# Online optimizing control: The link between plant economics and process control

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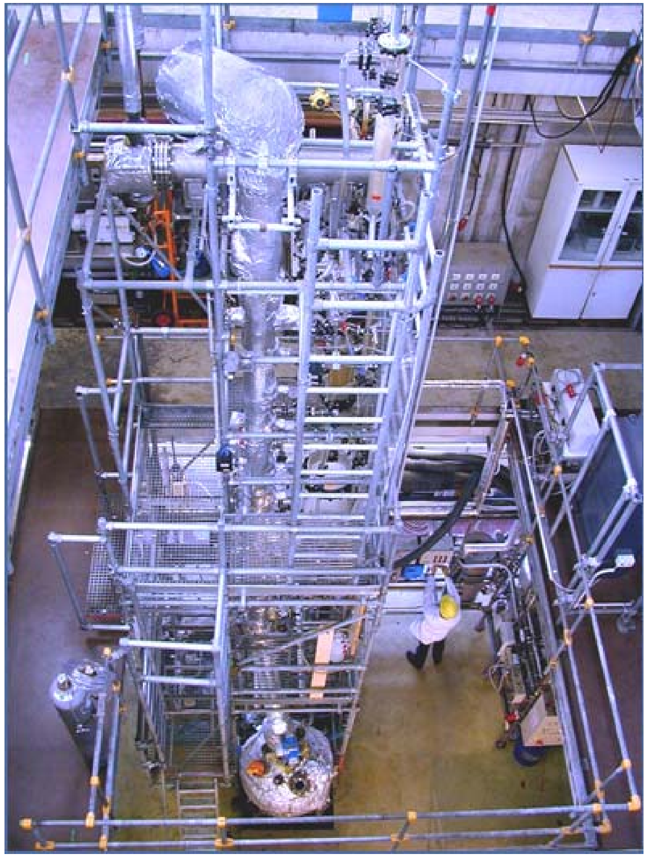
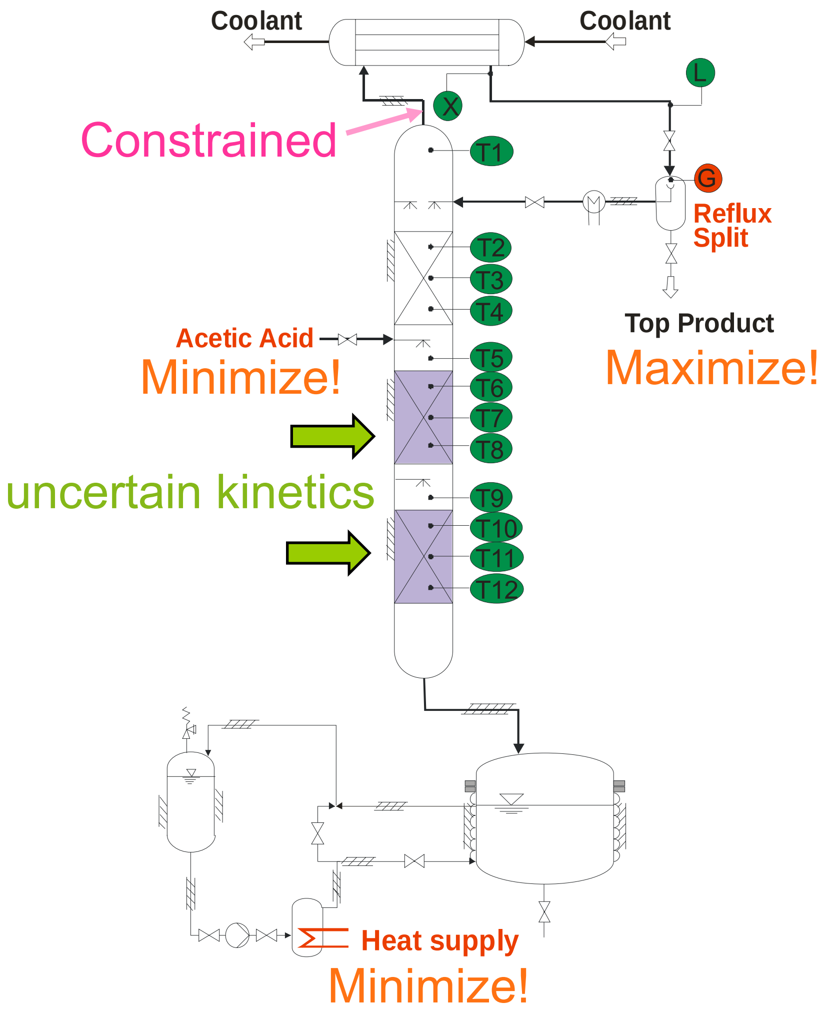
# The gap between process operations and controller design

# Process operations



Reactive distillation column



# Control engineering

**Standard task description:**

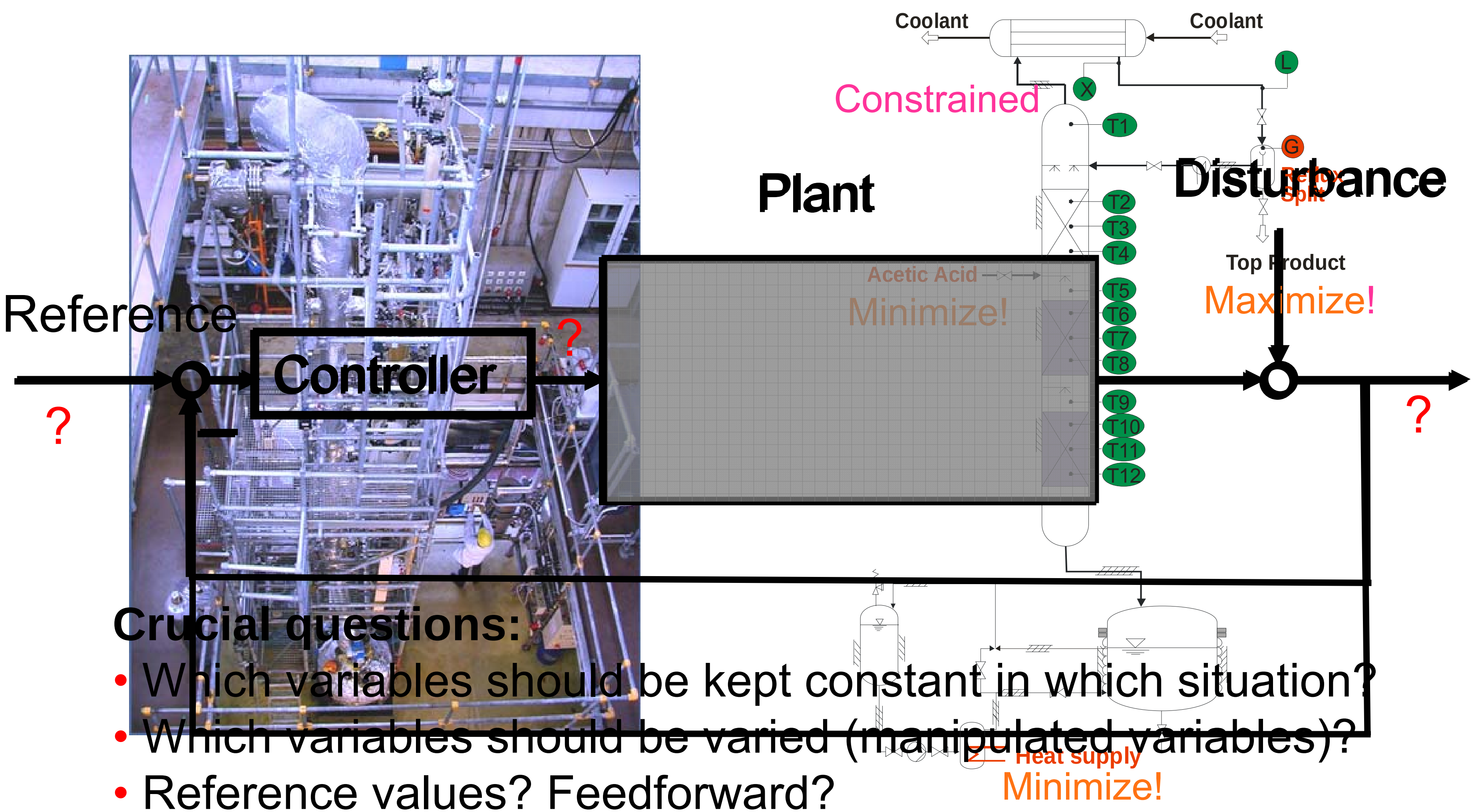
Choose and design feedback controllers for optimal

- disturbance rejection
- setpoint tracking

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

**“SERVO or REGULATION PROBLEM”**

# Control engineering reduction




**Crucial questions:**

- Which variables should be kept constant in which situation?
- Which variables should be varied (manipulated variables)?
- Reference values? Feedforward?

- In process control, the servo problem formulation is adequate for subordinate tasks:
  - Temperature control
  - Flow control
  - …
- Optimal solution of servo/regulation problems does not imply optimal plant operation – optimal plant operation is not necessarily a servo problem!
- Automatic (feedback) control is often considered as a necessary low level function but not as critical for economic success.

