 \\ 1.28 & -0.28 \end{bmatrix}$$

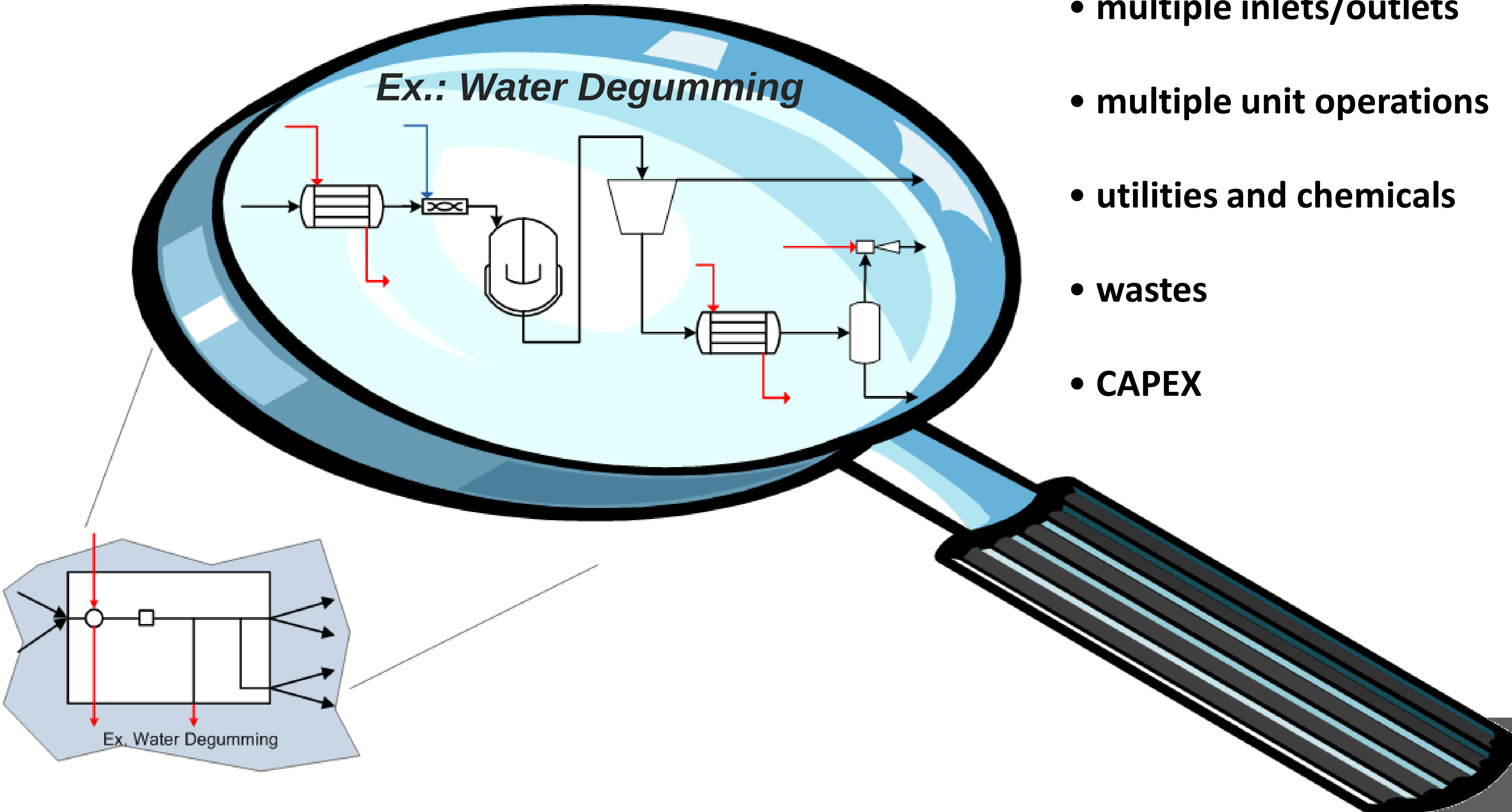
Model-based process synthesis-design





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

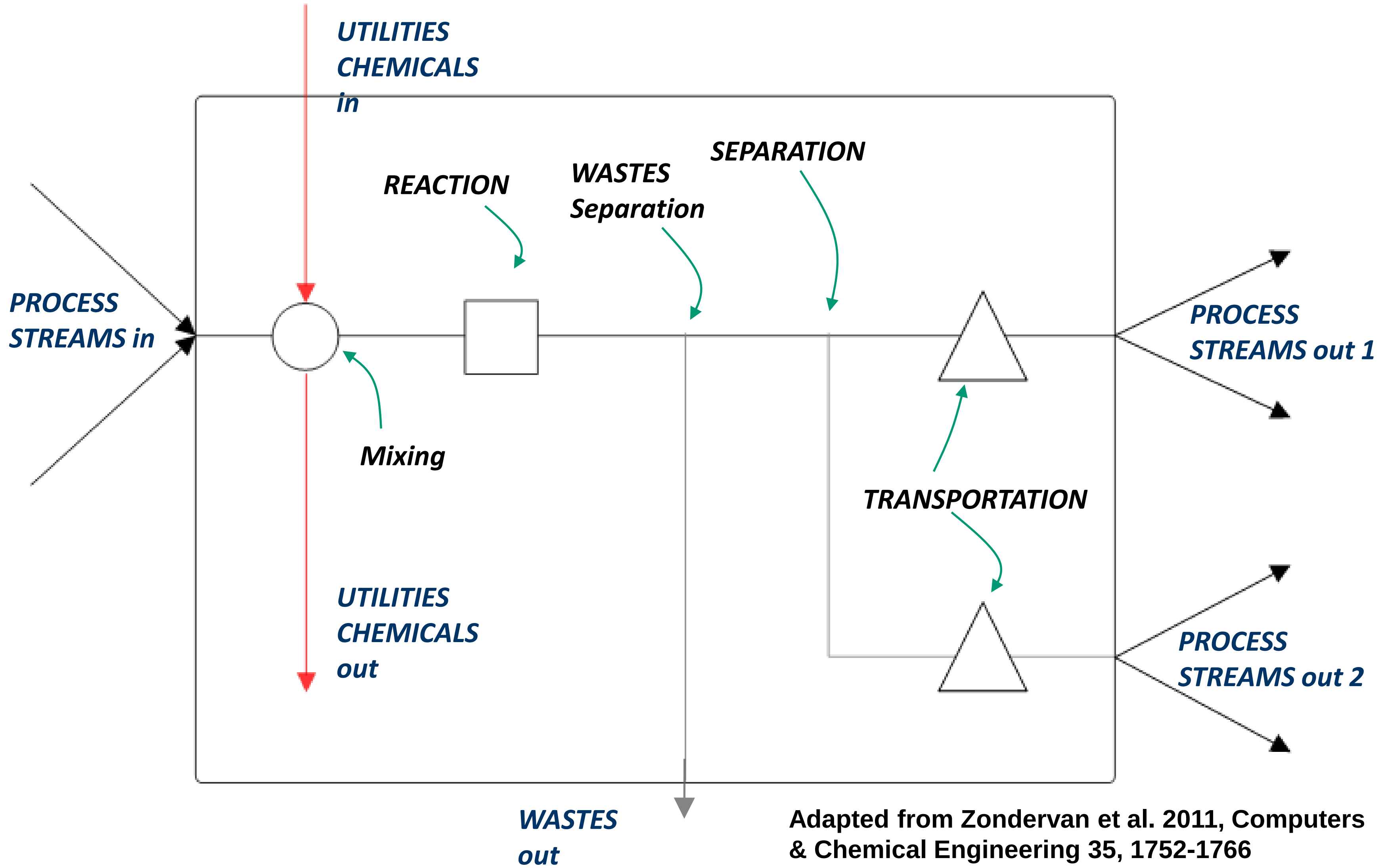
Model of the process-step interval network



