Process Performance Based Control Structure Selection

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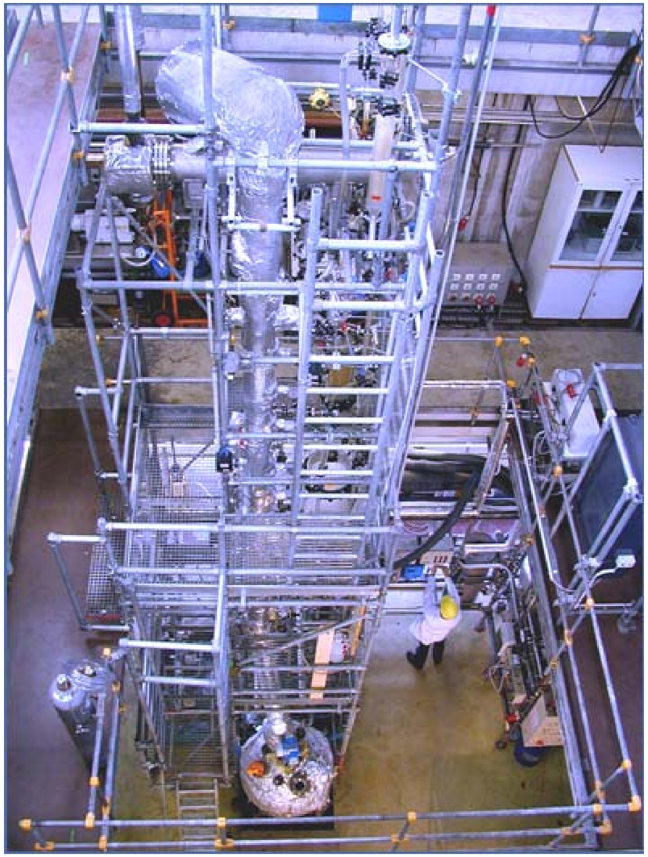
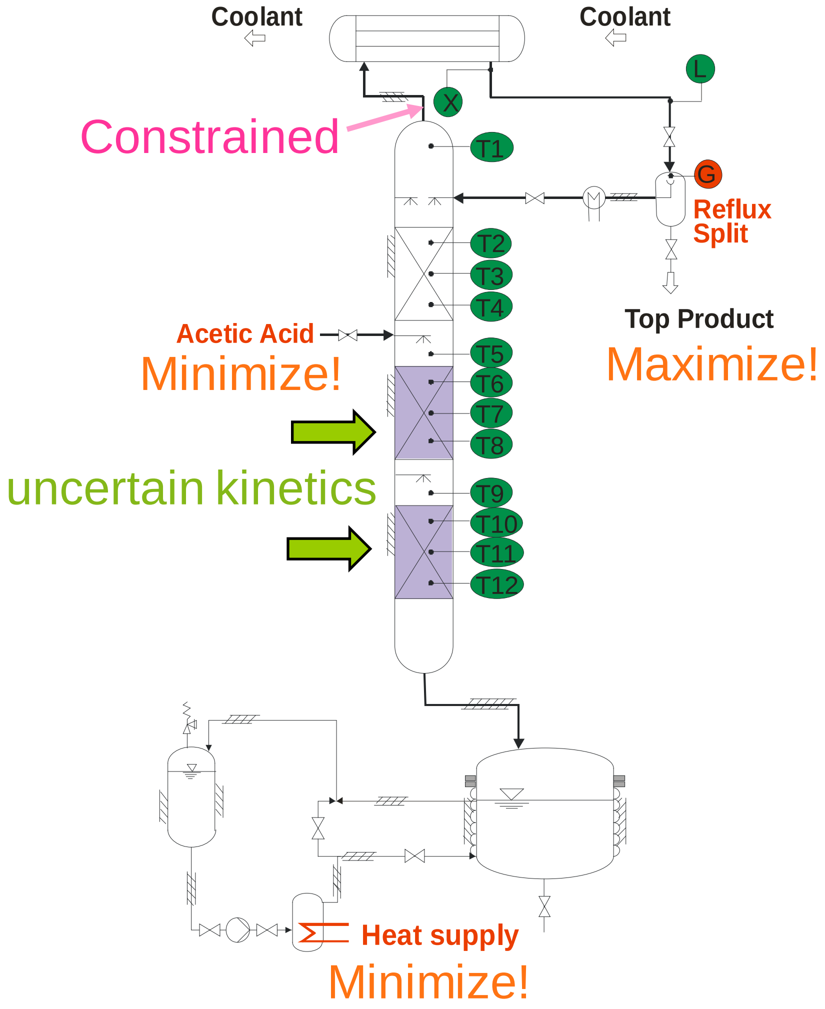
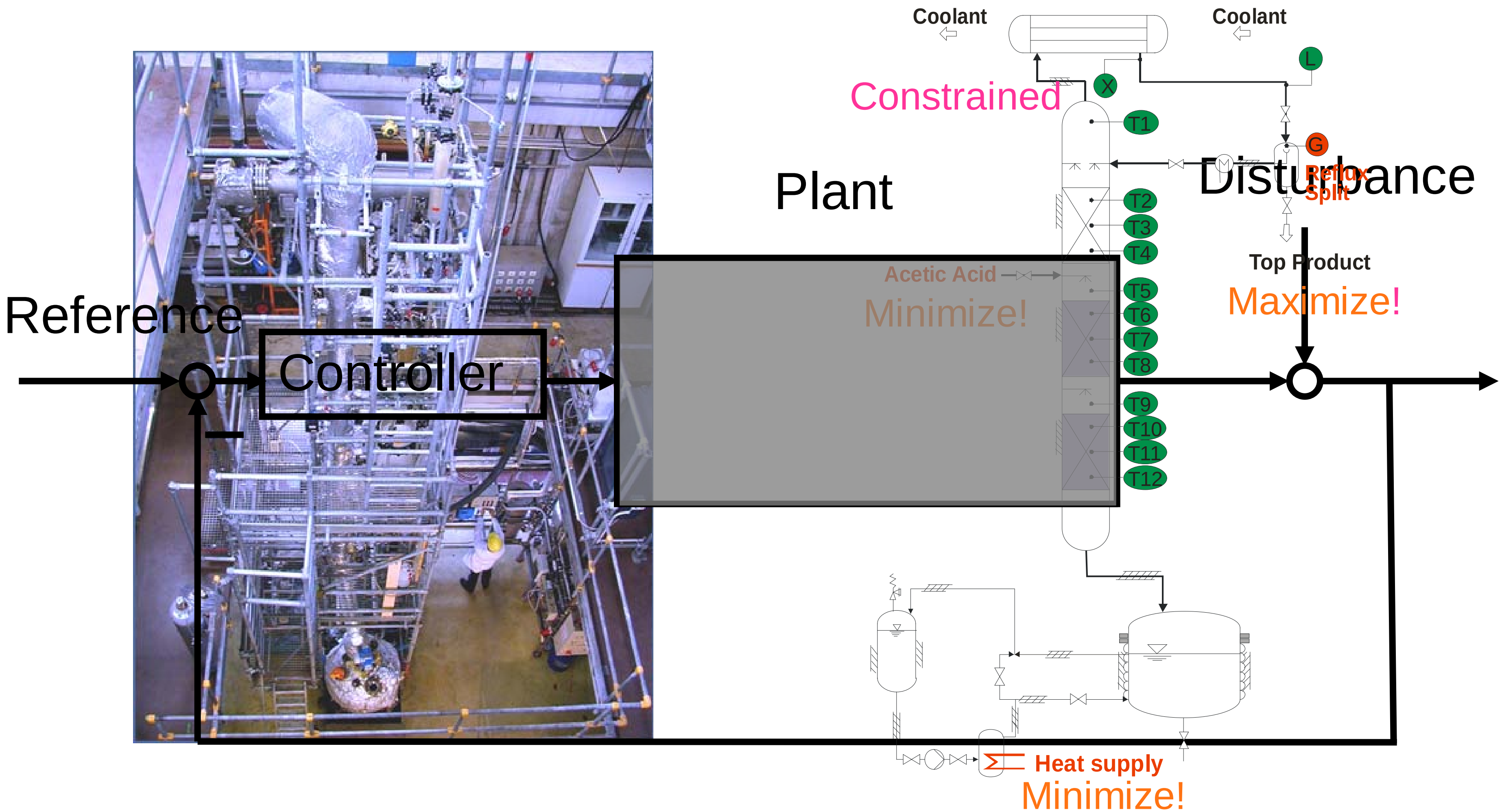
Process Operations: Challenge



Reactive distillation column



Control Engineering Reduction



Standard control task description:

Choose and design feedback controllers for optimal

- disturbance rejection
- setpoint tracking

for a given "plant" (i.e. inputs, outputs, dynamics, disturbances, references, model errors, limitations, …)

"SERVO or REGULATION PROBLEM"

Process Performance Optimization

- However, the purpose of good control is to optimize the performance of the process
- Tracking and disturbance rejection are means to an end, not the goal by themselves

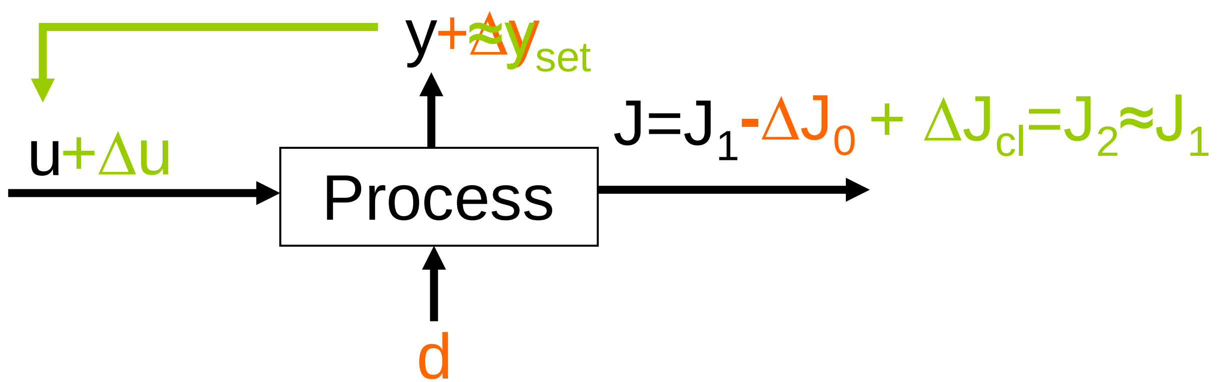
- This should be reflected in the approach to the selection of control structures