⇨ CONTROL FOR OPTIMAL PLANT OPERATION

# Outline: From control to optimal operation

- ✓ The gap between process control and process operations
- **Control structure selection**
- Real-time optimization
- From RTO to optimizing control
- Direct finite-horizon optimizing control
- Application example: SMB Chromatography
- Plant-model mismatch
- Summary, open issues and future work

# Control structure selection

- Choice of manipulated and controlled variables
  - Which variables should be controlled?
  - Which manipulated variables should be used?
  - Loop pairing (not considered here)
- Common methods:
  - Linear analysis: RGA, condition numbers, sensitivities, Jorge Trierweiler's RPN, optimization
  - Simulation studies

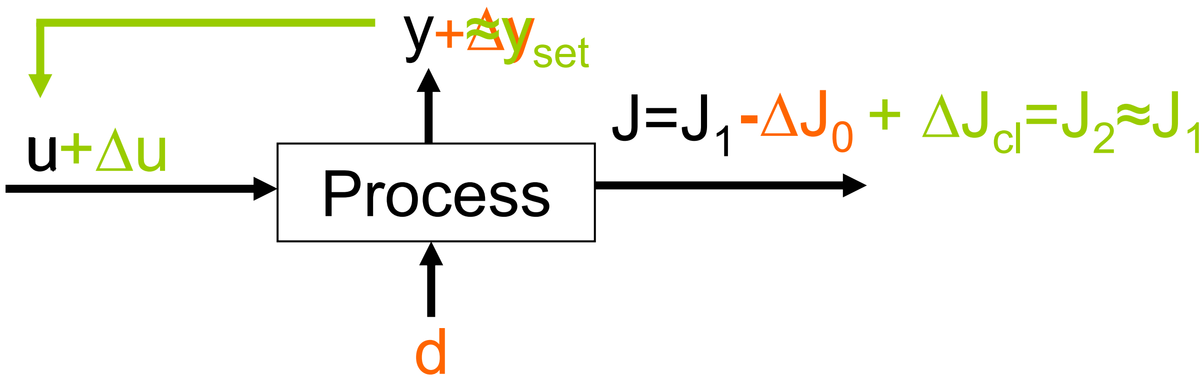
**Focus is on dynamics – methods address the servo problem but not optimal plant operation.**

# Plant performance-based control structure selection

- Skogestad (2000): “Self-optimizing control”
- Basic ideas:
  - Tracking of set-points is not always advantageous
  - Feedback control should guarantee cost effective operation in the presence of disturbances and plant-model mismatch
  - Stationary analysis (dynamics ignored)
  - Non-linear plant behavior considered by use of rigorous nonlinear plant models

# Plant performance-based control structure selection

- Decision based on the effect of regulation on the profit **J**




$$
\begin{aligned}
\Delta J = {} & J(\underline{u}_{nom}, d = 0) - J(\underline{u}_{nom}, \underline{d}_i) \quad (1)\\
& + J(\underline{u}_{nom}, \underline{d}_i) - J(\underline{u}_{opt}, \underline{d}_i) \quad (2)\\
& + J(\underline{u}_{opt}, \underline{d}_i) - J(\underline{u}_{con}, \underline{d}_i). \quad (3)
\end{aligned}
$$

(1) ≈ 0:

No regulatory control necessary

(1) >> 0 and (2) << 0 and (3) ≈ 0:

Closed-loop regulatory control recommended

(1) >> 0 and (2) << 0 and (3) >> 0:

Control with fixed set-point not advisable

# Comparison of feedback structures

- Feedback restricts the controlled variables to an interval around the set-points (due to measurement errors)
- Computation of the worst-case profit for possible control structures and several disturbance scenarios (guaranteed plant performance)

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

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

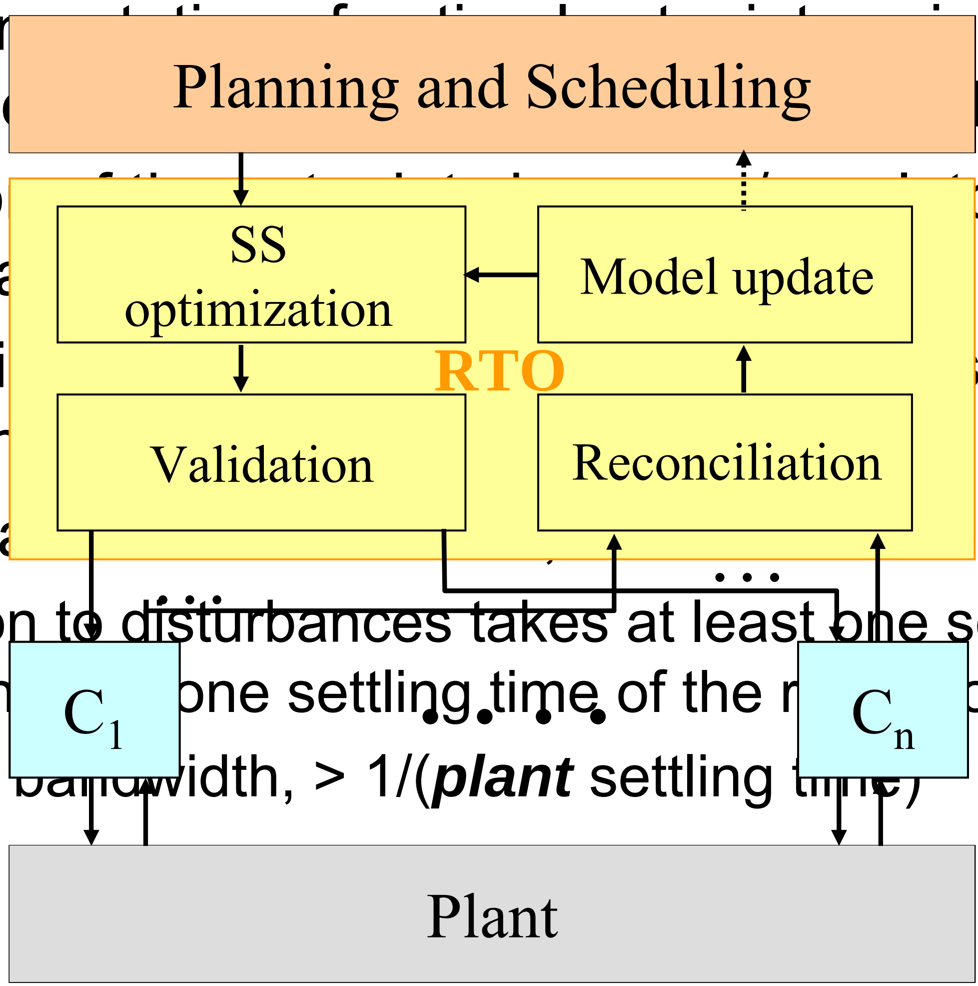
$$\underline{y} = \underline{m}(\underline{x}) = \underline{M}(\underline{u}, \underline{d}_i)$$

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

- Set-points optimized separately for a set of disturbances

# Two-layer architecture with RTO

- Online co… g nonlinear (mostly m… ka RTO)
- Realizatio… ory control, using linea… controllers)
- Optimizati… teady state of the plan…
- Clear sepa…
  - Reaction to disturbances takes at least one settling time of the plan… one settling time of the r… ory layer
  - Limited ba…width, > 1/(***plant*** settling time)



# From control to optimal operation

- ✓ The gap between process control and process operations
- ✓ Control structure selection
- ✓ Real-time optimization
- **From RTO to optimizing control**
- Direct finite-horizon optimizing control
- Application example
- Summary, open issues and future work

# From RTO to optimizing control

- Simple idea: (strict) RTO is too slow ...

  hence
- Do not wait for steady state → ***fast sampling RTO***
  - Current industrial practice:

    Sampling times of 10-30 mins instead of 4-8 hours

    ⇨ dynamic control without concern for dynamics
  - Stability enhanced by restricting the size of changes
  - Similar to gain scheduling control:
    Dynamic plant state is projected on a stationary point
  - Ad-hoc solution

# Integration of performance optimization in MPC

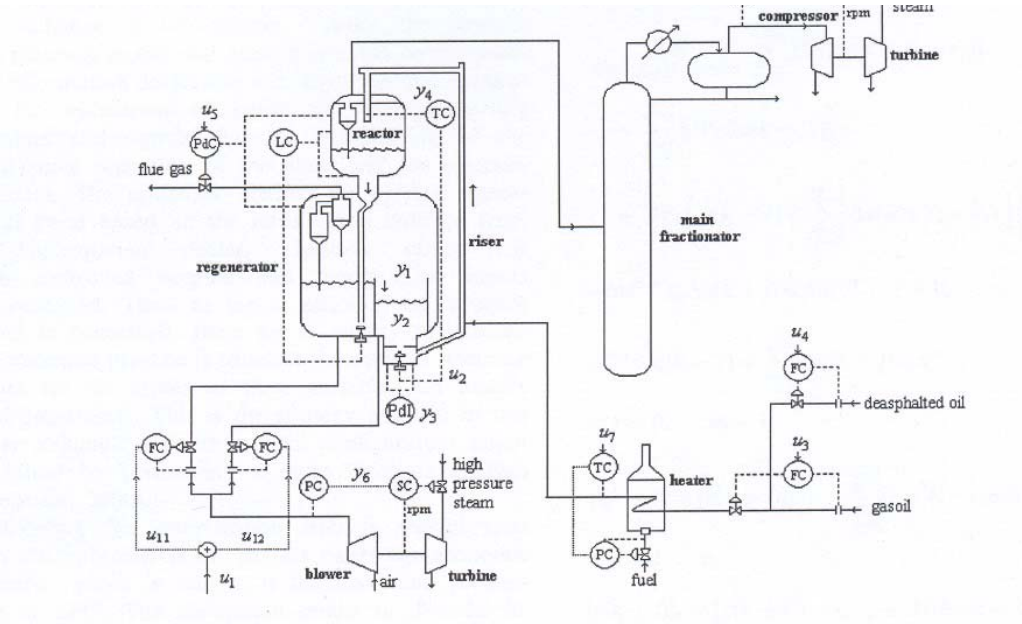
- Idea:
  - Add a term that represents the economic cost (or profit) to a standard (range control) MPC cost criterion
  - Zanin, Tvrzska de Gouvea and Odloak (2000, 2002):