PROCESS INTERVALS:

- **multiple inlets/outlets**
- **multiple unit operations**
- **utilities and chemicals**
- **wastes**
- **CAPEX**

The generic process interval model



Adapted from Zondervan et al. 2011, Computers & Chemical Engineering 35, 1752-1766

Generic Model Equations and Data

MIXING	$F^{M}_{i,kk} = \sum_{k} \left(F_{i,k,kk} \right) + \alpha_{i,kk} \cdot R_{i,kk}$ $R_{i,kk} = \mu_{i,kk} \cdot \sum_{i,k} \left(F_{i,k,kk} \right)$
REACTION	$F^{R}_{i,kk} = F^{M}_{i,kk} + \sum_{rr,react} \left(\gamma_{i,kk,rr} \cdot \theta_{react,kk,rr} \cdot F^{M}_{reac,kk} \right)$
WASTES SEPARATION	$F^{out}_{i,kk} = F^{R}_{i,kk} \cdot \left(1 - SW_{i,kk} \right)$
PRODUCT SEPARATION	$F_{i,kk,kk} = F^{out}_{i,k} \cdot S_{k,kk} \cdot \varepsilon_{i,k,kk}$
TRANSPORTATION	$Ctr_{k,kk} = \sum_{i} F_{i,k,kk} \cdot W_{k,\,kk} \cdot dist_{k,kk}$
CAPEX	$CAPEX_{kk} = P_{kk} \cdot \sum \left(F^{out}_{i,kk} \right)^{Q_{kk}}$
OBJECTIVE FUNCTION	$EBIT = \sum_{i,k} \left(P^{prod}_{k} F^{OUT}_{i,k} - P^{raw}_{k} F^{OUT}_{i,k} - P^{util}_{k} R_{i,kk} - P^{waste}_{i,k} Waste_{i,kk} - \frac{CAPEX_{k}}{t} \right)$

data

Data:	Source:
Alternatives	Company (all)
Process related	Engineering
Prices and Market related	Marketing, procurement
Product related	Product engineering
Regulations related	Regulatory