Control Structure Selection

- Choice of manipulated and controlled variables
  - Which variables should be controlled?
  - Loop pairing (not considered here)
- Common methods:
  - Linear analysis: RGA, condition numbers, sensitivities
  - Simulation studies
  - Heuristics
- **This lecture**:
  - Choice of controlled variables for maximum profit
  - Based upon rigorous non-linear plant models
  - References:
    - Engell, Scharf, Völker, IFAC WC 2005
    - Engell, Pham, PSE 2009

Plant Performance Based Control Structure Selection

- Discussed by Morari, Stephanopoulos and Arkun (1980)
- Skogestad (2000): “Self-optimizing control”
- Basic ideas:
  - Demand from process engineers and managers:
    - Guarantee cost effective operation in the presence of disturbances and plant-model mismatch
    - Tracking of set-points not necessarily essential
  - Decision based on the effect on the profit **J**



When is regulatory control needed and sufficient ?

$$J_2 = \underbrace{J(\underline{u}_{nom}, \underline{d}) - J(\underline{u}_{nom}, \underline{d} = \underline{0})}_{\text{Loss for open loop control}} \quad (1)$$

$$+ \underbrace{J(\underline{u}_{opt}, \underline{d}) - J(\underline{u}_{nom}, \underline{d})}_{\text{Benfit by optimisation}} \quad (2)$$

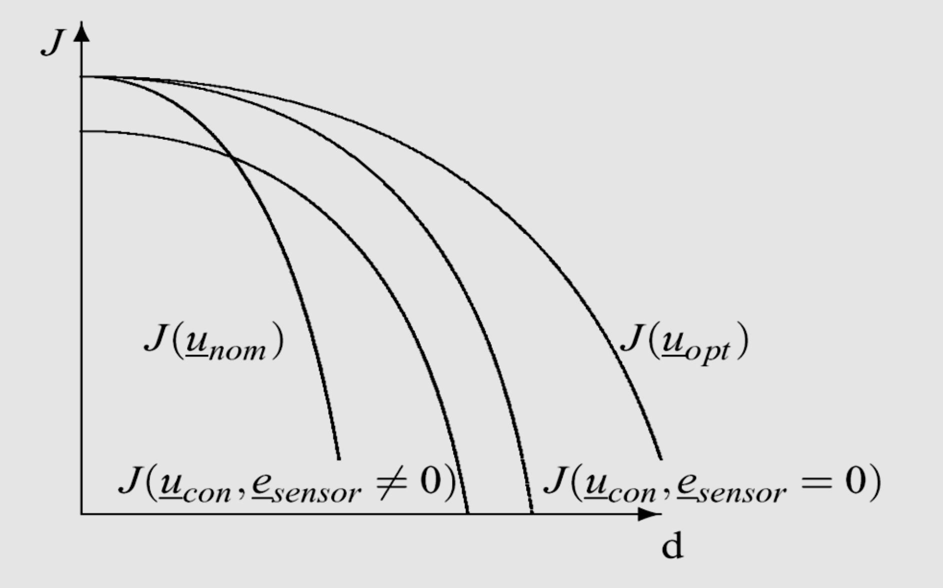
$$+ \underbrace{J(\underline{u}_{con}, \underline{d}) - J(\underline{u}_{opt}, \underline{d})}_{\text{Loss for closed loop control compared to optimisation}} \quad (3)$$

(1) ≈ 0:
: No closed loop control necessary

(2) >> 0 and (3) ≈ 0:
: Closed loop control recommended

(2) >> 0 and (3) >> 0:
: Control with fixed set-point not advisable, online optimization recommended

Basic Idea for Control Structure Selection



- Overall evaluation of the performance of a structure (theoretical)

$$\Delta J = \int_{-d_{1,\max}}^{d_{1,\max}} \int_{-d_{n,\max}}^{d_{n,\max}} w(d)(J(u_{nom}, d) - J(u_{con}, d)\, dd_1 \ldots dd_n$$

- Practically: Approximation by a finite set of disturbance scenarios

Control Structure Selection Procedure (Engell et al., 2005)

Complexity of the analysis

1. Define the economic optimization problem
2. Define critical disturbances
3. Pre-selection of control structures
4. Optimization of the set-points
5. Evaluation of the benefits for static disturbances
6. Performance for dynamic disturbances

Number of combinations

1. Definition of the Economic Optimization Problem

- Result of process design, starting point for control structure selection and controller design
- Determine the available degrees of freedom and choose a set of manipulated variables
- Determine the possible controlled variables
- Formulate a scalar profit function *J* and constraints that have to be satisfied

$$\max_{u} J(\underline{x}, \underline{u}, \underline{d}_i)$$

$$s.t \quad \text{system model}$$

$$\underline{h}(\underline{x}, \underline{u}) \leq 0$$

2. Definition of the Disturbances

- We distinguish between two types of disturbances:
  - Measurement errors the size of which can be estimated
  - External disturbances, e.g. errors in the assumed model, implementation errors of the controlled variables
- A priori knowledge about the disturbances is very useful as it makes the choice of the control structure more accurate.

3. Pre-selection of Control Structures

- Number of possible control structures:

$$C_n^k = \binom{n}{k} = \frac{n!}{(n-k)!\,k!}$$

  - n: degrees of freedom, k: number of measurements

  $\Rightarrow$ increases rapidly with the number of measurements
- Pre-screening is useful especially for large structures: RGA, SVD, RHP zeros, sensor sensitivity analysis (Engell et. al (2005))
- Common requirement for the measured variables:
  - Measurements should be sensitive to disturbances e.g. Sensor sensitivity analysis
  - Manipulated variables must affect the measurements

Pre-selection of Control Structures (2)

- Condition number of a matrix A:

$$\kappa(A) = \frac{\sigma_{\max}(A)}{\sigma_{\min}(A)}$$

  - Matrix with large condition number -> ill-conditioned matrix

- Relative gain array (RGA)

$$\Lambda(G) = G \times (G^{-1})^T$$

  - G: steady-state gain matrix
  - $\times$ denotes element by element multiplicatioin (Schur product)

Pre-selection of Control Structures (3)

- Generalized non-square relative gain array (NRGA):
  - Inverse is replaced by pseudo-inverse
  - The row sums of the NRGA are equal to the square of the output projections and should not be too small.
  - Consider not using outputs corresponding to the rows in the NRGA where the sum of elements is much smaller than 1.

Pre-selection of Control Structures (4)

- Sensor sensitivity analysis:

$$\underline{S} = diag(\Delta \underline{u})^{-1} \frac{\partial \underline{h}}{\partial \underline{y}} diag(\underline{e}_{sensor}); \ \underline{u} = \underline{h}(\underline{y})$$

$$\Delta \underline{u} = \max_{\underline{d}}(\text{argmax } J(\underline{u}, \underline{d})) - \min_{\underline{d}}(\text{argmax } J(\underline{u}, \underline{d}))$$

  - *h*: the inverse of the measurement mapping
  - *S* represents the propagation of the sensor errors to the manipulated variables
- Small singular values of *S* mean small influences of the sensor errors

  ⇒ Structures with large maximal singular values are excluded

Pre-selection of Control Structures (4)

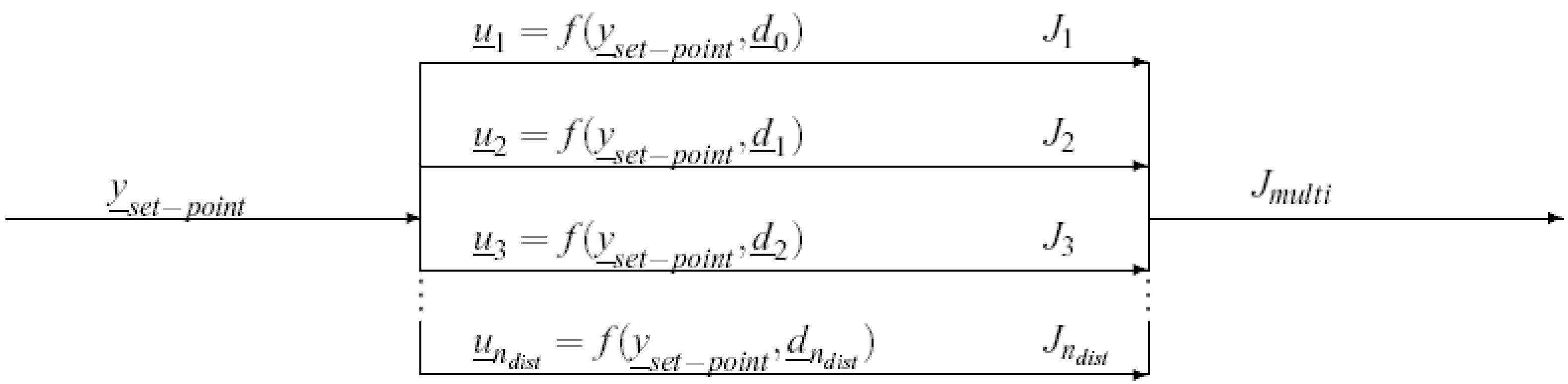
- RHP zeros:
  - The bandwidth of a feedback loop is restricted to 0.5 times the modulus of the smallest RHP zero

    $\Rightarrow$ rise time not smaller than the inverse of the zero.
  - Structures that yield small RHP should be excluded
- Negative elements of the RGA:
  - The system will become unstable for integral controllers when loops are opened if one of the RGA elements on the diagonal is negative at $\omega=0$. Structures with negative elements on the diagonal should be eliminated.

4. Optimization of the Set-points

Which set-point is optimal on the average and can be tracked in the presence of these disturbances?