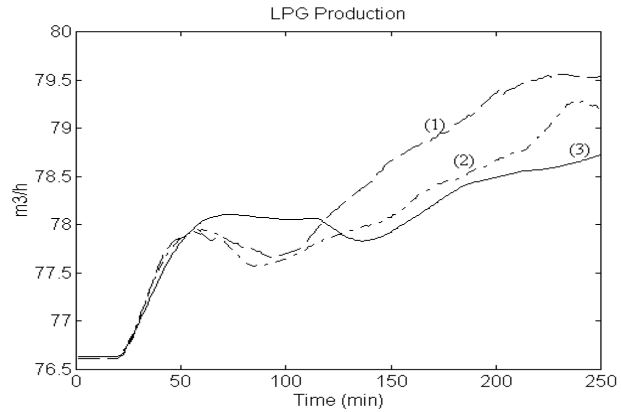
$$
\begin{aligned}
&\min_{\Delta u(k+i);i=0,\dots,m-1} \sum_{j=1}^{p} \left\| W_1 (y(k+j) - r) \right\|_2^2 \\
&+ \sum_{i=0}^{m-1} \left\| W_2 \Delta u(k+i) \right\|_2^2 + W_3 f_{eco}(u(k+m-1)) \\
&+ \left\| W_5 (u(k+m-1) - u(k-1) - \Delta u(k)) \right\|_2^2 \\
&+ W_6 [ f_{eco}(u(k+m-1), y(k+\infty)) \\
&- f_{eco}(u(k), y'(k+\infty)) ]^2
\end{aligned}
$$

# Application to a real industrial FCC

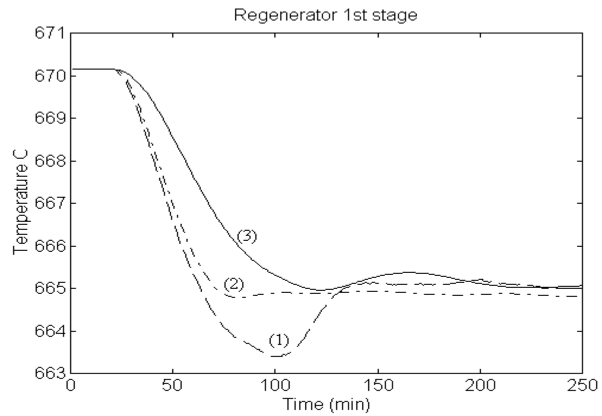
7/6 inputs, 6 outputs

Economic criterion: LPG-production




(1) *W3*=100, (2) *W3*=1, (3) *W3*=0.1




Problems: Acceptance by operators

Concerns for vulnerability

# From control to optimal operations

- ✓ The gap between process control and process operations
- ✓ Control structure selection
- ✓ Real-time optimization
- ✓ From RTO to optimizing control
- **Direct finite-horizon optimizing control**
- Application example
- Plant-model mismatch
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# Direct Finite Horizon Optimizing Control

- Idea:
  - Optimize - over a finite moving horizon - the (main) degrees of freedom of the plant with respect to process performance rather than tracking performance
  - Represent the relevant constraints for plant operation as constraints in the optimisation problem and not as setpoints
  - Quality requirements are also formulated as constraints and not as fixed setpoints

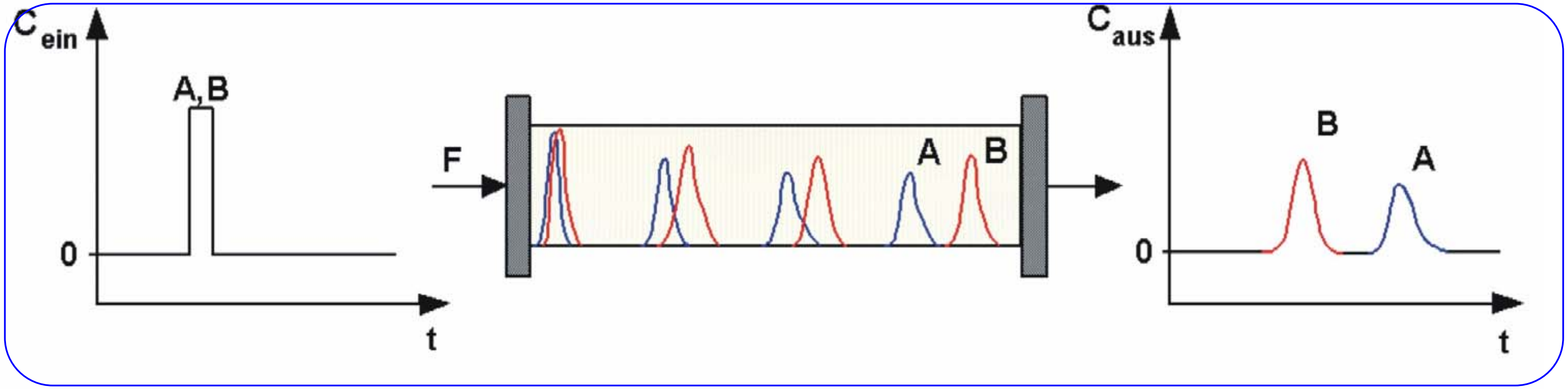
⇨ Maximum freedom for economic optimization

# Direct Finite Horizon Optimizing Control

- Advantages:
  - Degrees of freedom are fully used.
  - One-sided constraints are not mapped to setpoints.
  - No artificial constraints (setpoints) are introduced.
  - No waiting for the plant to reach a steady state is required, hence fast reaction to disturbances.
  - Non-standard control problems can be addressed.
  - No inconsistency arises from the use of different models on different layers.
  - Economic goals and process constraints do not have to be mapped to a control cost whereby inevitably economic optimality is lost and tuning becomes difficult.
  - The overall scheme is structurally simple.

# Application study: SMB chromatography

# Chromatography: Principle, batch process

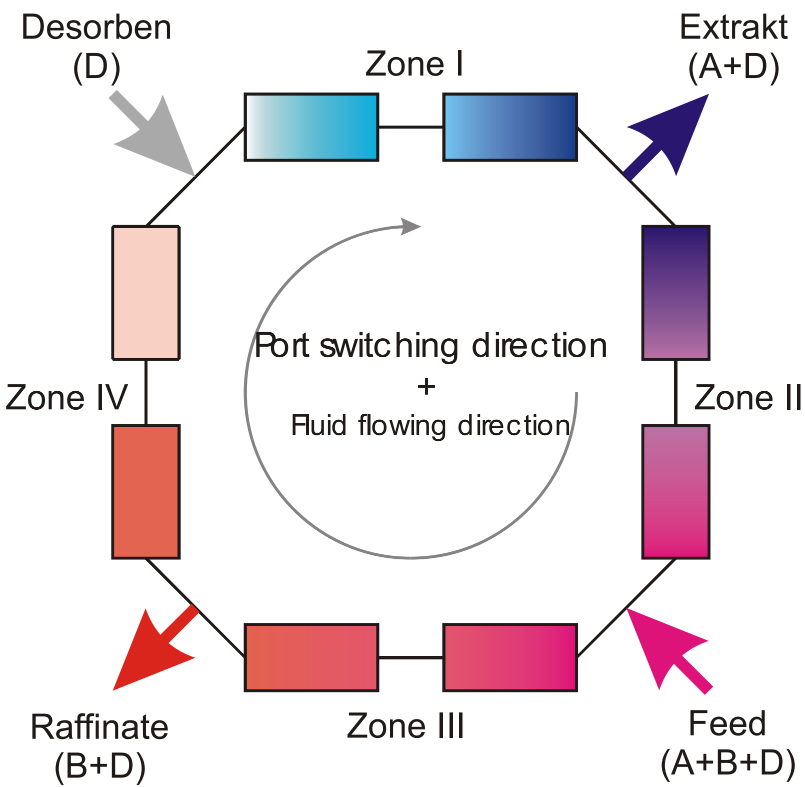



- Separation is based on different adsorption affinities of the components to a fixed adsorbent.
- Gradual separation while the mixture is moving through the column
- Fractionating of the products at the column outlet