Large number of equations and data

Multiple data type and sources

↓

Need for Automation of problem formulation

General mathematical problem

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

Process-product model

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

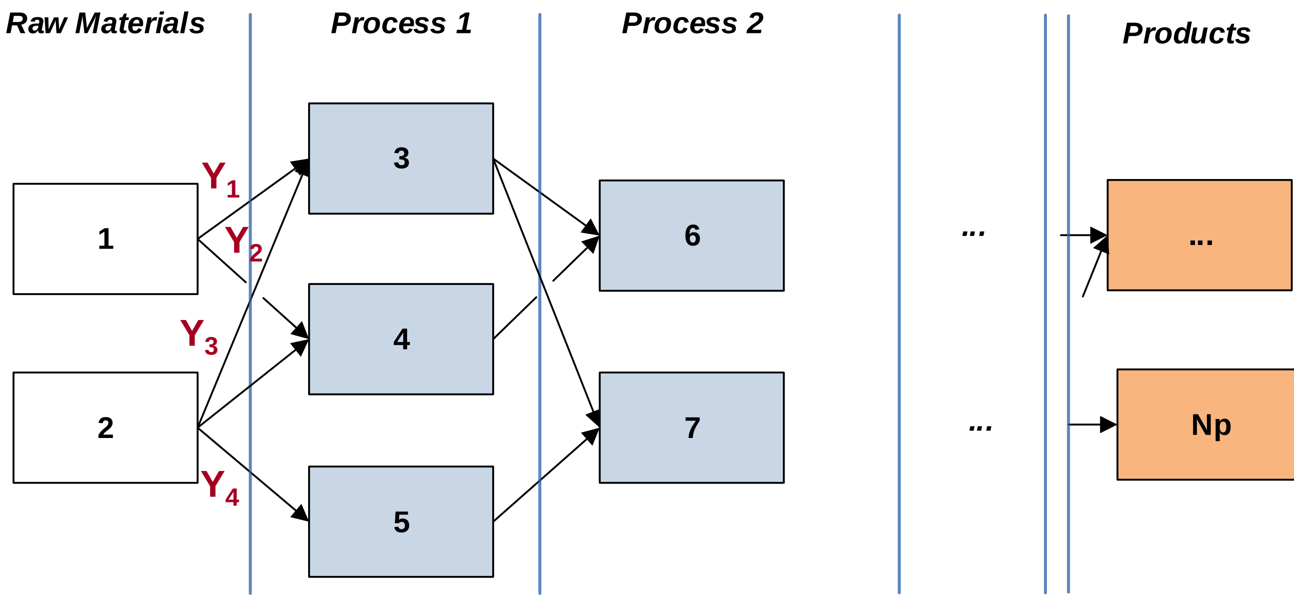
Process-product

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

Equipment-material

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

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



Flowhseet-chemical alternatives

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

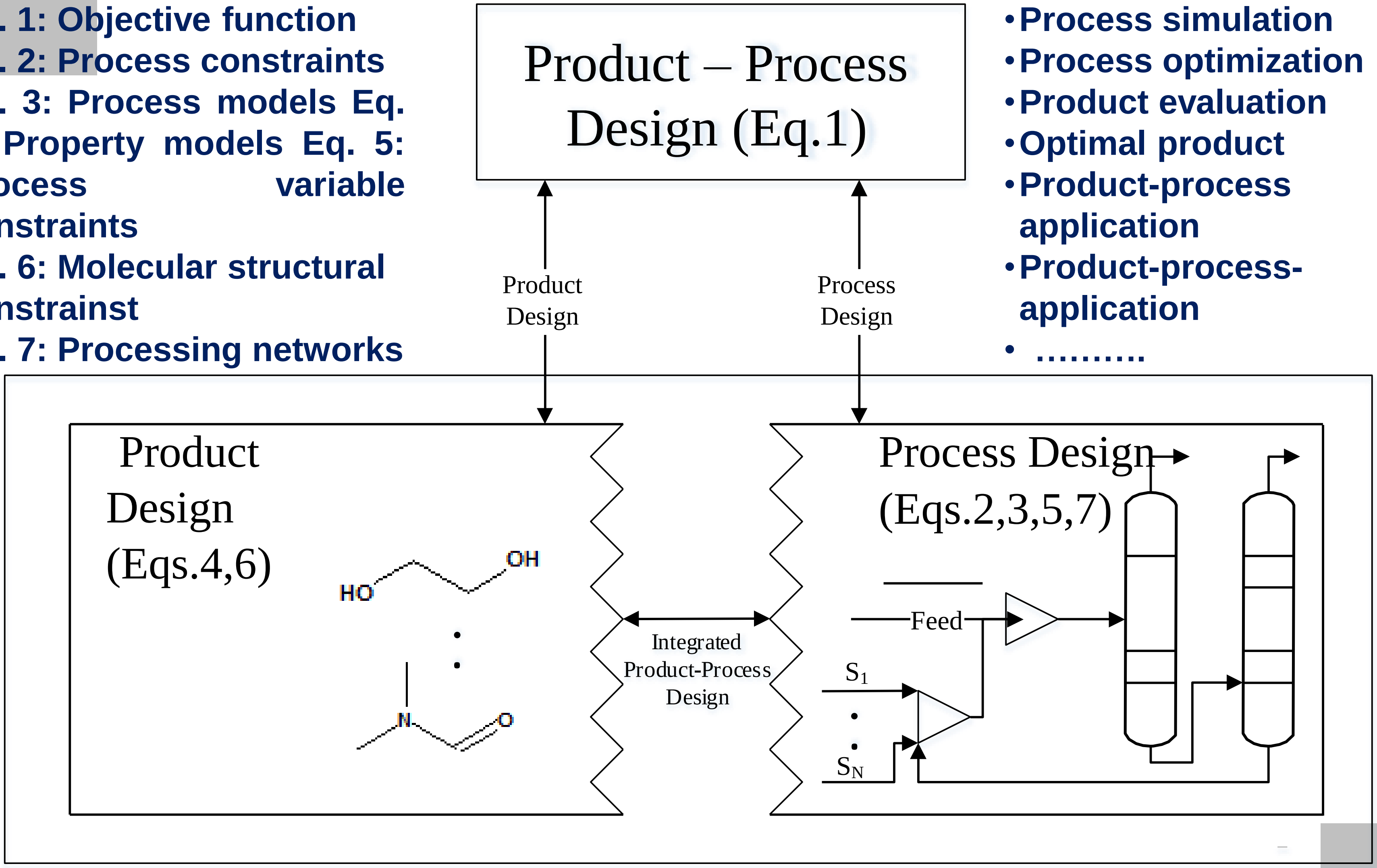
$\Sigma Y_i = 1$ or $1 \geq \Sigma Y_i \leq 2$

Or, Set $Y_2 = 0$

Integration of process-product design problems

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

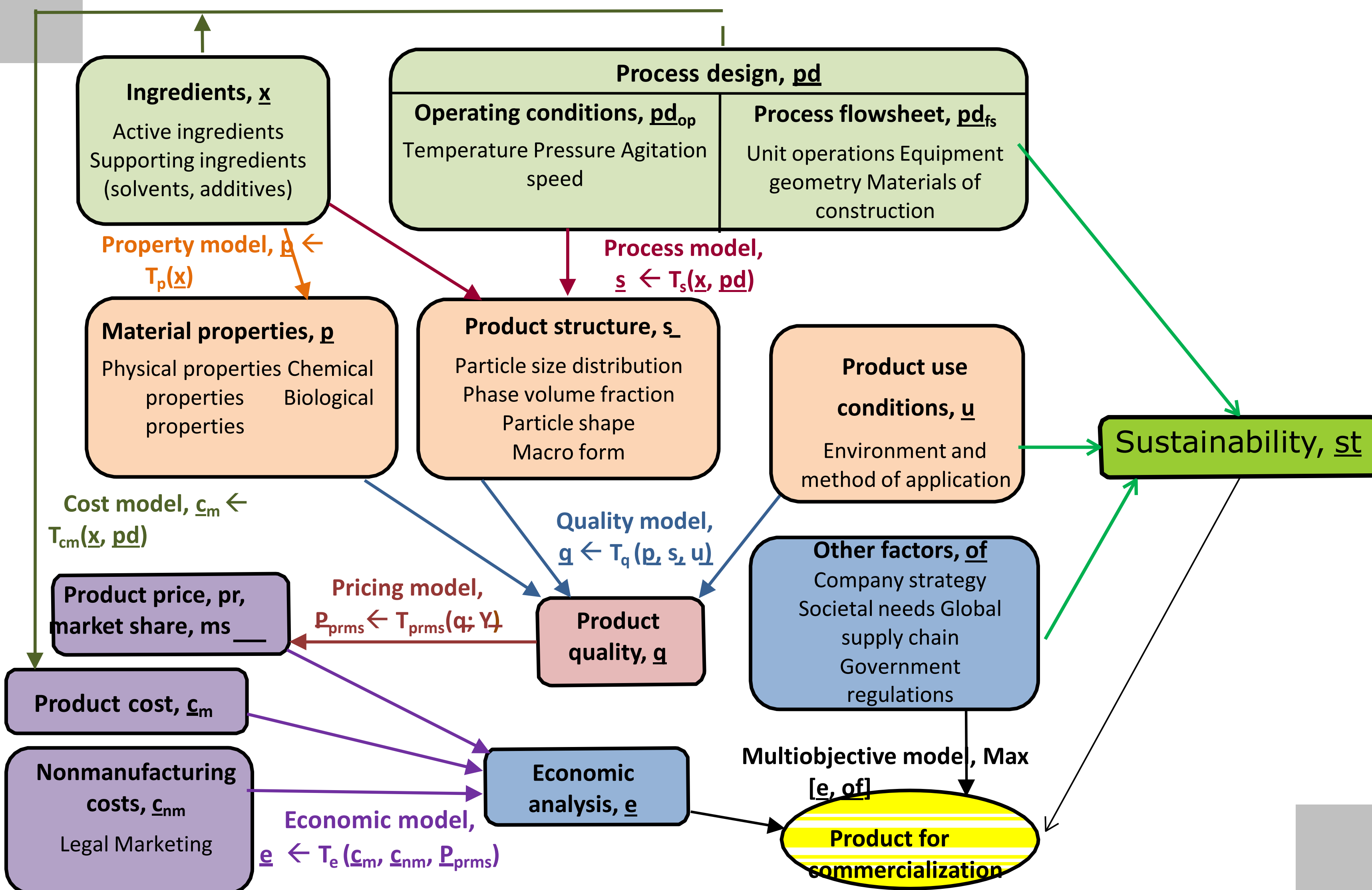
- **Process simulation**
- **Process optimization**
- **Product evaluation**
- **Optimal product**
- **Product-process application**
- **Product-process-application**
- **……….**