- Multi-scenario optimisation



- Optimization formulation:

$$\max_{\underline{u}_i, \underline{y}_{set-point}} \sum_{i=1}^{n_{dist}} J(\underline{x}, \underline{u}_i, \underline{d}_i)$$

$$s.t.: \forall \underline{d}_i :$$

$$\dot{\underline{x}} = f(\underline{x}, \underline{u}_i, \underline{d}_i) = 0$$

$$\underline{y}_{set-point} = \underline{m}(\underline{x})$$

5. Evaluation of the Benefits for Static Disturbances

$$\min_{\underline{u}} J = J(\underline{u}, \underline{d}_i, \underline{x})$$

$$s.t.: \underline{\dot{x}} = f(\underline{u}, \underline{d}_i, \underline{x}) = 0$$

$$\underline{h}(\underline{x}, \underline{u}) \leq 0$$

$$\underline{y} = \underline{m}(\underline{x}) = \underline{M}(\underline{u}, \underline{d_i})$$

$$\underline{y}_{set-point} - \underline{e}_{sensor} \leq \underline{y} \leq \underline{y}_{set-point} + \underline{e}_{sensor}$$

- Minimization: **worst case profit** is considered

Evaluation of the Benefits for Static Disturbances (2)

- Different levels of disturbances are considered:
  - E.g. -1; -1/3; 0; 1/3; 1 of maximum value
  - Smaller deviations more probable
- All levels of all disturbances are considered individually
- Structures are evaluated according to the average performance
- Small number of good control structures retained.

6. Performance for Dynamic Disturbances

- Option 1: Design classical controllers and simulate
  - Controller design (SISO / MIMO)
  - Comparison of the economic performance
- Difficulty:
  - For classical controllers, the performance depends on the controller type (PI, PID…) and the controller parameters used
    → performance depends on the structure and of the design
- Alternative: Best possible performance
  - Multivariable NMPC controller

Performance for Dynamic Disturbances (2)

- Lower layer: NMPC controller tracks the set-points

$$P(t_k) = \min_{\mathbf{u}} \left(\int_{t=t_k}^{t_k+H_P} \left(\left\| y(t) - y_{set\text{-}point} \right\|_P + \left\| u(i) - u_{set\text{-}point} \right\|_Q \right) dt \right)$$

$$s.t.: \quad \dot{x}(t) = f(x(t), u(t), d(t)) \qquad (P1)$$

$$y(t) = m(x(t))$$

- Upper layer: Optimization of the weights *P*, *Q* (DFO)

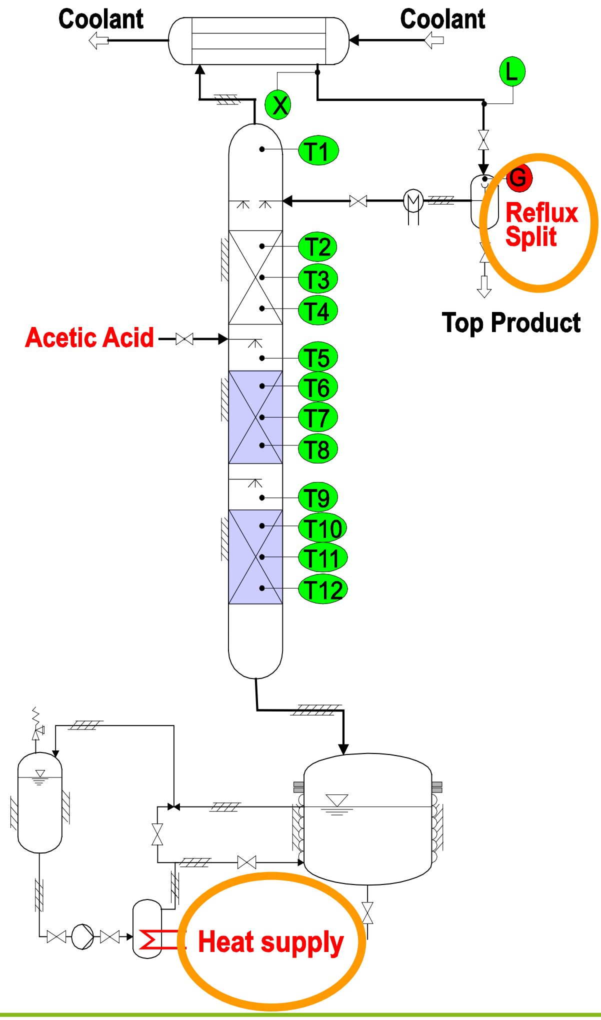
$$\max_{P,Q} \int_{t=0}^{t=t_{end}} \sum_{i=1}^{n} J(\underline{x}, \underline{u}_i, \underline{d}_i) dt$$

$$s.t.: P, Q \succ 0$$

$$(P1)$$

Example 1: Reactive Distillation Column

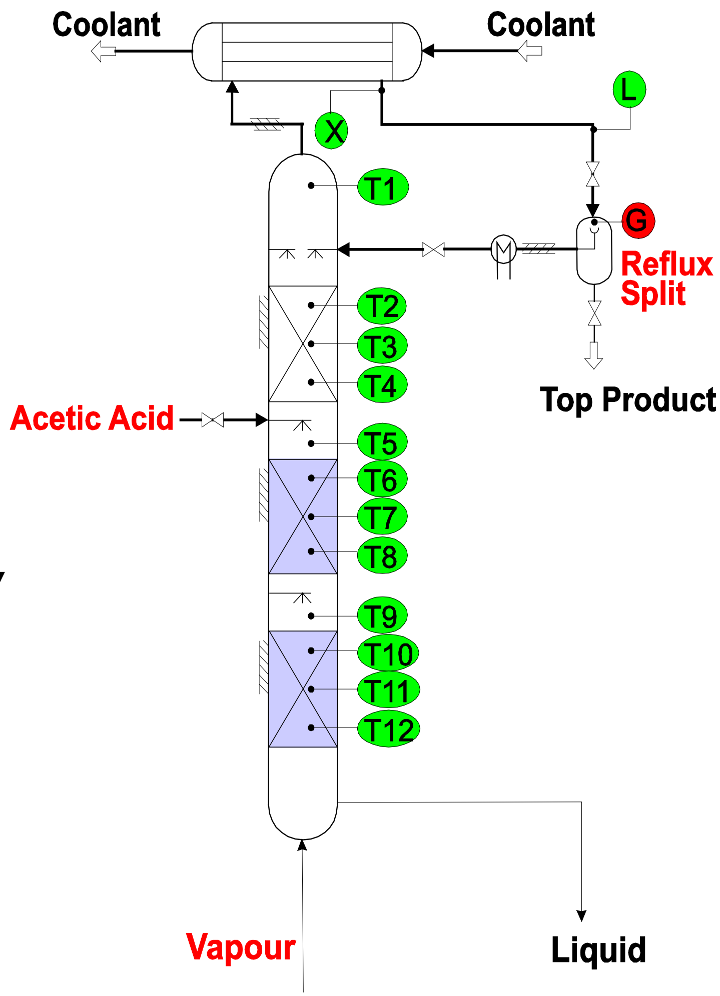
- **Engell, Scharf, Völker, 2005**
- **Process:**
  - MeOH + HAc ⇆ MeAc + H_2O
  - Heterogenously catalysed
  - 17 measurements
  - 2 manipulated variables
- **Model:**
  - Dynamic, non-linear equilibrium stage model
  - Approx. 650 algebraic, 100 differential equations



Reactive Distillation (2)

- *Semi-batch process*
- *Further investigation:*
  - *Quasi-steady state model*

⇨ *Heat supply ➯ vapour flow*
  - *Liquid flow to reboiler neglected*



Problem Definition for the RD Process

- 2 manipulated variables: reflux split and heat supply
- 17 possible controlled variables: temperatures on each tray, concentrations in the vapor stream, condensate flow
- Profit function:

$$\max_{\underline{u}} J(\underline{u}, \underline{x})$$

$$s.t.: J = c_{MeAc}\dot{n}_{MeAc} - c_{HAc}\dot{n}_{HAc} - c_{heat}q_{heat}$$

$$x_{MeAc} \geq 0.8$$

Selection of Disturbances for the RD Process

- Considered disturbances:
  - Heat loss -500…500 W (of about 3000 W)
  - Reaction rate 90…110% of the nominal value
  - Subcooling of the condensate by 0…40K (boiling temp. 60° C)
  - Change in the vapour composition (5…11h → 90…73% MeOH in the vapour)

- Worst case Scenario:

$$\min_{\underline{d}} J = c_{MeAc}\dot{n}_{MeAc} - c_{HAc}\dot{n}_{HAc} - c_{heat}q_{heat}$$

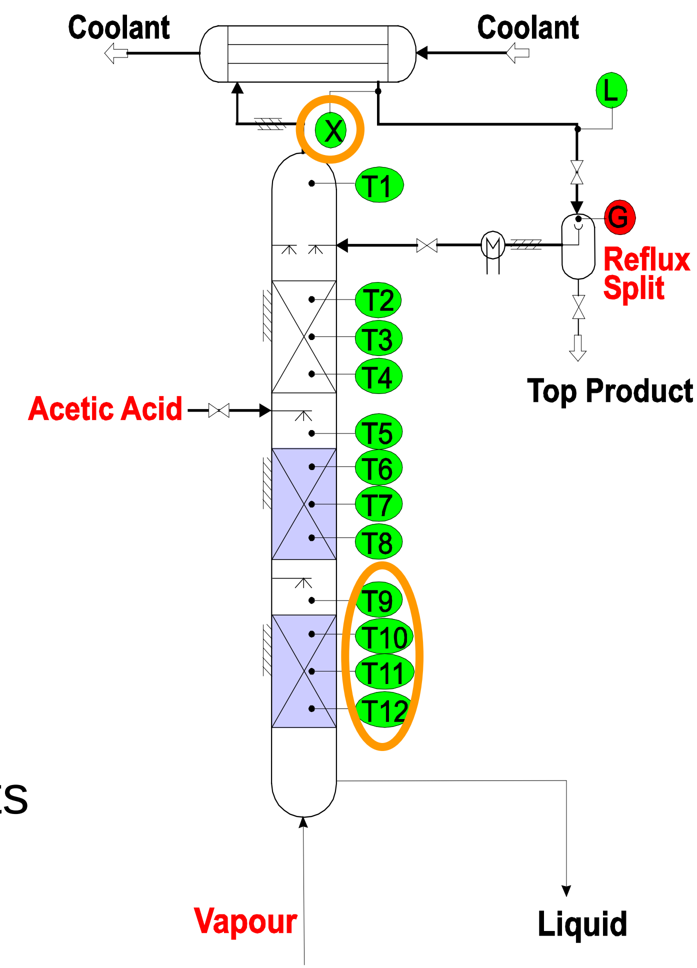
- All disturbances at upper/lower bounds