☺ Simple process, high flexibility

☹ High operating costs,
high dilution of the products, and
low productivity

# Simulated-Moving-Bed process

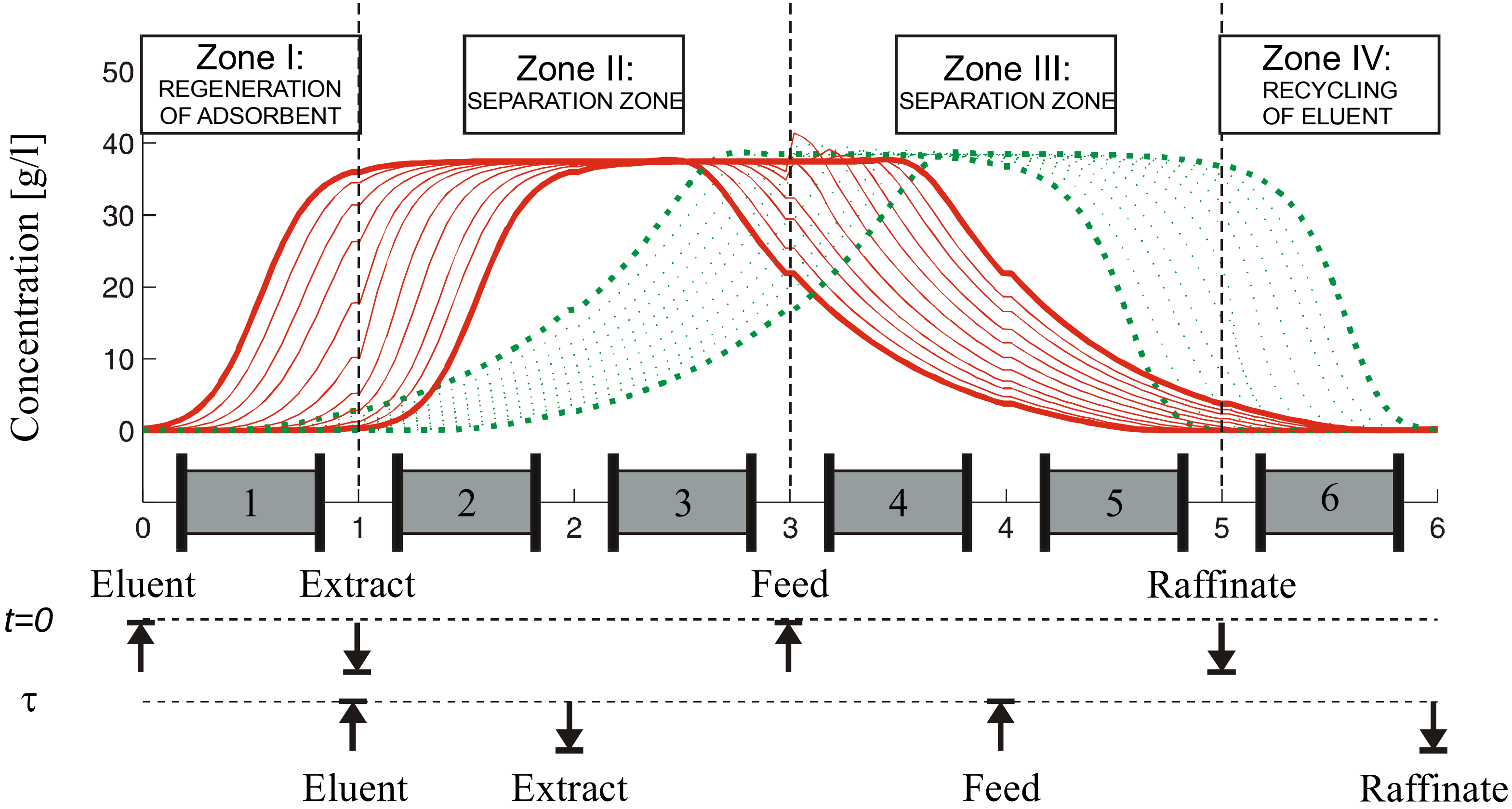



- A number of chromatographic columns are connected in series
- The inlet and outlet ports move to the next column position after each swichting period ($\tau$)
- Quasi-countercurrent operation is achieved ("simulated") by cyclic port switching

☺ Continuous operation, higher productivity, and lower separation cost

☹ Complex dynamics, very slow reaction to changes

# SMB dynamics

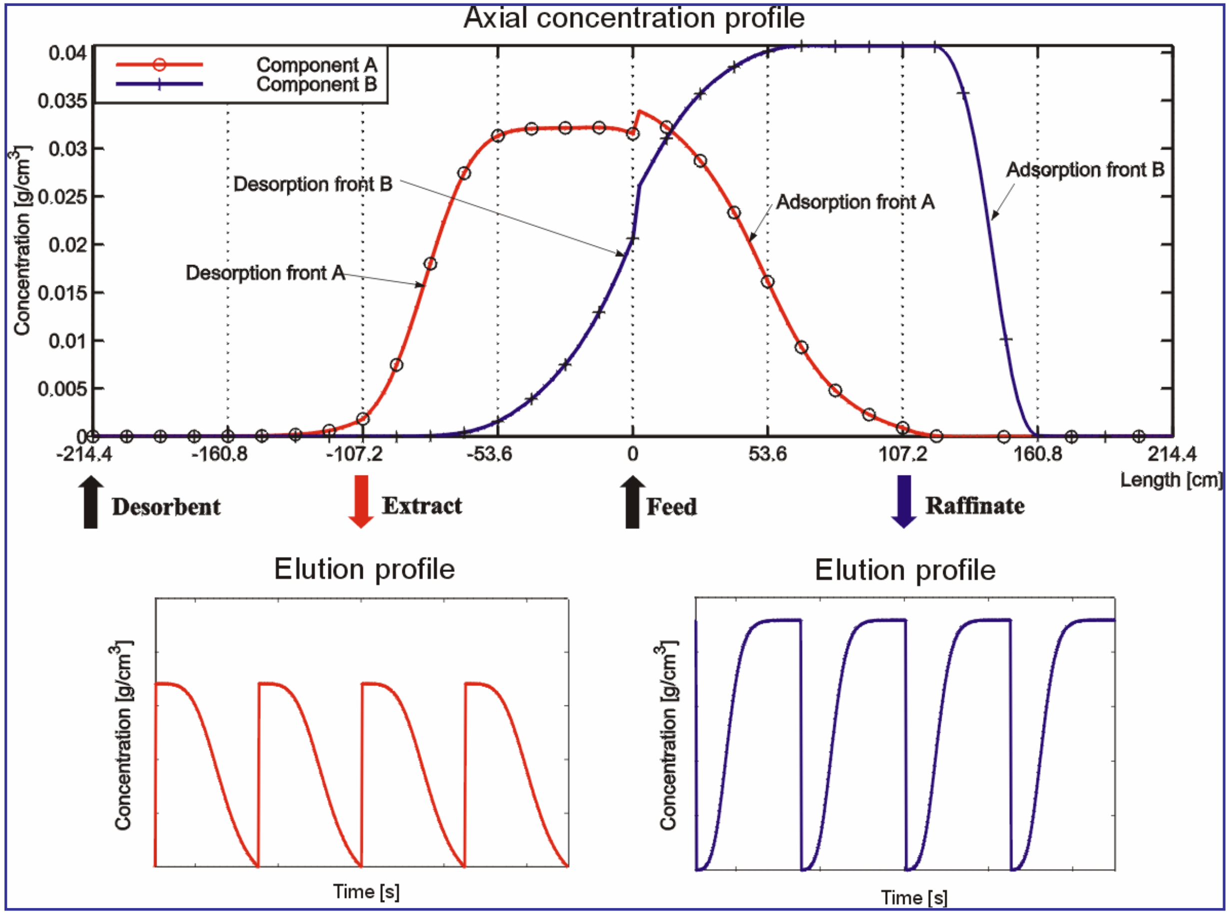



$$\mathbf{c}_{\mathbf{ax,k}}(t=\tau)=\mathbf{P}\mathbf{c}_{\mathbf{ax,k}}(t=0)$$

# SMB concentration profiles

- Continuous flows and discrete switchings
- Axial profile builds up during start-up
- Same profile in different columns in **cyclic** steady state