Simultaneous Product – Process Design

SPEED

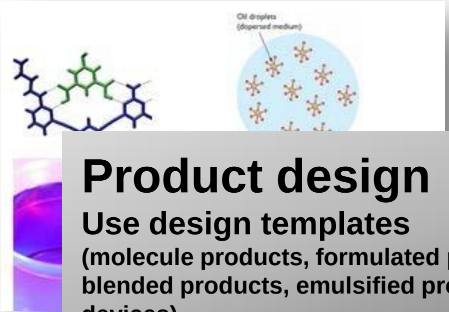
The grand chemical product design model



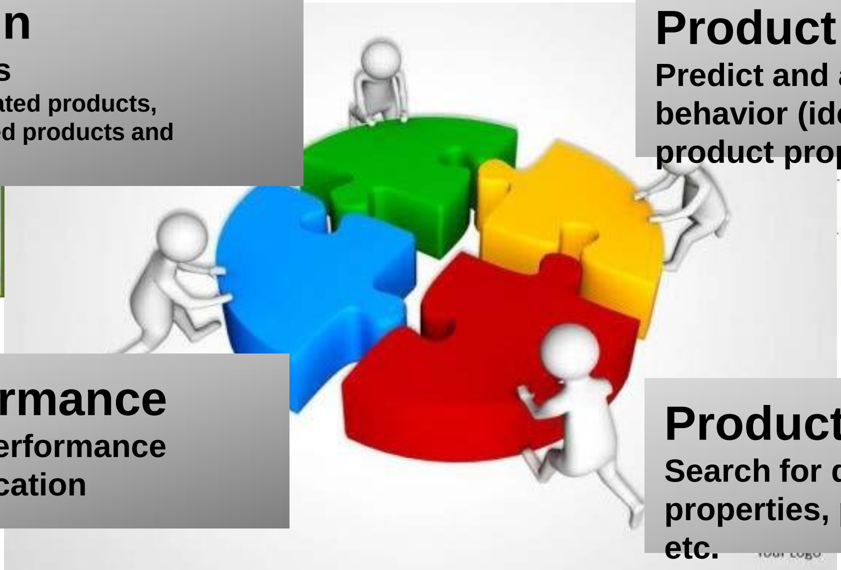
PSE for SPEED

Chemical product design simulator

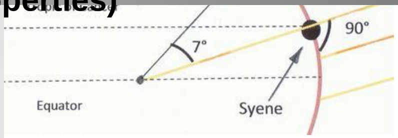
There is a need for a product simulator with the same and more useful features than a typical process simulator.
Based on available data, models, methods and analysis tools, the first chemical product simulator has been developed: ***ProCAPD***



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



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

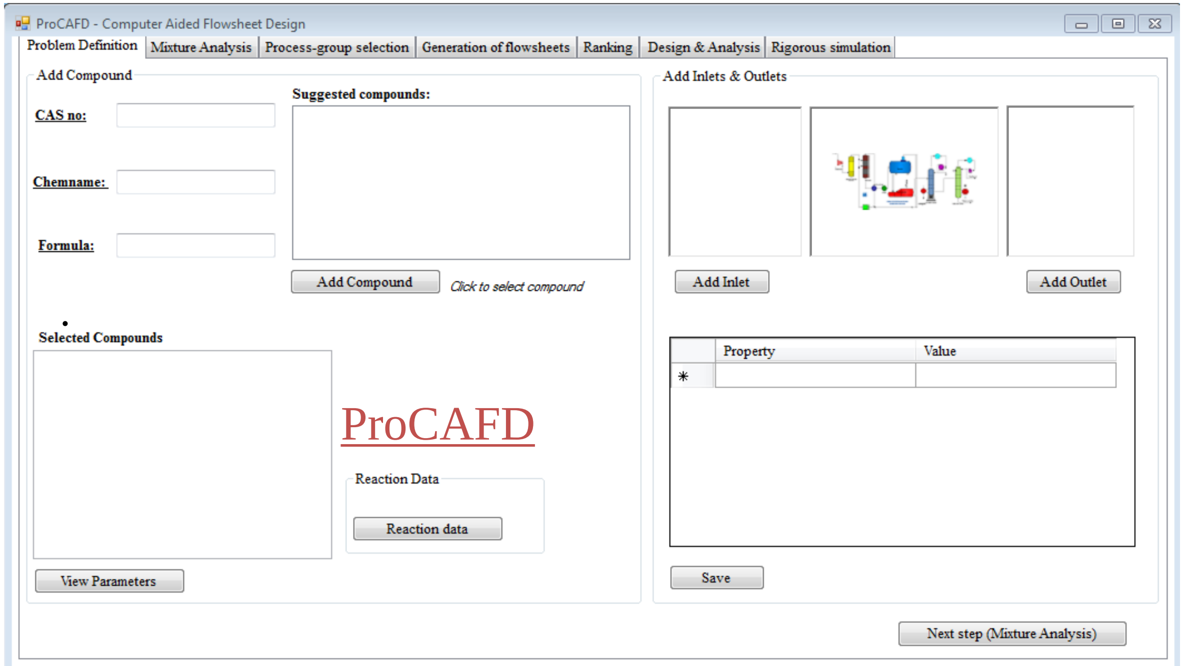


Product performance
Simulated product performance through virtual application experiments

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

Model-based process synthesis-design tool

Synthesis Problem : The **objective** of Process Synthesis is to find the best processing route, among numerous alternatives for converting given raw materials to desired products subject to design constraints and predefined performance criteria.