- Largest effect on the profit: Reaction rate

Pre-selection for the RD Process

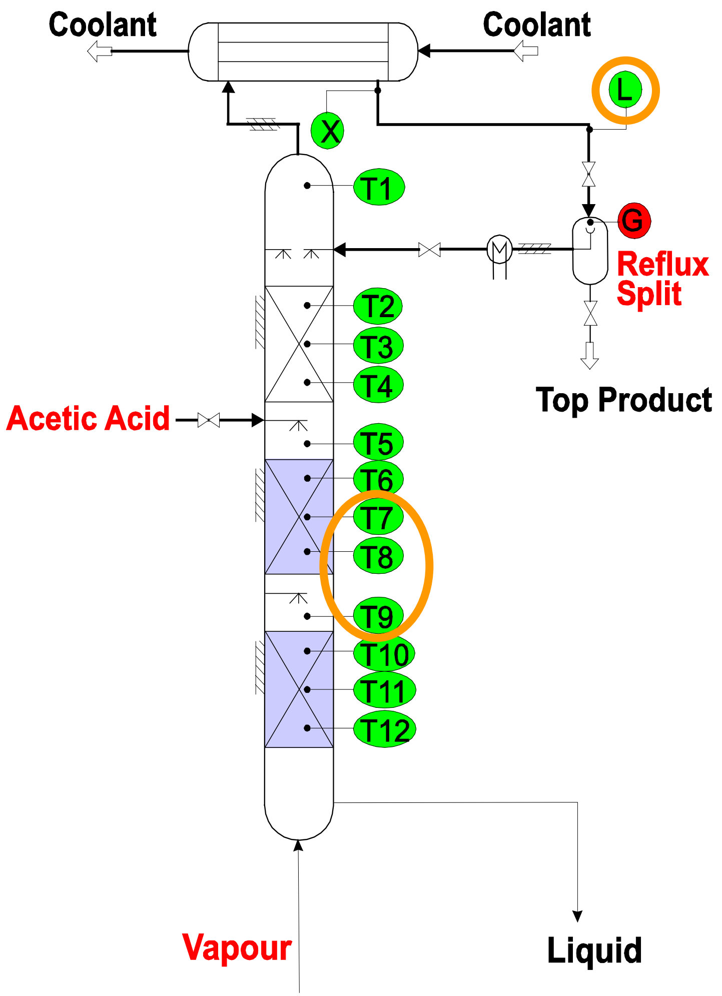
- 17 measurements, 2 manipulated variables
  - ⇨ 136 structures
- Pre-selection based on sensitivities:
- $\sigma_{max}(\underline{S})$ 10 times larger than for the best case

⇨ Rejection of 66 structures
  - ⇨ Structures using temperatures near the bottom of the column
  - ⇨ Structures using measurements with large relative error (e. g. x_{HAc})



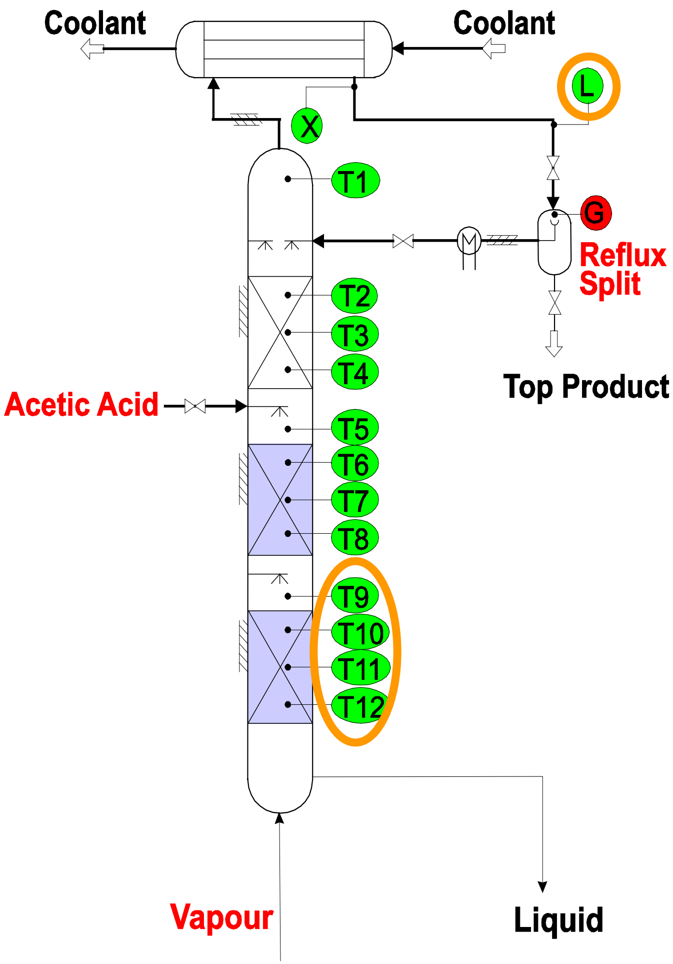
Choice of Set-points for the RD Column

- No common set-point found for 8 structures
  - Structures that use the condensate flow
    - Only affected by the heat supply
  - Structures that use the temperatures $T_7 \ldots T_9$
    - Only represent drift in vapour composition



Selection of Structures

- 4 Disturbance scenarios,66 structures
  - 264 optimisations
- 7 structures can not meet the requirement on MeAc concentration
  - Structures that use adjacent measurements
- 10 structures excluded because ΔJ>30%
  - Structures that use the condensate flow
  - Structures that use temperatures in the lower reactive packing



Combined Disturbances for the RD Process

- Non-linear process:
  - Summation of the effects of disturbances not reasonable
  - ⇨ Optimisation for scenarios of all combinations of
    - Vapour composition (5h,11h)
    - Subcooling (0K,13K, 40K)
    - Heat loss (-500W, -167W, 0, 167W, 500W)
    - Reaction rate (90%, 96,7%, 100%, 103,3%, 110%)

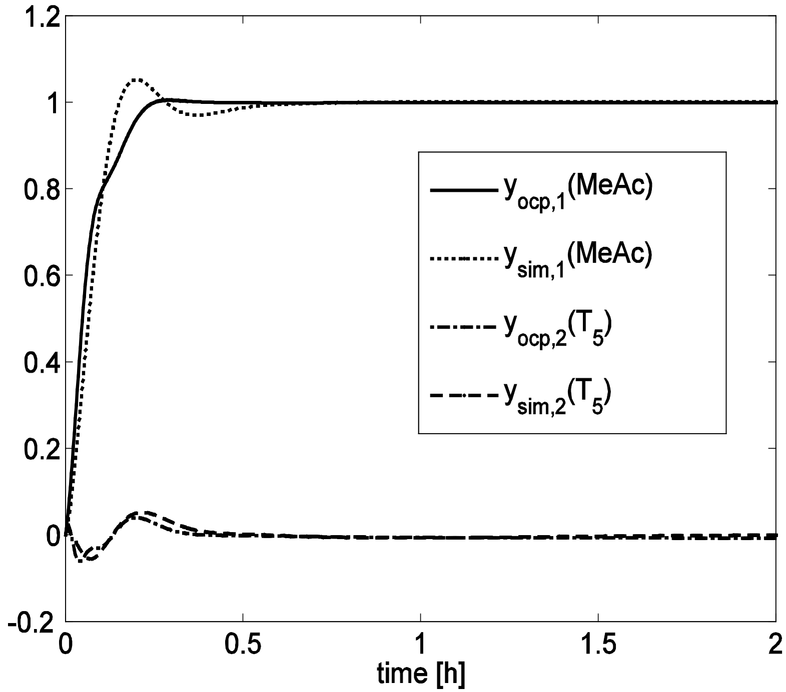
⇨ $\Delta J_{average}$ < 5%, all structures suitable

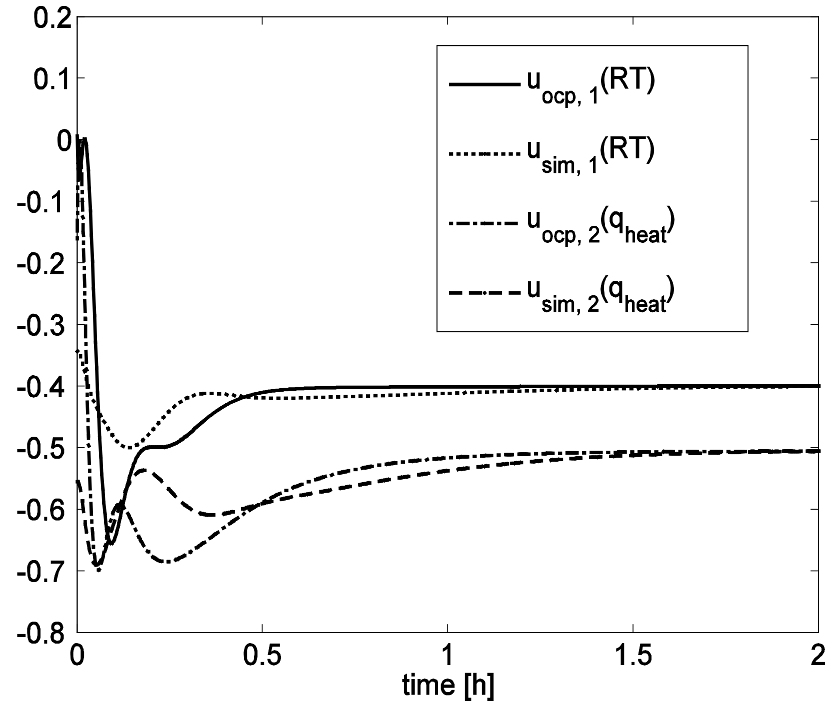
Dynamic Analysis

- Analysis of linear controllability measures for the 41 best structures
  - No right half-plane zeros < 0.01
    - Excludes 11 structures
  - Condition number < 10 at frequencies $10^{-2} \ldots 10^{-3}$
    - Excludes 5 structures
- For the remaining 25 structures:
  - Computation of the attainable control performance using convex optimisation for linearized models
  - Simplification of the controller using frequency response approximation