⇨ Periodic output concentrations

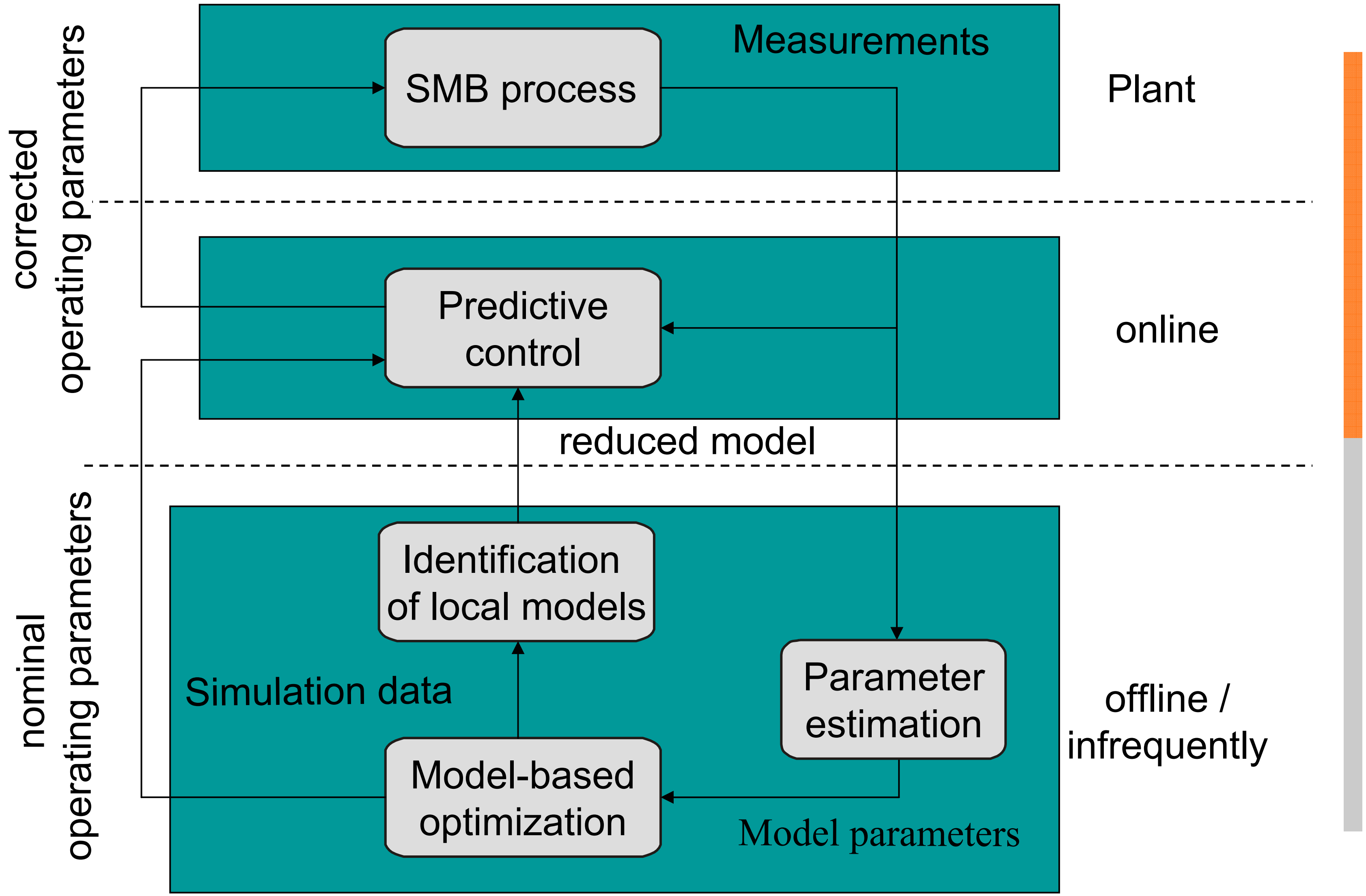


# SMB optimization and control problem

- **Goal:** Maintain specified purity at minimal operating cost
- Periodic process described by switched pde‘s
- Strongly nonlinear behaviour especially for nonlinear adsorption isotherms
- Drifts may lead to breakthrough of the separation fronts → long periods of off-spec production
- Intuitive determination of a near-optimal operating point is difficult.
- Optimal operation is at the purity limit.
- Operating cost is caused by solvent consumption and the cost of the adsorbent per (gram of) product

⇨ **Minimization of the solvent flow rate while meeting the specs for purity and recovery**

# Hierarchical control scheme (Klatt et al.)

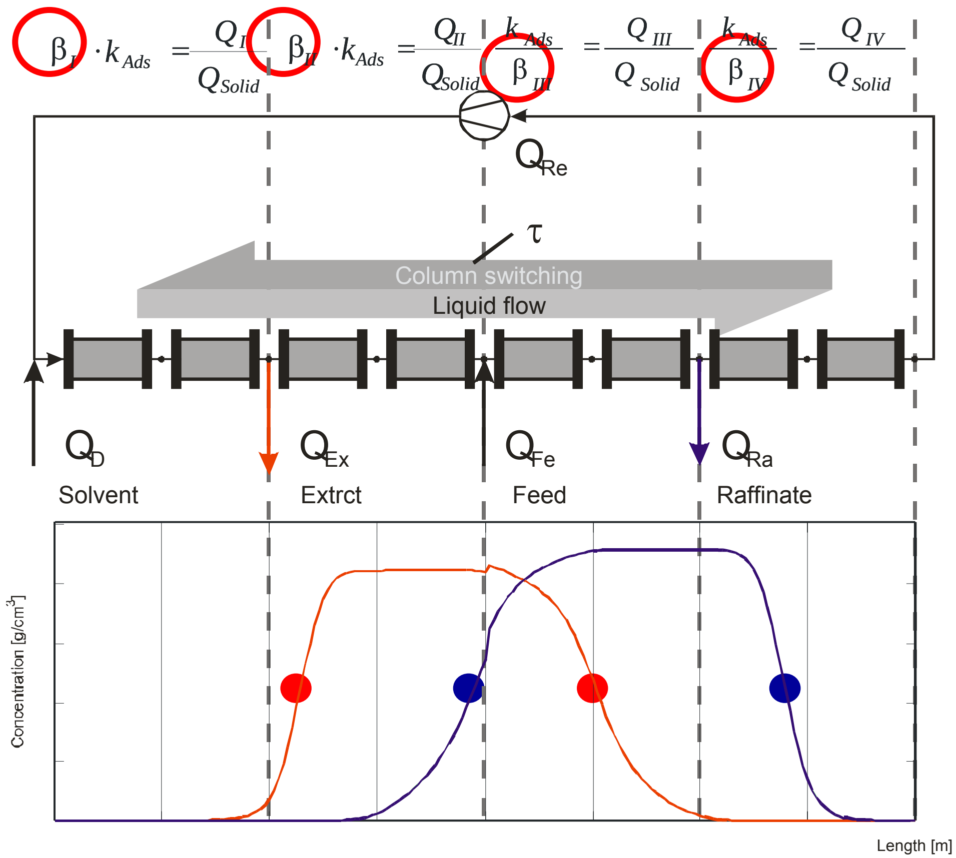


# Stabilizing the concentration profile

- Front positions taken as controlled variables
- Choice of manipulated variables: β-factors

⇨ Decoupled influence on the zones of the SMB process

- Successful application to process with linear isotherm



# Problems of the hierarchical approach

- Extension to nonlinear isotherms possible but control scheme quite complex (NN-based LPV MPC) (Wang and Engell, 2003)
- Fronts can only be detected accurately in the recycle stream, not in the product streams
- Optimality and desired purities cannot be guaranteed by front position control if the model has structural errors, e.g. in the form of the isotherm.

  → additional purity control layer necessary

  → scheme becomes very complex, optimality is lost.

⇨ Use **economic** online optimization directly to control the plant (Toumi and Engell, Chem. Eng. Sci., 2004)

# Formulation of the online optimization problem

$$\min_{[\beta_k, \beta_{k+1}, \ldots, \beta_{k+H_r}]} \sum_{j=k+1}^{k+H_p} (\Theta(j) + \Delta\beta_j{}^T R_j \Delta\beta_j)$$

Θ: economic criterion: solvent consumption

$\beta_k$ degrees of freedom – transformed flow rates and switching time

s.t.

$$\begin{cases} x_{k+1,0} = Mx_k \\ \dot{x} = f(x,u,p) \\ y = h(x,u) \end{cases}$$

Rigorous hybrid process model

$$\sum_{j=k+1}^{k+H_p} Pur_{Ex,j} + \Delta Pur_{Ex} \geq Pur_{Ex,\min}$$

Purity requirements (with error feedback, log. scaled)

$$\sum_{j=k+1}^{k+H_p} Rec_{Ex,j} + \Delta Rec_{Ex} \geq Rec_{Ex,min}$$

Recovery (with error feedback)

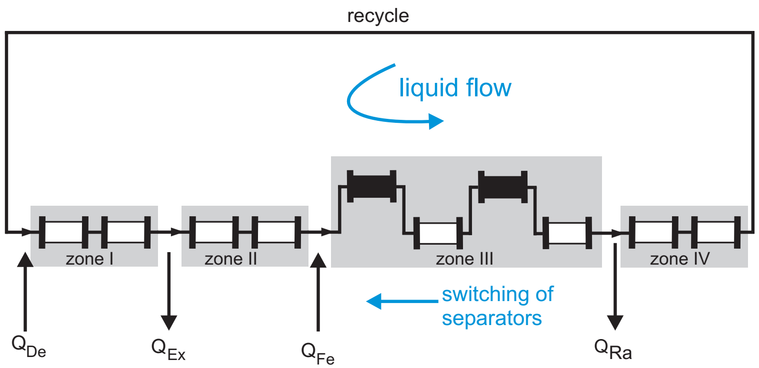
$$\Delta p_j \leq \Delta p_{\max}$$

max. pressure loss

$$j = k, \ldots, k + H_p$$

# Reactive SMB processes

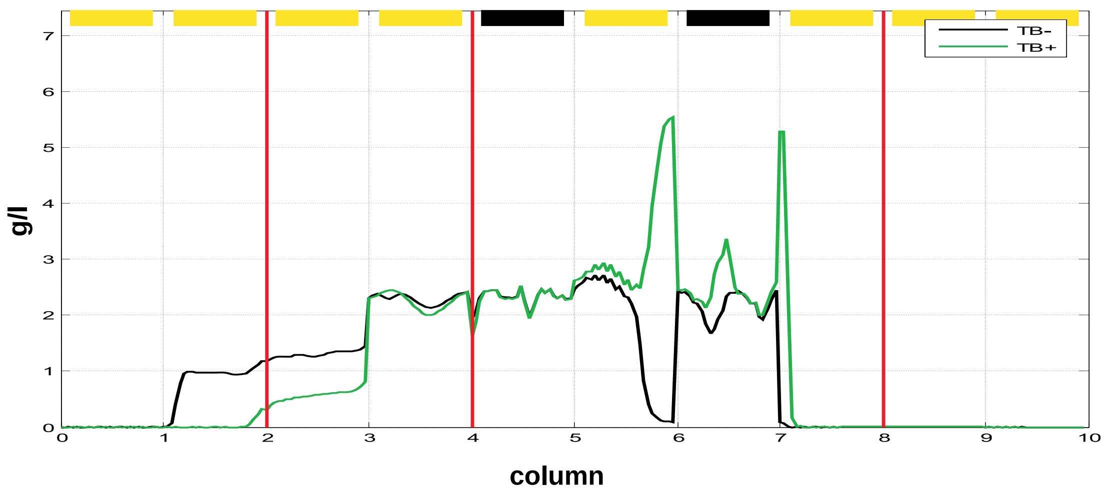
- Integration of reaction and separation can overcome equilibria and reduce energy and solvent consumption
- Fully integrated process however is severely restricted
- Hashimoto SMB-process:
  - Reaction and separation are performed in separate columns
  - Reactors remain fixed in the loop at optimal locations
  - Optimal conditions for reaction and separation can be chosen