A Computer-Aided Tool to:

- ❖Generate all feasible process flow-sheets (To generate novel/innovative solutions).
- ❖Quick & efficient evaluation of alternatives.
- ❖Design & Analysis of Alternatives
- ❖That requires minimal computation resources and expert knowledge.

Other examples of model based systems

Examples:

Model-based system for design/analysis of process analytical technology (PAT) systems

Model-based system for optimization of refinery (petroleum & bio) operations

Model-based system for design/analysis of hybrid reaction-separation systems

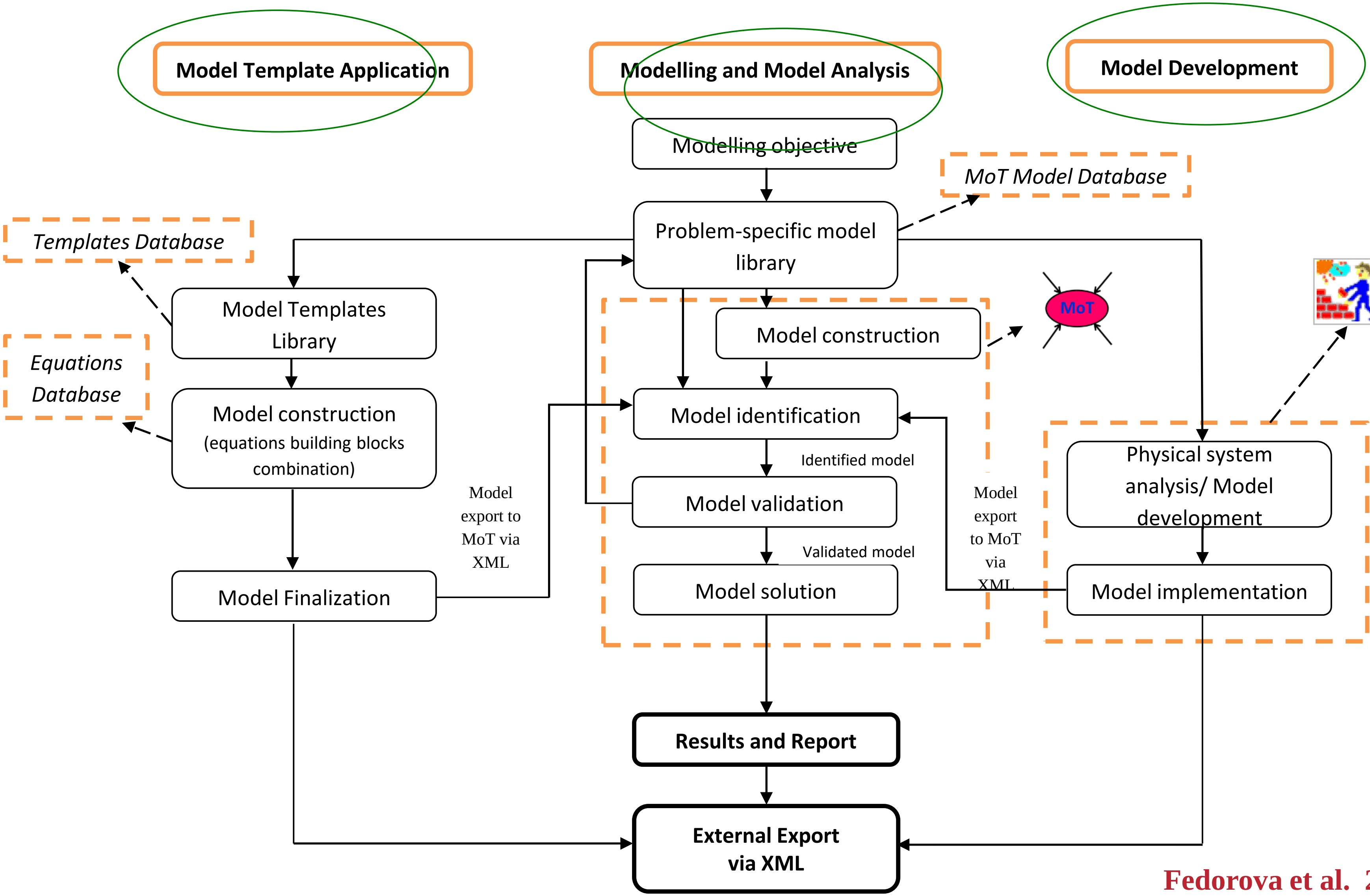
Model-based systems for integrated design-control of chemical processes

Model-based systems for product-process design/analysis (pharmaceuticals, agrochemicals, food, solvents, …)

……..