Linear Dynamic Simulation of the Controller

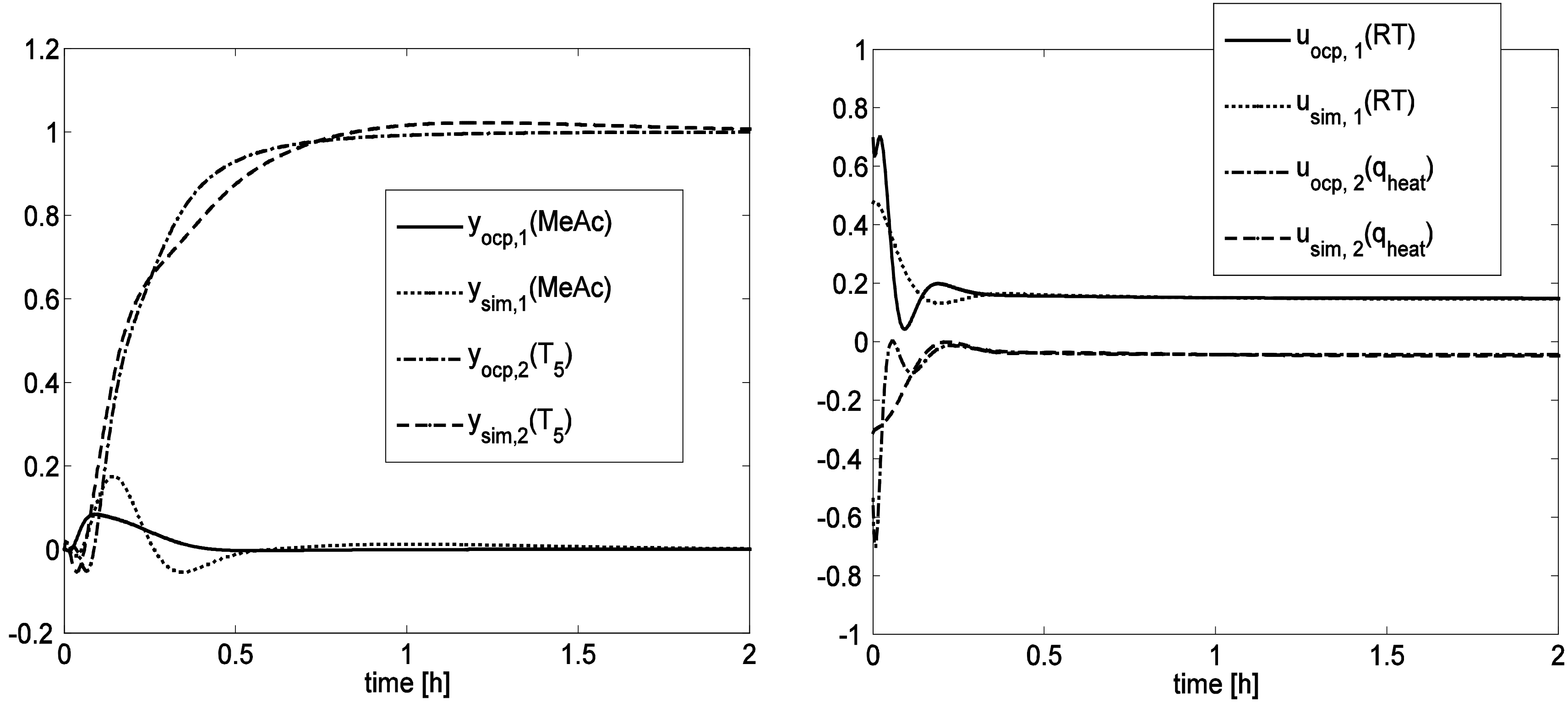
- Set-point step of 5 mol%



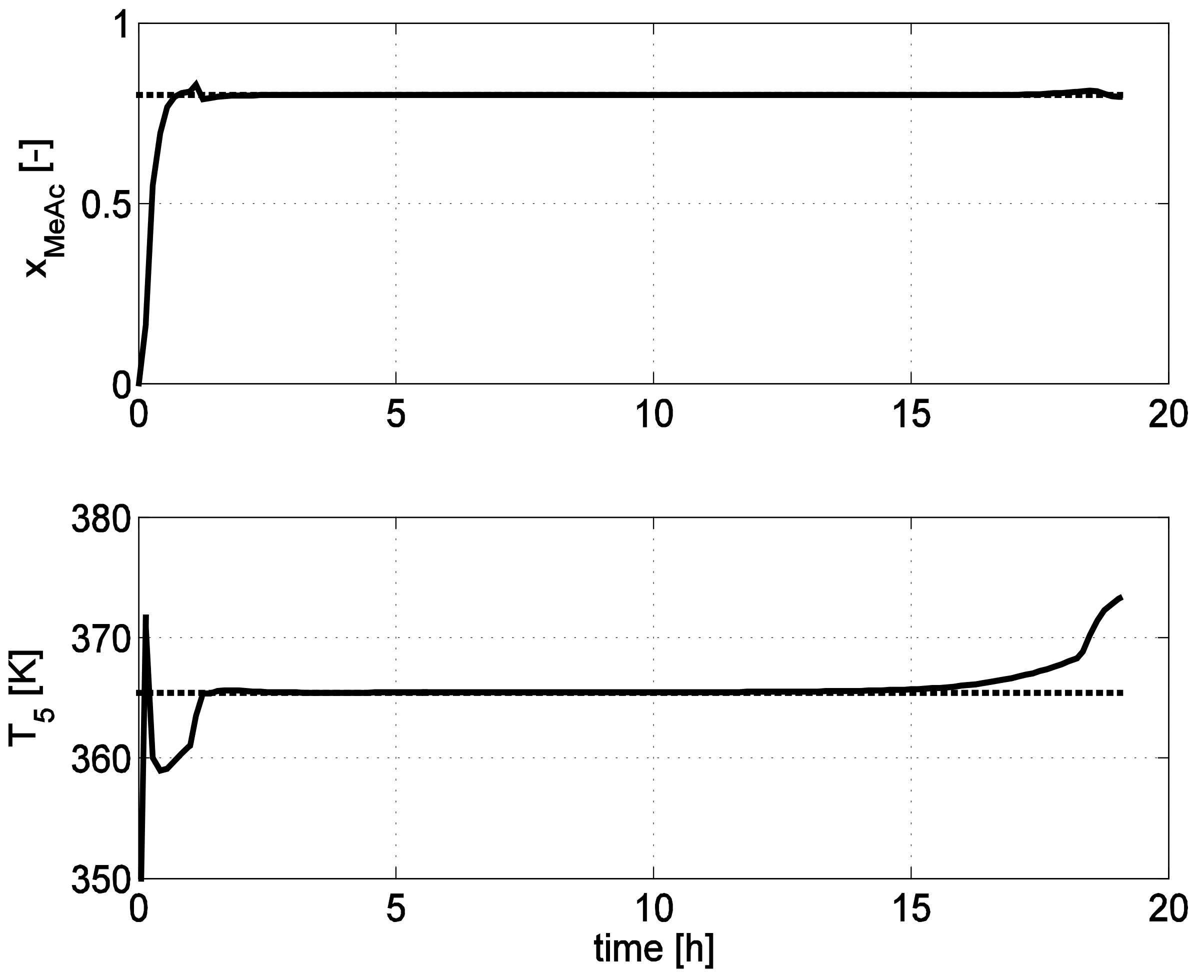


Linear Dynamic Simulation of the Controller

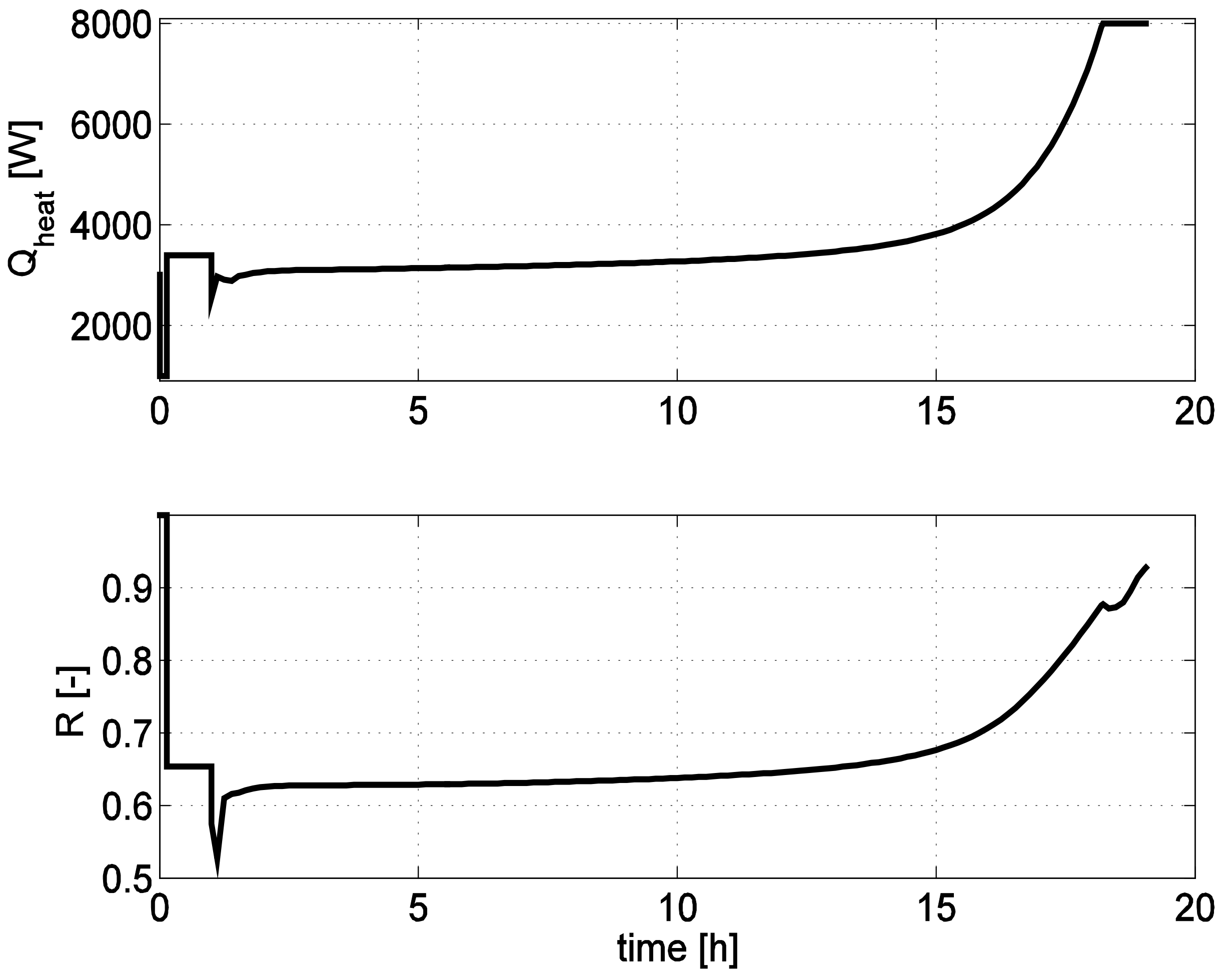
- Set-point step of 5K:



Simulated Batch Run, Controlled Variables

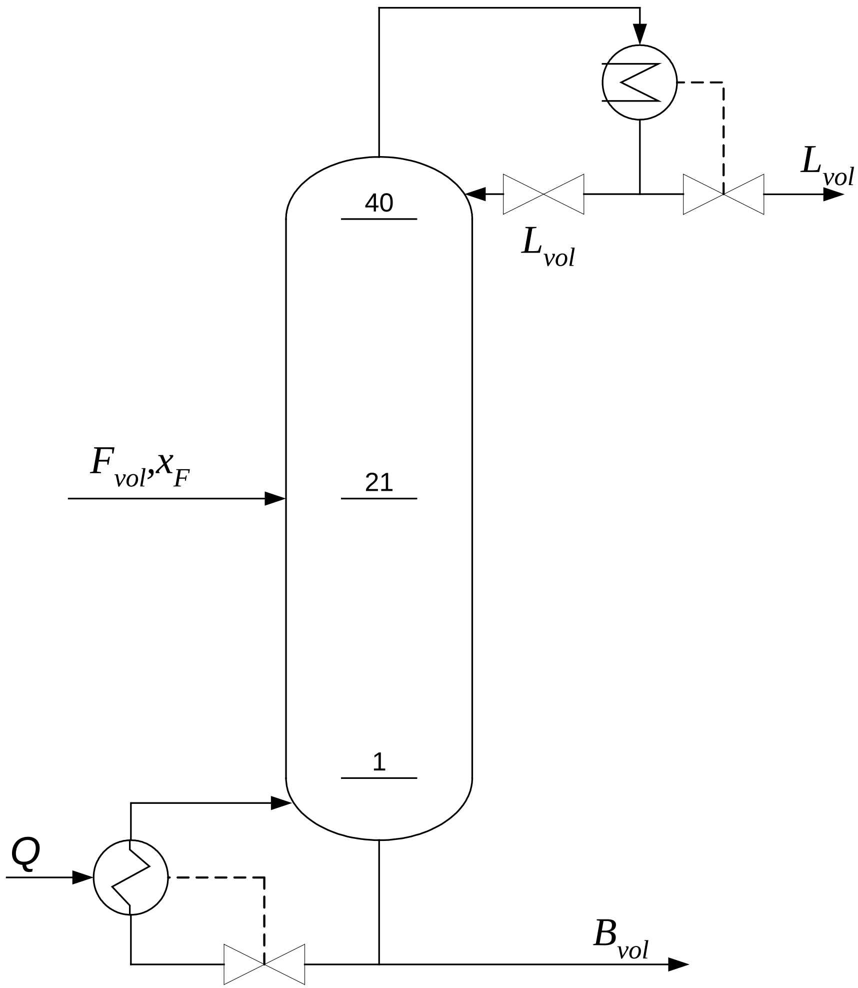


Simulated Batch Run, Manipulated Variables



Case Study 2 : Binary Distillation Column

- Process:
  - Separation of a mixture of methanol, *n*-propanol
  - Column has 40 trays, feed tray: 21
  - 2 manipulated variables
  - 41 measurements
- Rigorous Model:
  - Dynamic, non-linear equilibrium stage model
  - Stiff DAE with 204 variables



Control Structure Selection Procedure

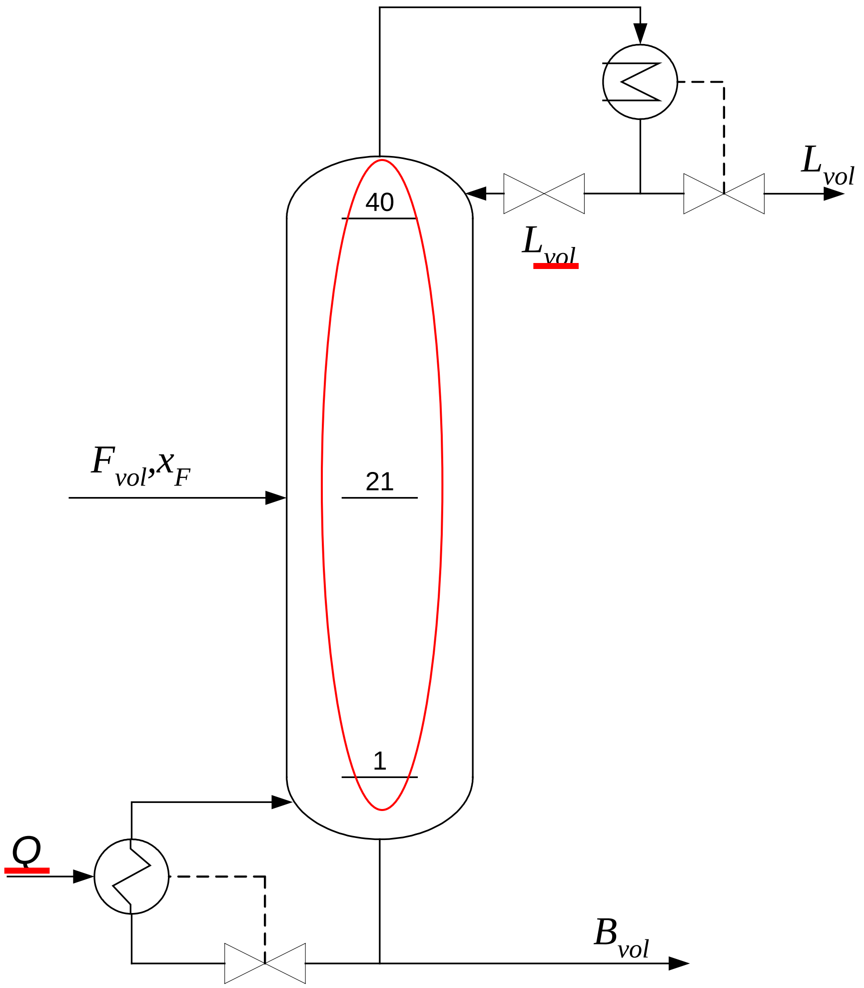
Complexity of the analysis

1. Define the economic optimization problem
2. Define critical disturbances
3. Pre-selection of control structures
4. Optimization of the set-points
5. Evaluation of the benefits for static disturbances
6. Performance for dynamic disturbances

Number of combinations

Problem Statement

- 2 manipulated variables: Heat input and reflux flow rate
- Possible controlled variables: temperatures on 40 trays



Economic Optimization Problem

- Profit function: Income of top product – cost of the heat input.
- Purity requirements:

  Distillate purity: 99%, bottom impurity 1%
- Problem formulation:

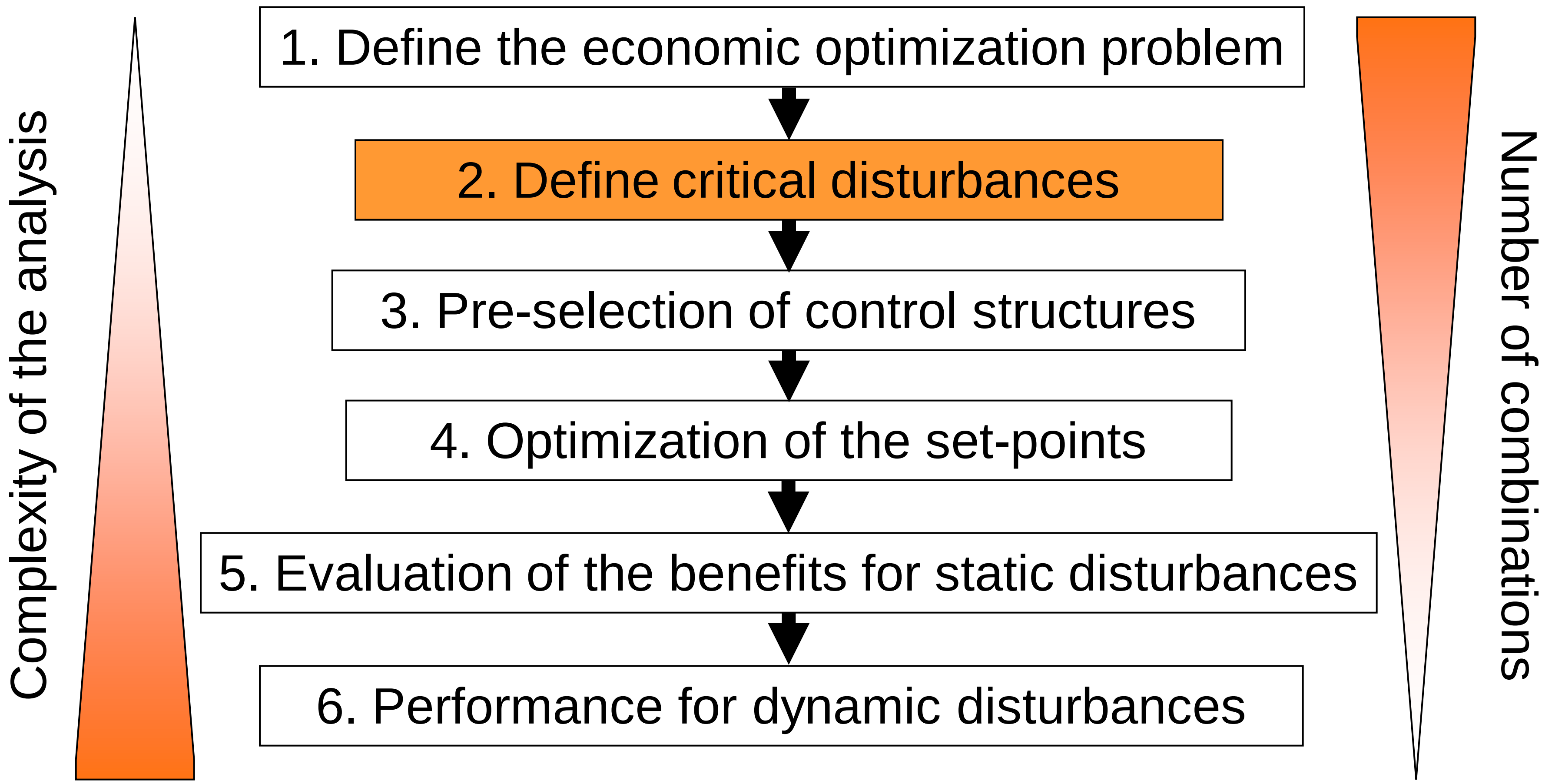
$$\max_{\underline{u}} J(\underline{u}, \underline{x})$$