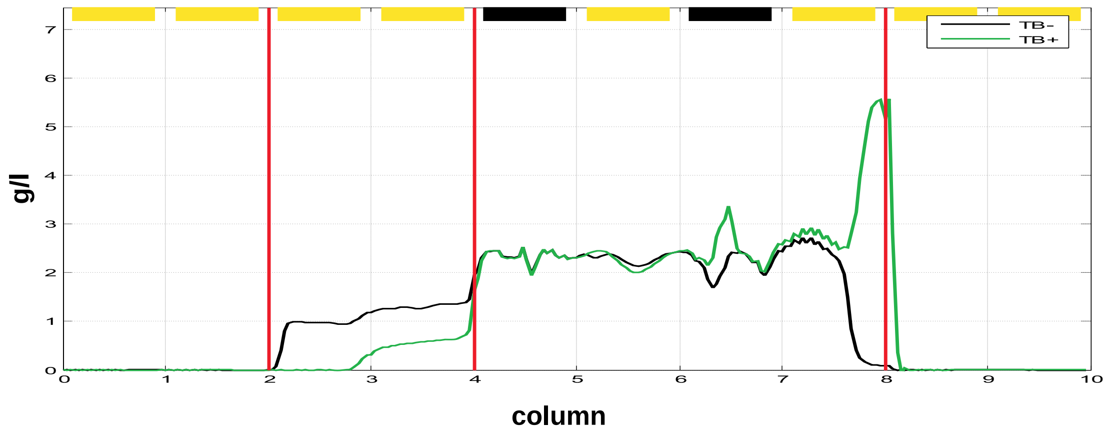

  - Disadvantage: complex valve shifting for simulated movement of reactors

# Racemization of Tröger's Base (TB): Profiles

Beginning of a period




End of a period



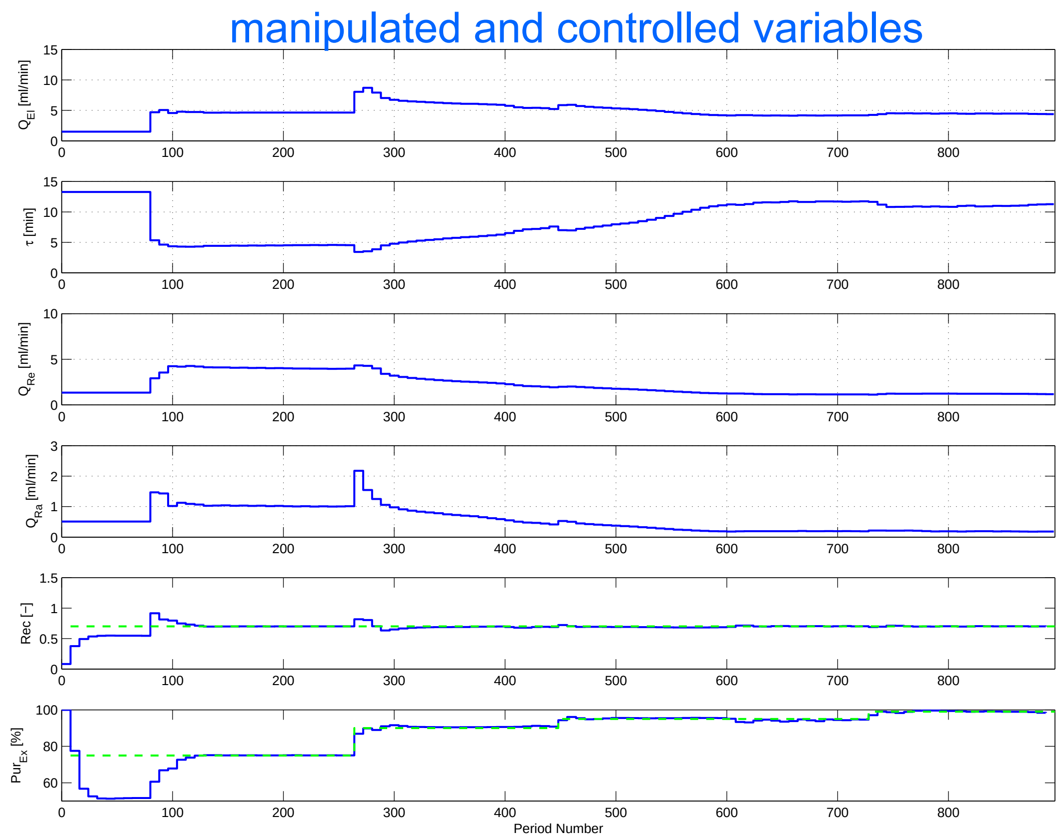

Eluent Extract Feed Raffinate

# Simulation of the optimizing controller

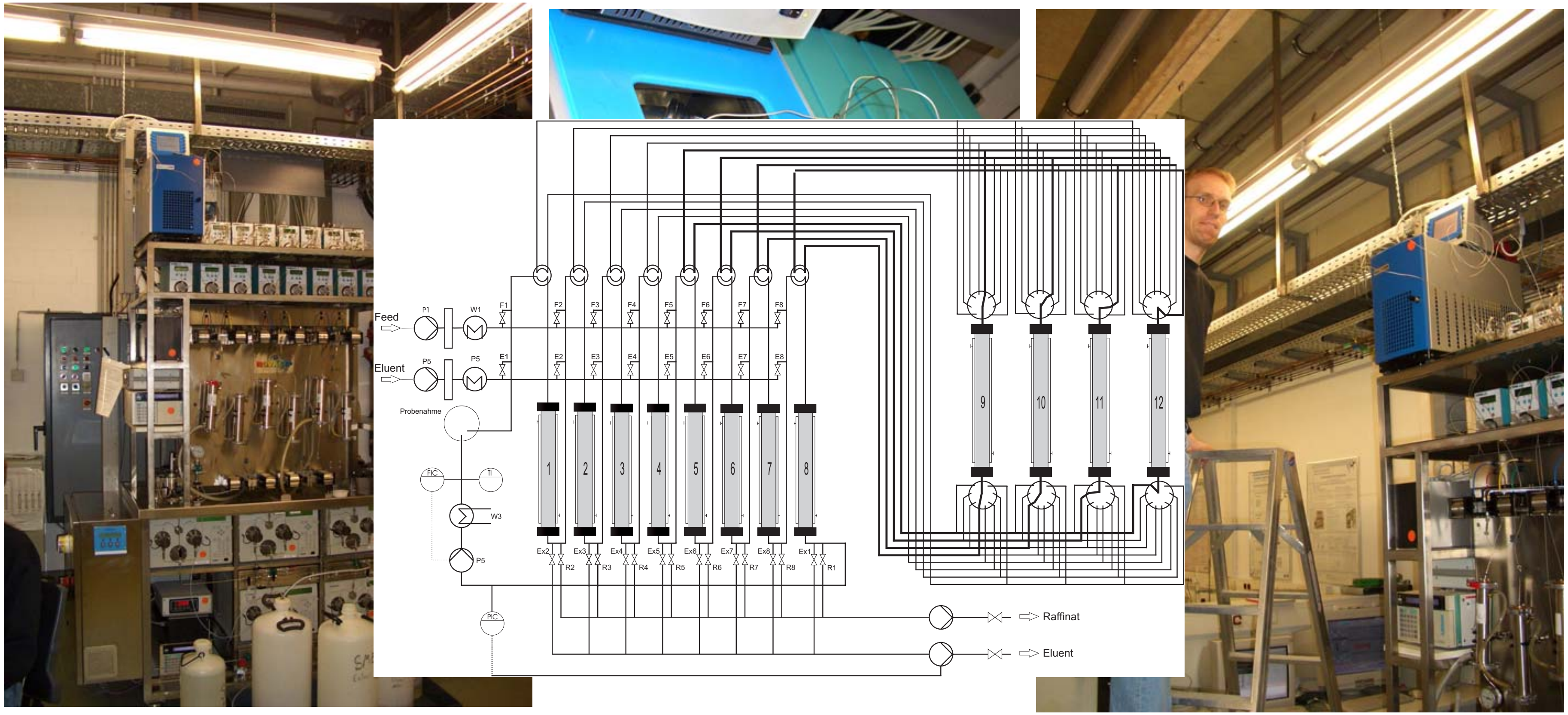
- Purity and recovery constraints enforced
- Plant/model mismatch

  ($H_A$ +10%, $H_B$ -5%)