Integration of work-flow & data-flow for problem specific solution

Computer-aided modelling tool: ICAS-ModTem



Fedorova et al. 2014

Future Research Challenges in PSE

* Truly innovative solutions to problems related to
  - Energy
  - Water
  - Resources
- Establish modeling as an enabling technology
- Establish solution strategies for multiscale & multidisciplinary nature of problems
  - Handling of large datasets
  - Handling of models from different disciplines
  - Handling of conflicting objectives
- Models not just working with unit operation scale – true predictive models are needed both for process and product

Modelling case study – I

Develop a model for the evaporation of a chemical from a water droplet

Stage-1: Develop models for pure component properties of water and chemical-A (for example, methanol) – includes parameter estimation
Stage-2: Develop activity coefficient model (including parameter estimation)
Stage-3: Develop evaporation model
Stage-4: Combine all models for evapoaration of methanol from water droplet

Note: Corresponding MoT-file will be provided in class

Modelling case study - II

Develop a steady state model for a short-path evaporation process

Stage-1: Derive the process model equations for a given set of constitutive equations and model assumptions – Model is a DAE in 2 spatial directions

Stage-2: Discretize the DAE model in horizontal direction and integrate in vertical direction

Stage-3: Transfer discretized model to MoT

Stage-4: Solve model in MoT

Note: Corresponding MoT-file will be provided in class

Lecture 10: Additional topics

- Data acquisition & analysis
- Process modelling for control & diagnosis
- Modelling of discrete event systems
- Modelling of hybrid systems

Model-Based Process Control

- *Definitions (controllability, observability)*
- *Feedback*
- Pole-placement Control
- Linear Quadratic Regulator
- State Filtering
- *Model-based Predictive Control*

State Controllability

A system is said to be "(state) controllable" if for any t_0 and any initial state $x(t_0) = x_0$ and any final state x_f, there exists a finite time $t_1 > t_0$ and control $u(t)$, such that $x(t_1) = x_f$

A LTI system with the state equation

$$\dot{x} = Ax + Bu$$

is controllable iff the controllability matrix

$$U = \left[B, AB, A^2B, \ldots, A^{n-1}B\right]$$ has rank n

State Observability

A system is said to be "(state) observable" if for any t_0 and any initial state $x(t_0)= x_0$ there exists a finite time $t_1 > t_0$ such that knowledge of $u(t)$ and $y(t)$ for $t_0 \leq t \leq t_1$ suffices to determine x_0

A LTI system with the state space model

$$\dot{x} = Ax + Bu$$

$$y = Cx$$

is observable iff the observability matrix

$$V = \left[C, CA, CA^2, \ldots, CA^{n-1}\right]^{\mathrm{T}}$$ has rank n

MATLAB functions (V4.2)

- Controllability

$$co = ctrb(A, B)$$

% uncontrolled states

$$unco = length(A) - rank(co)$$

- Observability

$$ob = obsv(A, C)$$

% unobserved states

$$unob = length(A) - rank(ob)$$

In ICAS, the matrix manipulations can be done by supplying the matrices A, B & C

Example

Model equations

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} -7.1847 & -50.0415 \\ 50.0415 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} 1 \\ 0 \end{bmatrix} u$$

$$y_1 = \begin{bmatrix} 1.9558 & -0.04761 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

Controllability

$$A = [-7.1847\ -50.0415;\ 50.0415\ 0];$$

$$B = [\,1;\quad 0];$$

$$co = ctrb(A,B) = \begin{bmatrix} 1.0 & -7.1847 \\ 0 & 50.0415 \end{bmatrix};\ rank(co) = 2$$

Observability

$$A = [-7.1847\ -50.0415;\ 50.0415\ 0];$$

$$C = [1.9558\ \ -0.04761];$$

$$ob = obsv(A,C) = \begin{bmatrix} 1.9558 & -0.0476 \\ -16.4343 & -97.8712 \end{bmatrix};\ rank(ob) = 2$$

Structural properties of systems

A dynamic system possesses a structural property if "almost every" system with the same structure has this property

("same structure" = identical structure graph)

Properties include:

- Structural controllability
- Structural observability
- Structural stability

What is the relation to design?

Model Structure Simplification

Elementary simplification steps

- **variable removal:**

  steady state assumption on a state variable
  removes the vertex and all adjacent edges
  and conserves the paths.

- **variable lumping:**
  for a vertex pair with similar dynamics,
  it lumps the two vertices together,
  unites adjacent edges
  and conserves the paths.

Structural Rank

The structural rank (s-rank) of a structure matrix [Q] is its maximal possible rank when its structurally non-zero elements get numerical values

$$[\mathbf{Q}] = \begin{bmatrix} \overline{\times} & 0 & 0 & \times & 0 \\ 0 & \overline{\times} & 0 & 0 & 0 \\ \times & 0 & 0 & \overline{\times} & 0 \\ 0 & 0 & \overline{\times} & 0 & 0 \end{bmatrix} , \quad \mathbf{Q}' = \begin{bmatrix} 1 & 0 & 0 & 2 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 1 & 0 & 0 & 2 & 0 \\ 0 & 0 & 5 & 0 & 0 \end{bmatrix}$$

$$s-rank([\mathbf{Q}]) = 4 \quad , \quad rank(\mathbf{Q}) = 3$$

Structural Controllability

A system is structurally controllable if the structural rank (s-rank) of the block structure matrix *[A,B]* is equal to the number of state variables *n*

$$[\mathbf{A},\mathbf{B}] = \big[\, [\mathbf{A}] \,\big|\, [\mathbf{B}] \,\big], \quad \mathbf{U}(\mathbf{A},\mathbf{B}) = \big[\, \mathbf{B} \,\big|\, \mathbf{AB} \,\big|\ldots\big|\, \mathbf{A}^{n-1}\mathbf{B} \,\big]$$

$$s-rank([\mathbf{A},\mathbf{B}]) \rightarrow rank(\mathbf{U}(\mathbf{A},\mathbf{B}))$$

Structural Controllability

A system is **structurally controllable** if:

- the state structure matrix [A] is of full structural rank.
- the structure graph of the state space realization ([A],[B],[C],[D]) is input connectable.

Structural rank: pairing of columns and rows.

Input connectable: path to every state vertex from at least one input vertex.

Structural Observability

A system is **structurally observable** if the structural rank (s-rank) of the block structure matrix $[C,A]^T$ is equal to the number of state variables n

$$[\mathbf{C},\mathbf{A}]^{T}=\left[\frac{[\mathbf{C}]}{[\mathbf{A}]}\right],\quad \mathbf{V}(\mathbf{A},\mathbf{C})=\begin{bmatrix}\underline{\mathbf{C}}\\ \underline{\mathbf{CA}}\\ \underline{\cdots}\\ \mathbf{CA}^{n-1}\end{bmatrix}$$

$$s-rank([\mathbf{C},\mathbf{A}]^{T})\rightarrow rank(\mathbf{V}(\mathbf{A},\mathbf{C}))$$

Structural Observability

A system is **structurally observable** if:

- the state structure matrix [A] is of full structural rank.
- the structure graph of the state space realization ([A],[B],[C],[D]) is output connectable.

Structural rank: pairing of columns and rows.

Output connectable: path from every state vertex to at least one output vertex.