$$s.t.: J = c_{Distillate}\dot{n}_{Distillate} - c_{heat}q_{heat}$$

$$x_{Distillate} \geq 0.99$$

$$x_{Bottom} \leq 0.01$$

Control Structure Selection Procedure

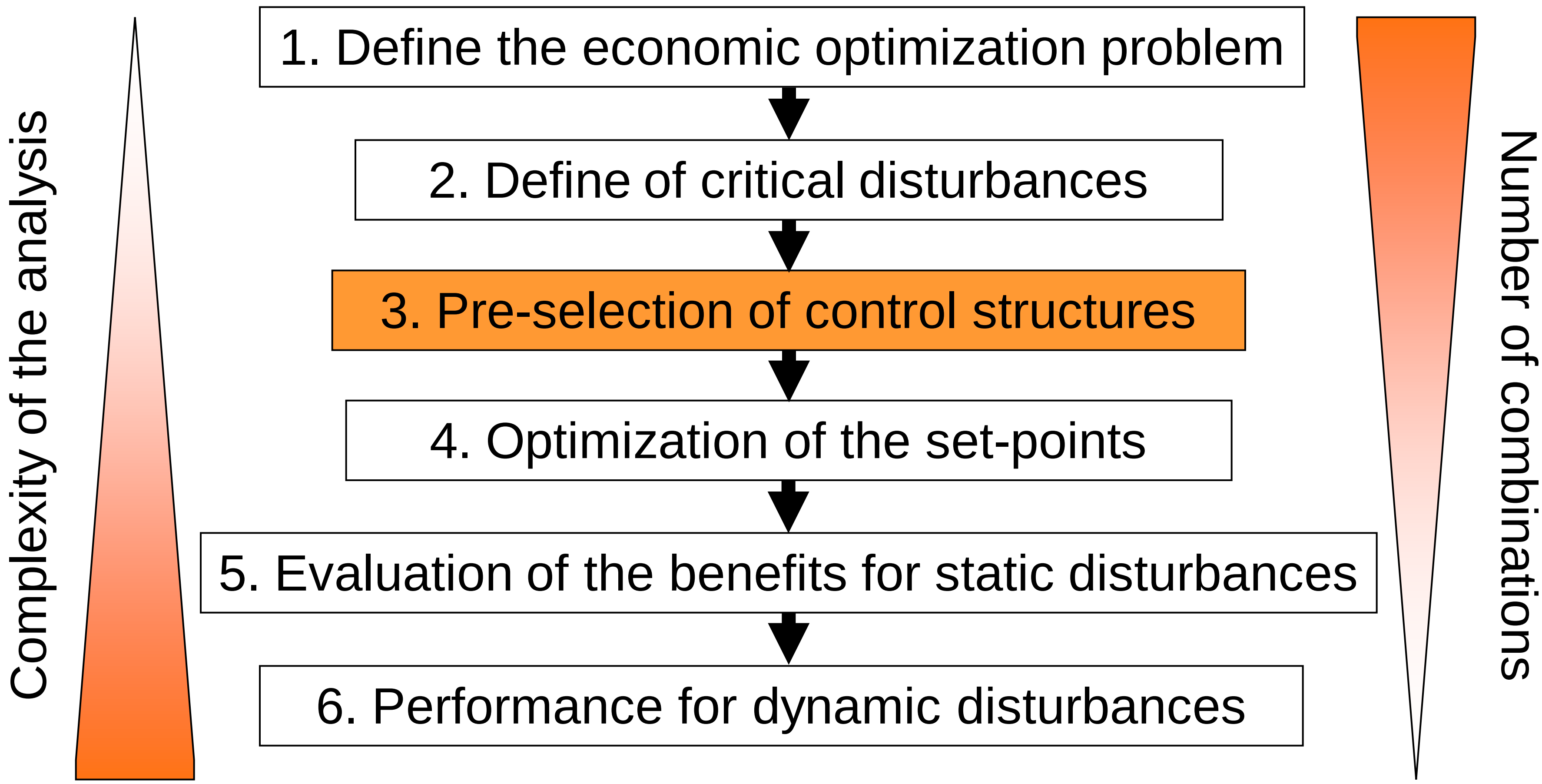


2. Definition of Critical Disturbances

- 5 disturbances, uniformly distributed

Disturbances	Value
Feed rate	±4 l/h
Feed temperature	±5 °C
Feed composition	±0.1
Reboiler heat input	±0.2 kW
Condenser temperature	±5 K

Control Structure Selection Procedure



Pre-selection of Control Structures

- 40 possible measurements, 2 manipulated variables, number of structures:

$$C_{40}^{2} = \binom{40}{2} = \frac{40!}{(40-2)!2!} = 780$$

- Method:
  - Generalized non-square relative gain array (NRG)
  - Negative elements of the RGA
  - Sensor sensitivity analysis (Engell et. al (2005)
    - Structures with $\sigma_{max}(\underline{S})$ smaller than 0.05 are excluded

$\Rightarrow$ Screens out 702 unpromising structures out of 780

Control Structure Selection Procedure

Complexity of the analysis

1. Define the economic optimization problem
2. Define critical disturbances
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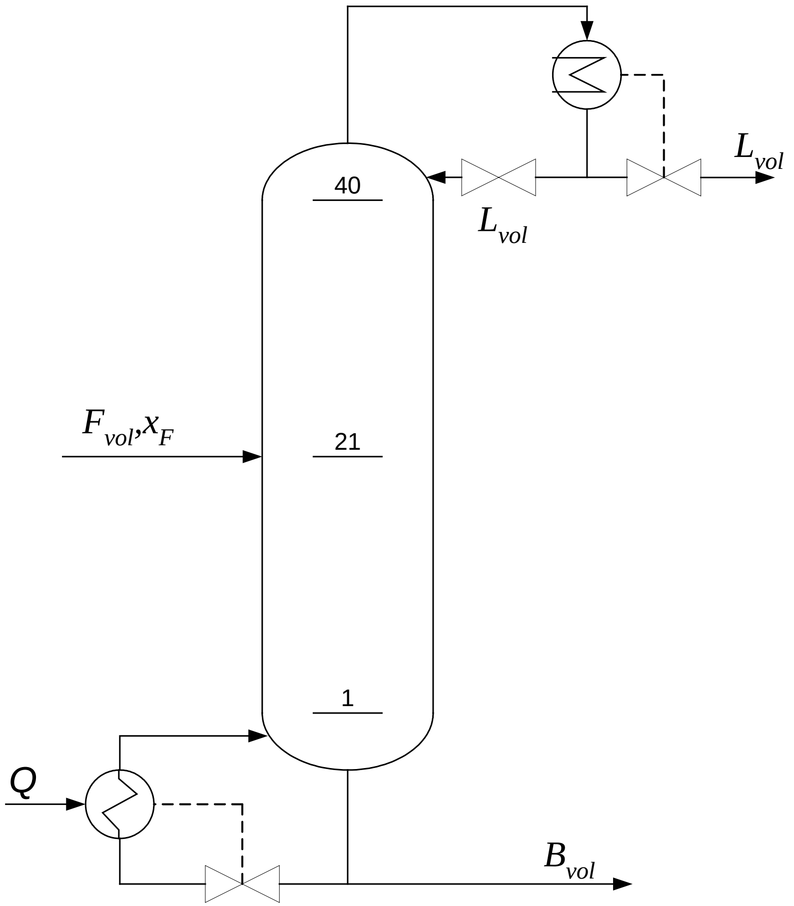
6. Performance for dynamic disturbances

Number of combinations

Choice of Set-points for the Distillation Column

- Static optimization using TOMLAB with SNOPT 6.0
- All structures have common set-points

⇒ 78 structures go to the next step



Control Structure Selection Procedure

Complexity of the analysis

1. Define the economic optimization problem
2. Define critical disturbances
3. Pre-selection of control structures
4. Optimization of the set-points
5. Evaluation of the benefits for static disturbances
6. Performance for dynamic disturbances

Number of combinations

Combined Disturbances for the Binary Distillation Column

- Non-linear process:
  - Summation of the effects of disturbances not reasonable

  ⇒ Optimization for scenarios of all combinations of
  - Feed rate (-4l/h, -1.3l/h, 0, +1.3l/h, +4l/h), nominal: 14l/h
  - Feed temperature (-5°C, -1.66°C, 0, +1.66°C, +5°C), nominal: 71°C
  - Feed composition (-0.1, -0.033, 0, +0.1, +0.033), nominal: 0.32
  - Reboiler heat input (-0.2kW, -0.066kW, 0kW, +0.066kW, +0.2kW), nominal: 2.35kW
  - Condenser temperature (-5°C, -1.66°C, 0, +1.66°C, +5°C), nominal: 47.2°C