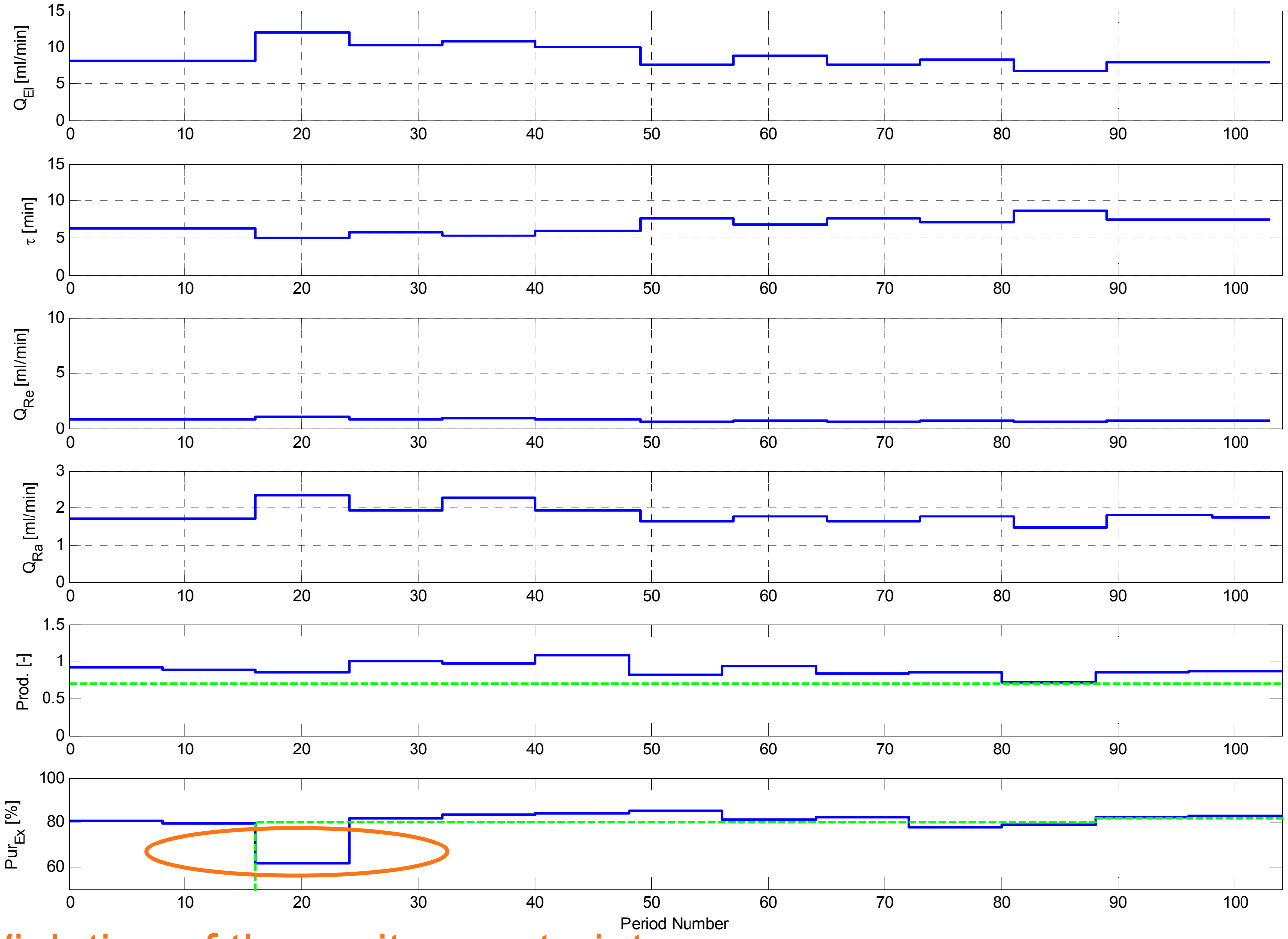
- Controller reduces the solvent consumption
- Satisfaction of process requirements



# Experimental Hashimoto SMB reactor



# Experimental results

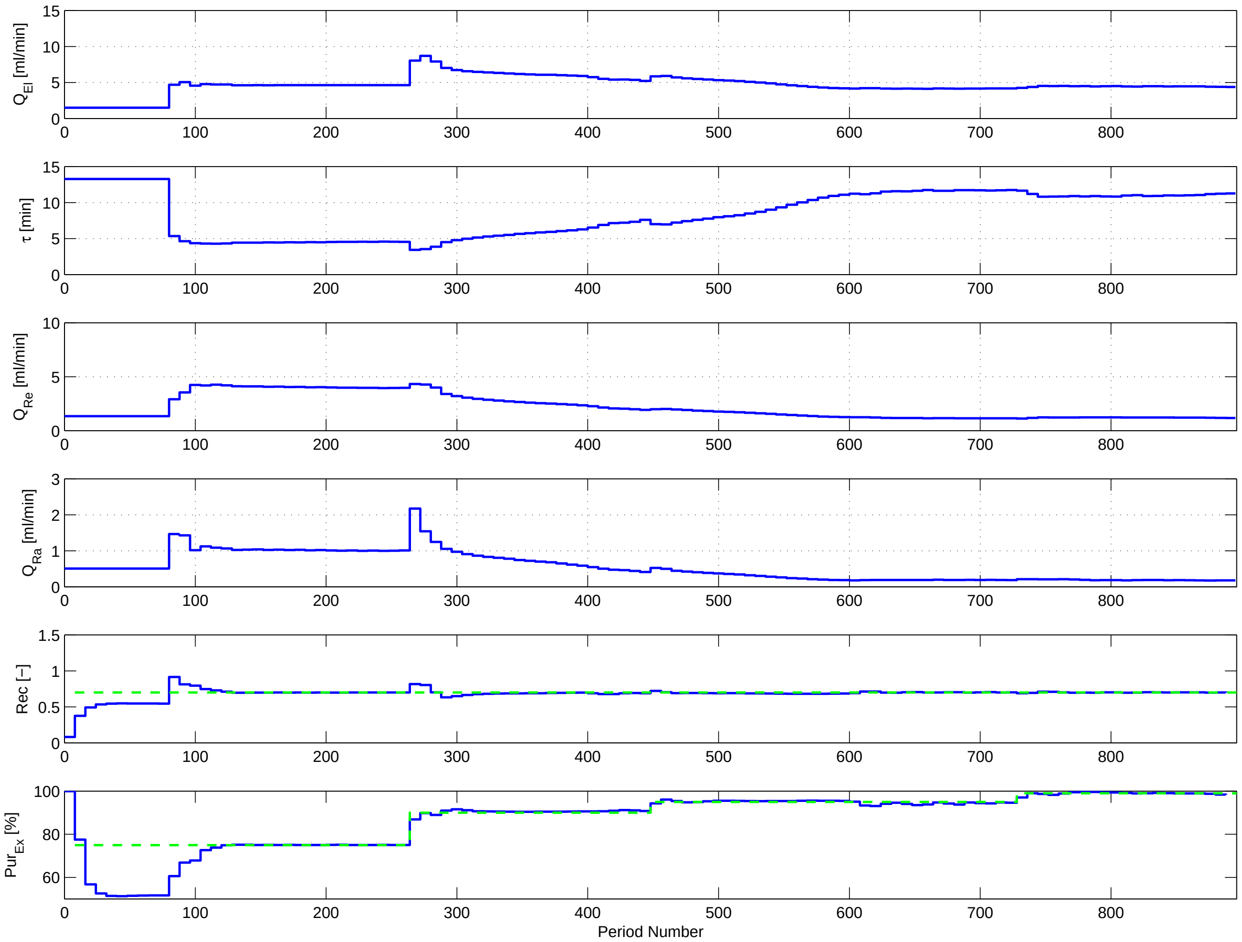



Violation of the purity constraint
because of a pump failure

# Conclusion from the case study

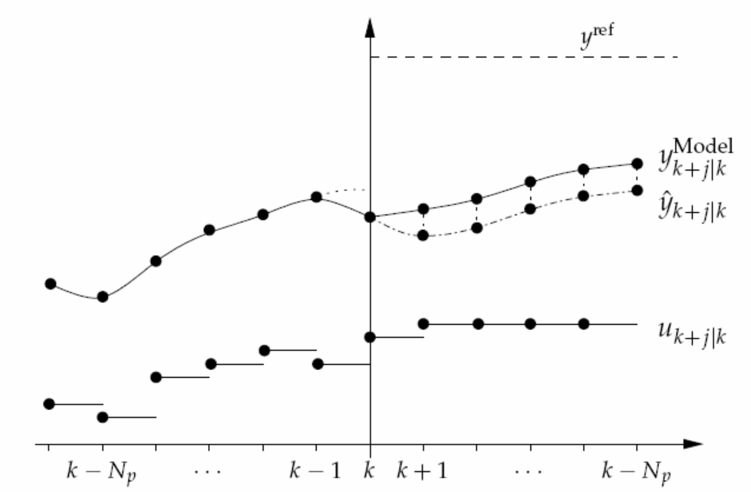
- Direct optimizing control is feasible!
- Numerical aspects:
  - General-purpose NLP algorithms for dynamic problems provide sufficient speed for slow processes (Biegler et al., Bock et al.)
  - Special algorithms taylored to online control for short response times (~ s) (Bock, Diehl et al.)
- **Main advantages**
  - Performance
  - Clear, transparent and natural formulation of the problem, few tuning parameters, no interaction of different layers
- **But there is a problem ...**