Structural Stability

- Method of **circle families**
  conditions depending on the sign of non-touching circle families (computationally hard)
- Method of **conservation matrices**

$$\text{sign pattern:} \qquad a_{\mathrm{ii}} < 0 \ , \ a_{\mathrm{ij}} \geq 0 \ \ i \neq j$$

$$\text{dominant diag:} \ \ |a_{ii}| \geq \sum_{i \neq j} a_{ij} \quad , \ i = 1, \ldots, n$$

If the state matrix A is a conservation matrix then the system is structurally stable.

Feedback

Open-loop system model

$$dx/dt = \mathbf{f}(x,u) \quad , \quad y = \mathbf{g}(x,u)$$

- State feedback

  $$u = \mathbf{F}(x)$$

  \- full state, linear, static feedback

  $$u = \mathbf{K}\,x \quad , \quad \mathbf{K} : \text{control gain}$$

- Output feedback

  $$u = \mathbf{F}(y)$$

Model-based Predictive Control

Given:

- discrete time parametrized predictive dynamic model

$$y^{(M)}(k+1) = \mathcal{M}(\mathcal{D}[1,k];\ p^{(M)}) \quad , \quad k = 1, 2, \cdots$$

- measurement record

$$\mathcal{D}[1,k] = \{\ (u(\tau), y(\tau) \mid \tau = 1, \cdots, k\}$$

- loss functional with N, $y^{(ref)}$, **Q**, **R**

$$J^{(N)}(y^{(M)} - y^{(r)}, u) \ = \ \sum_{i=1}^{N} [\ r^T(k+i) Q r(k+i) \ + \ u^T(k+i) R u(k+i)\ ]$$

$$r(k) = y^{(r)}(k) - y^{(M)}(k) \quad , \quad k = 1, 2, \cdots$$

Compute: the discrete time control signal $\{\ u(k+i),\ i=1,\ldots,N\ \}$ that minimizes the loss

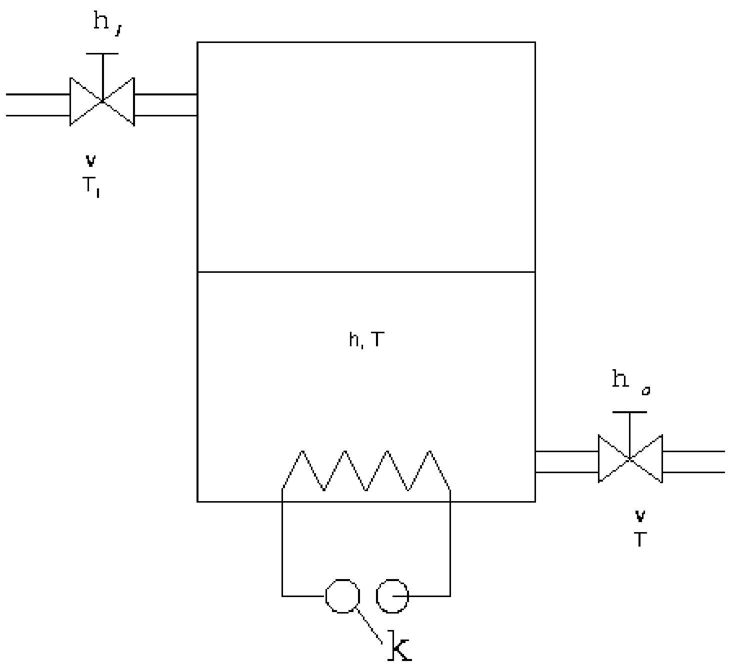
Model-Based Process Diagnosis

- Prediction-based Diagnosis
- Identification-based Diagnosis

Basic idea: build models which describe
- normal non-faulty (healthy) behaviour
- faulty behaviour (identified by fault mode label)

use measured data to determine the fault mode of the system

Simple Example: Batch Water Heater



$$\frac{dh}{dt} = \frac{v}{A}\eta_I - \frac{v}{A}\eta_O$$

$$\frac{dT}{dt} = \frac{v}{Ah}(T_I - T)\eta_I + \frac{H}{c_p \rho h}\kappa$$

where the variables are

t	time $[s]$
h	level in the tank $[m]$
v	volumetric flowrate $[m^3/s]$
c_p	specific heat $[Joule/kgK]$
ρ	density $[kg/m^3]$
T	temperature in the tank $[K]$
T_I	inlet temperature $[K]$
H	heat provided by the heater $[Joule/sec]$
A	cross section of the tank $[m^2]$
η_I	binary input valve $[1/0]$
η_O	binary output valve $[1/0]$
κ	binary switch $[1/0]$

Characteristics of Discrete Event System Models

- The range **space** (value) of signals (state, input, output) is discrete

  $$x(t) \in \mathbf{X} = \{\, x_0, x_1, \ldots, x_n \,\}$$

- **Event:** an occurrence of a discrete change
- **Time** is also discrete
  - $T = \{ t_0, t_1, \ldots, t_n, \ldots \} = \{ 0, 1, \ldots \}$
  - Only the event **sequence** is important
- Focus is on sequential and parallel events
- Application areas: scheduling, operating procedures, resource allocation

Approaches to Solving DES Models

- **Problem statement**

  Given

  - formal DES model (automata, Petri net)
  - initial state
  - external events (input sequence)

  Generate: internal (state and output) events

- Solution: **algorithmic**

  non-polynomial (NP-hard)