Application to the Binary Distillation Column

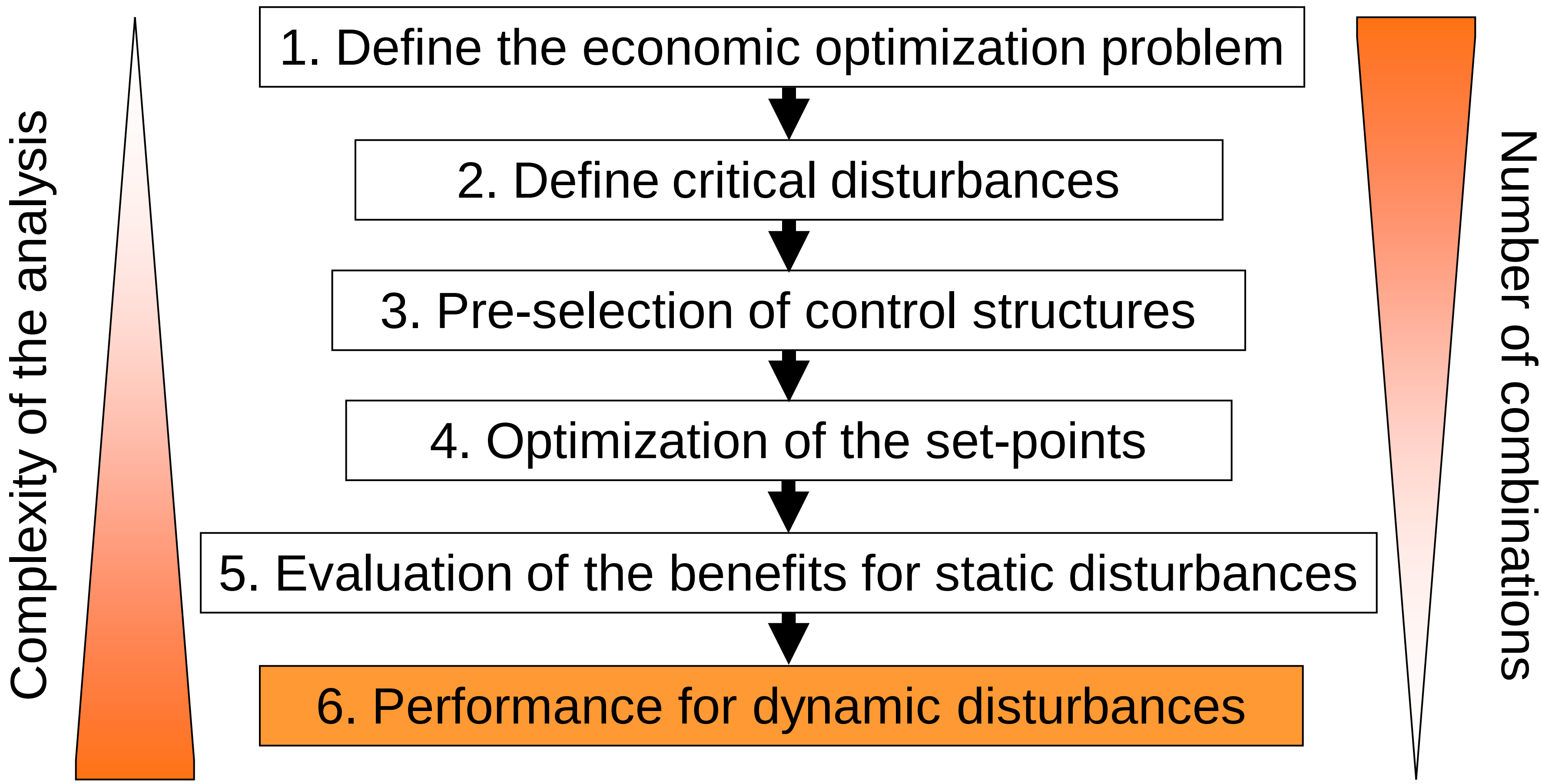
- "Softened" cost function

$$J = H\left(x_{Distillate} - 0.99\right) c_{Distillate} \dot{n}_{Distillate} - c_{heat} q_{heat}$$

- Evaluation of the performance for static disturbances
  - 12 structures are chosen for the final step

Structure	Profit
(6,35)	113.51
(7,30)	112.07
(7,33)	113.16
(7,35)	111.49
(9,30)	110.26
(10,28)	112.38
(10,29)	111.61
(10,30)	110.56
(11,31)	111.82
(11,32)	109.31
(11,35)	110.12
(17,27)	112.75

Control Structure Selection Procedure



Numerical Algorithms

- The NMPC simulation is done by MUSCOD-II (***MU***ltiple ***S***hooting ***CO***de for ***D***irect Optimal Control) developed by IWR Heidelberg (Bock et al.)
  - Solves general optimal control problems with dynamics described by DAE and constraints
  - Multiple shooting: The optimization horizon is divided into subintervals, differential equations are solved independently on each subinterval by a ODE or DAE solver.
  - The resulting large but structured NLP problem is solved by an SQP algorithm

Optimization of the Weights

- Conventional optimization algorithms can not be used here:
  - Objective function results from a complex numerical procedure, expensive to evaluate
  - Convergence can be slow
- Derivatives free optimization (DFO) is more suitable
  - CONDOR (***CO***nstrained, ***N***on-linear, ***D***irect, parallel, multi-objective ***O***ptimization using trust ***R***egion method for high-computing load, noisy objective functions)
  - Can only solve problems with simple constraints

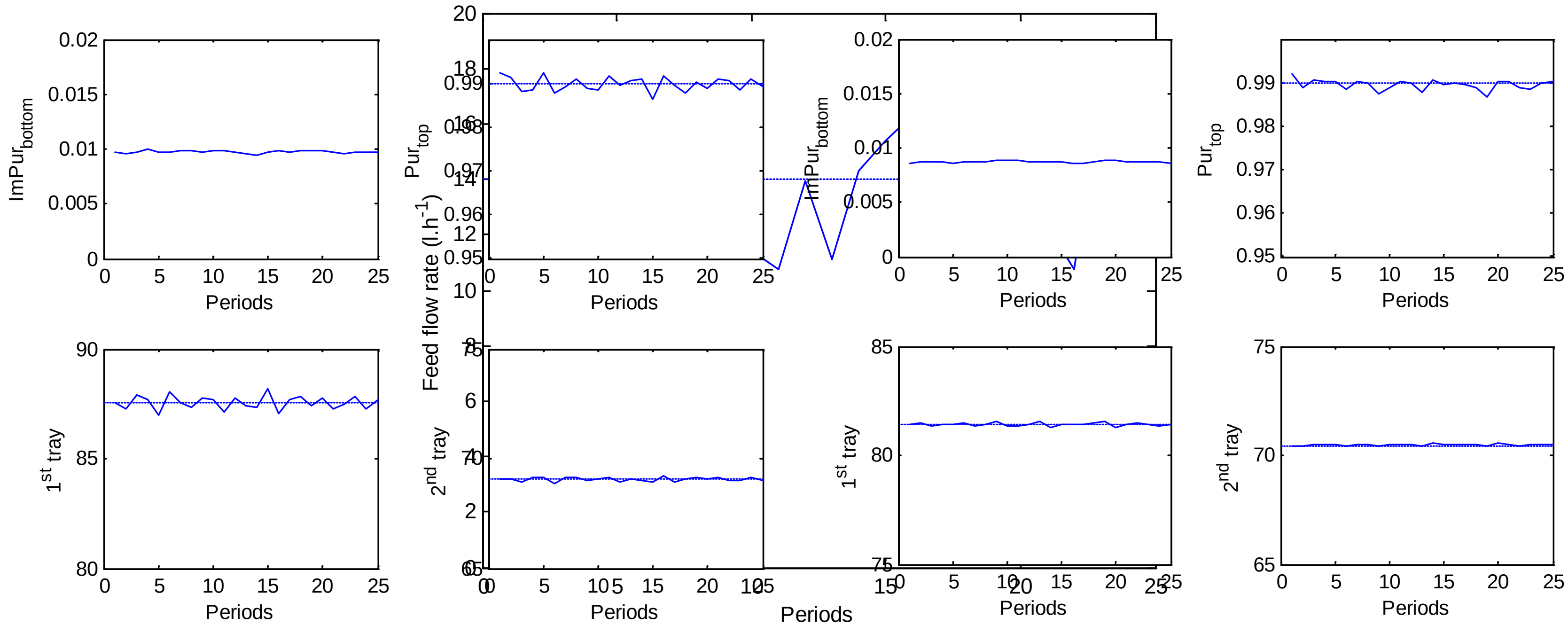
  ⇒ P, Q are assumed to be diagonal, positive-definiteness of matrix is equivalent to positiveness of the diagonal elements

Performance for Dynamic Disturbances

- Same cost function as in step 5
- Quantitative evaluation for dynamic disturbances
  - First linear MPC is used: 3 structures are chosen
  - Next NMPC is performed: Best structure: (10, 28)

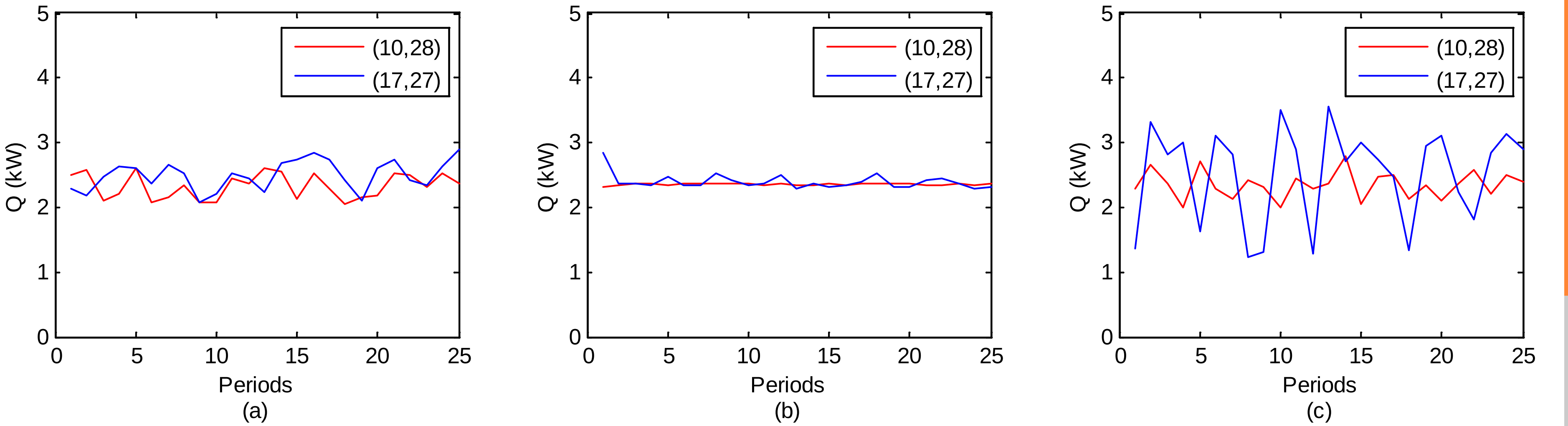
Structure	Profit
(10,28)	113.54
(10,31)	112.56
(17,27)	109.09

Dynamic Simulations (NMPC Controller)



Structure (10,28) Disturbances in feed flow rate Structure (17,27)

Dynamic Simulations (NMPC Controller) (2)



Heat input in 3 disturbances cases:

a) Feed flowrate, b) Feed temperature, c) Feed composition

Summary

- Systematic, exhaustive method for control structure selection
- Measurement errors, static and dynamic performance are taken into account
- Applied to several other case studies, e.g. reactive distillation of butyl acrylate, ternary distillation