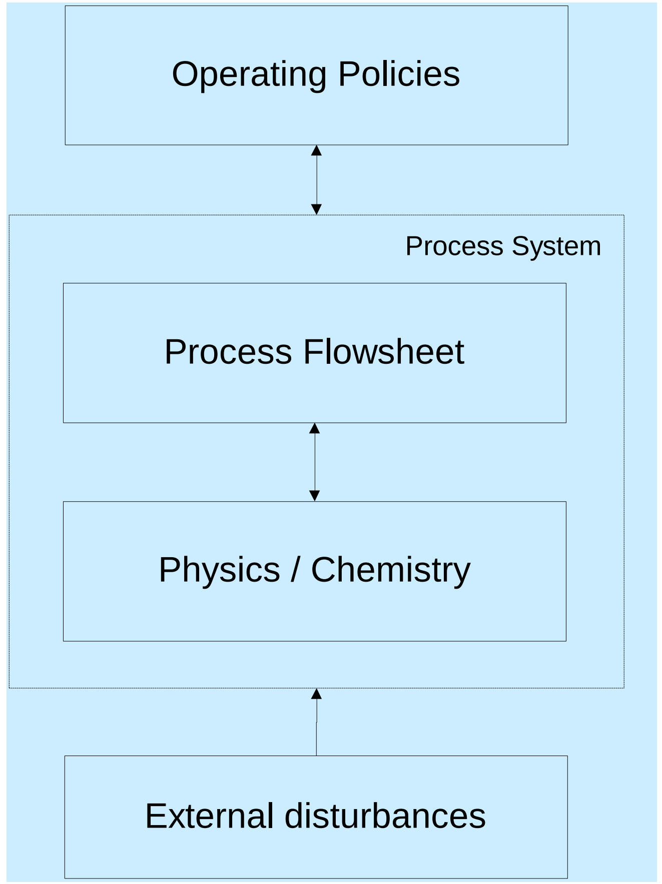
Modelling of Hybrid Systems

Characteristics and Issues

<u>All process engineering systems are hybrid in nature</u>

Sources of discrete behaviour

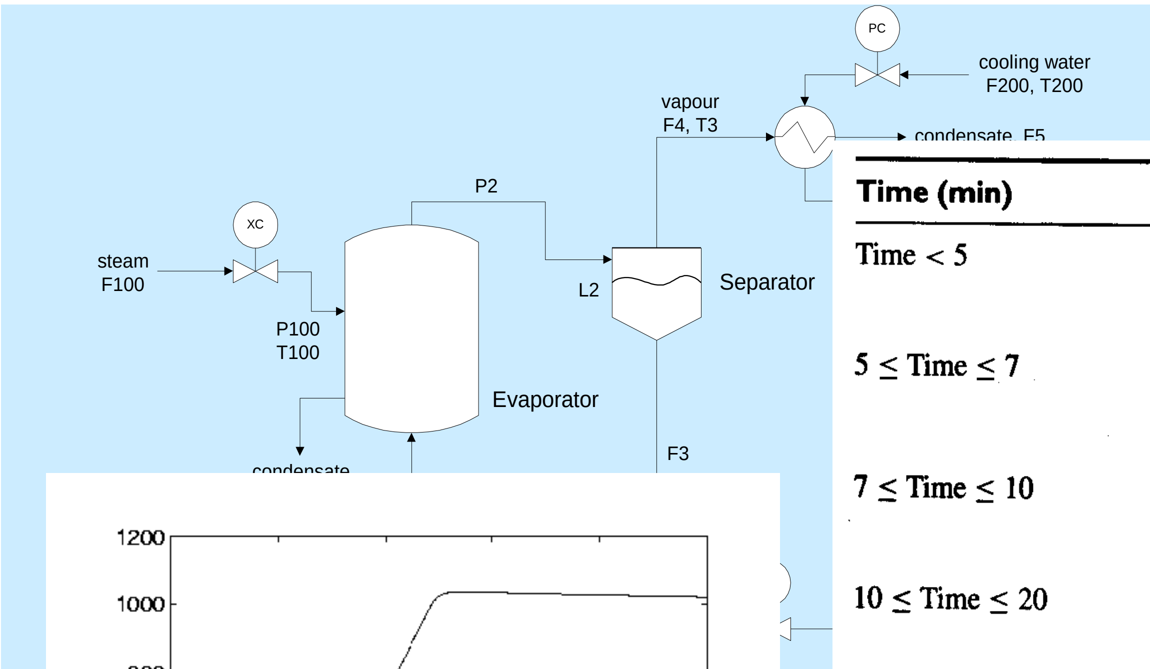
- process flowsheet
- physics and chemistry
- operational policies
- external disturbances

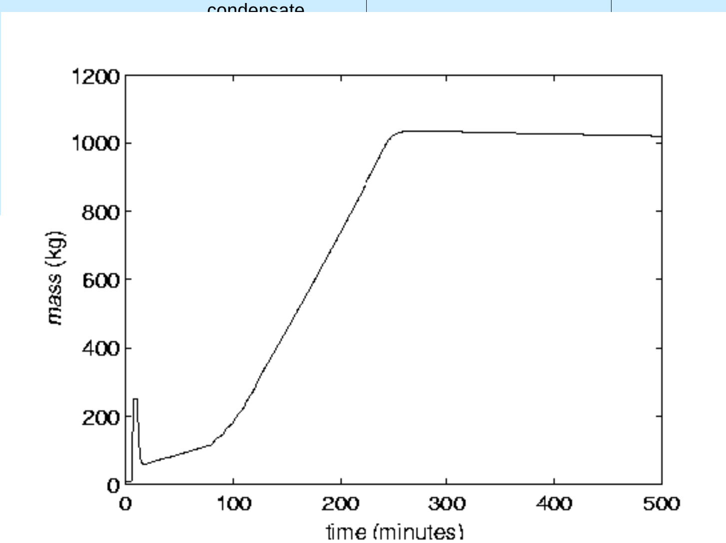


Key application areas of hybrid system modelling

- batch processes for specialty chemicals, pharmaceuticals and paints
- continuous processes during start-up, shut-down and product changeover
- manufacturing systems where discrete items are processed on discrete machines
- design of systems with units described by discrete variables such as staged operations and binary variables (0,1) where they are present (1) or not present (0)

An Example: Startup of an Evaporator





Time (min)	Status or operation to be done
Time < 5	Feed flow = 0 Recirculation flow = 0 All controllers in manual with 0 output
5 ≤ Time ≤ 7	Set feed flow to fill shell in 2 min All controllers in manual with 0 output Recirculation flow = 0
7 ≤ Time ≤ 10	Feed flow = 0 Recirculation flow = 0 All controllers in manual with 0 output
10 ≤ Time ≤ 20	Feed flow ramped to 5 kg/min Recirculation flow ramped to 50 kg/min Level controller set to automatic, setpoint = 1 m Pressure controller set to automatic, setpoint = 50.5 kPa Composition controller set to automatic, setpoint = 25%
20 ≤ Time ≤ 80	Feed flow constant at 5 kg/min Recirculation flow constant at 50 kg/min
Time > 80	Feed flow increased to 10 kg/min
Time > 90	Feed flow increased to 15 kg/min
Time > 100	Feed flow increased to 20 kg/min
Time > 110	Feed flow increased to 25 kg/min
Time > 120	Feed flow increased to 30 kg/min