# Simulation of the optimizing controller

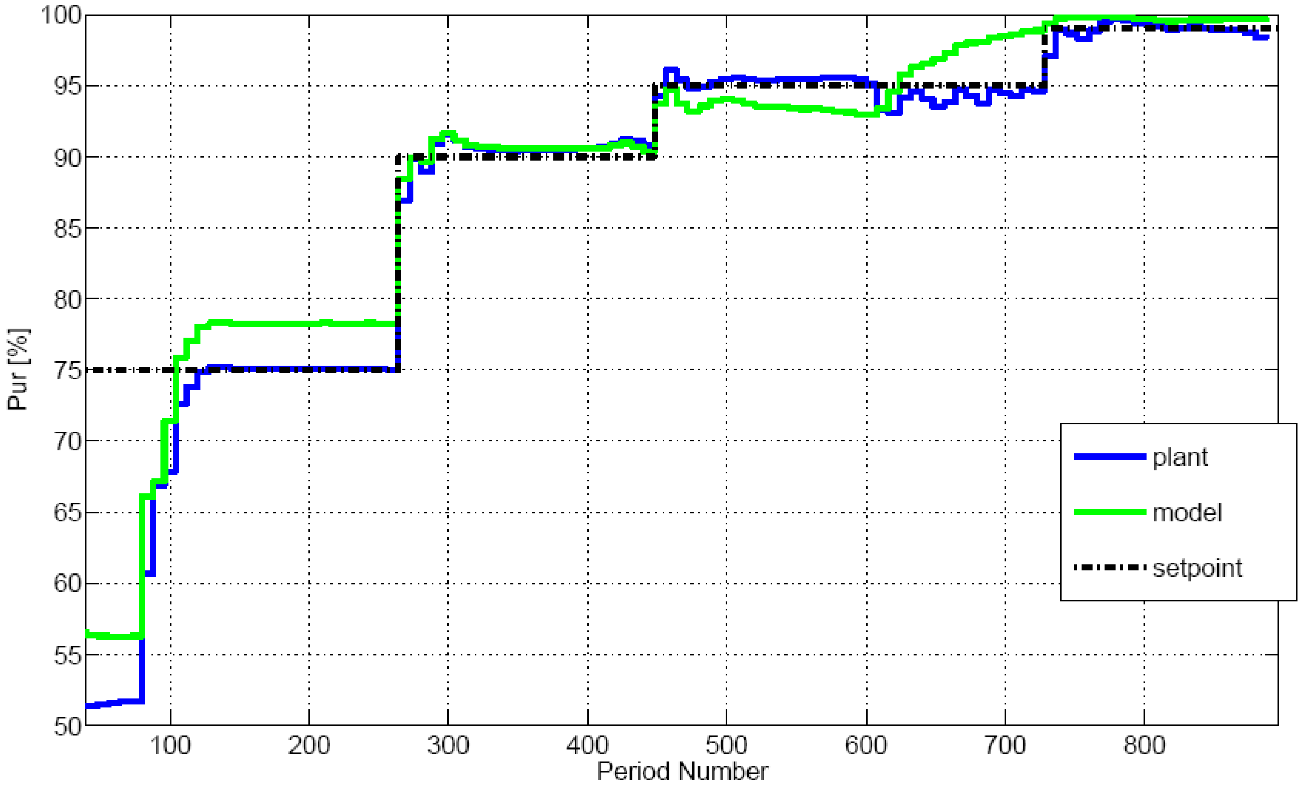


# NMPC and model accuracy

- The idea of (N)MPC is to solve a forward optimization problem repeatedly
- Quality of the solution depends on the model accuracy
- Feedback only enters by re-initialization and error correction (disturbance estimation) term
- Model errors are usually taken into account by a constant extrapolation of the error between prediction and observation



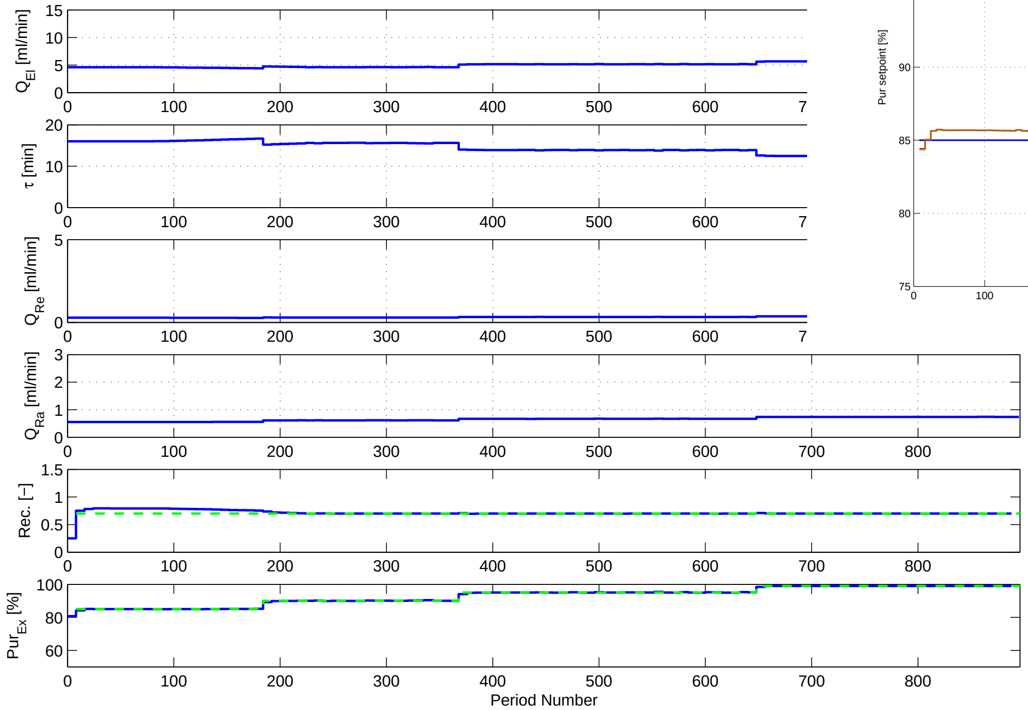
# Plant-model mismatch for Hashimoto SMB

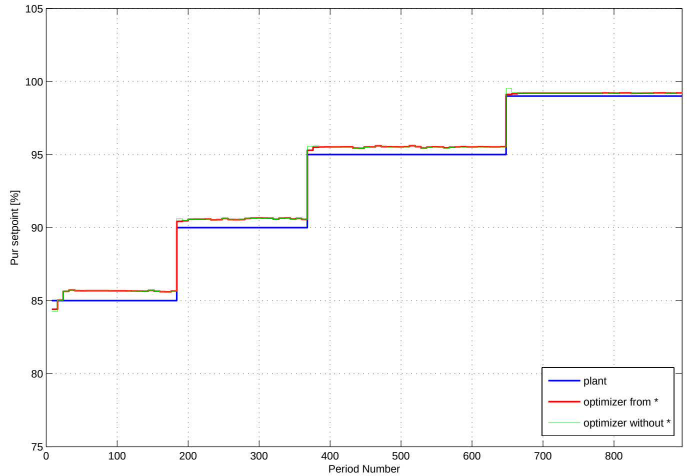


# Modification of the cost function

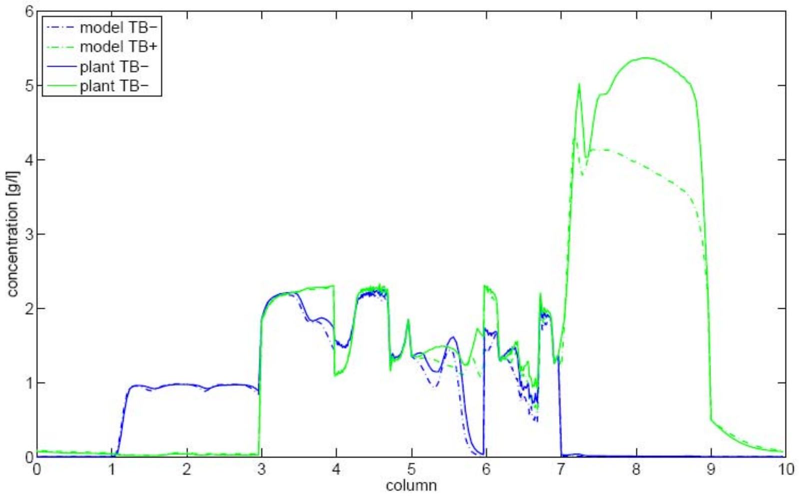
- Penalty term for breakthrough
- Same simulation experiment as before

manipulated and controlled vari



# Modification of the cost function



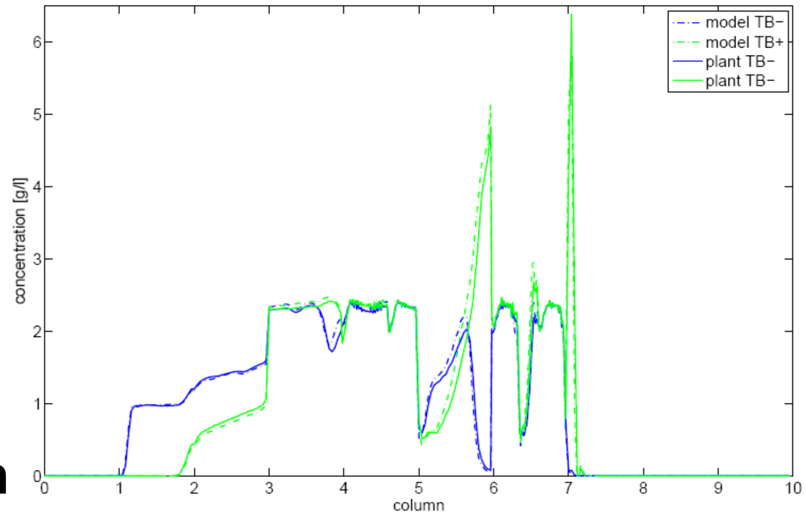

$$\min \sum_{j=k}^{k+H_p} (\Theta(j) + \Delta\beta_j{}^T R_j \Delta\beta_j)$$

**Solvent consumption optimal but not robust against model errors**

Modification of the cost function to avoid breakthough

$$\min \sum_{j=k}^{k+H_p} (\Theta(j) + \Delta\beta_j{}^T R_j \Delta\beta_j + \gamma \int_0^{T_j} Q_{re}(c_{A,re} + c_{B,re})dt$$

**Robust operating regime but increased solvent consumption**



# How to include robustness in optimizing control?

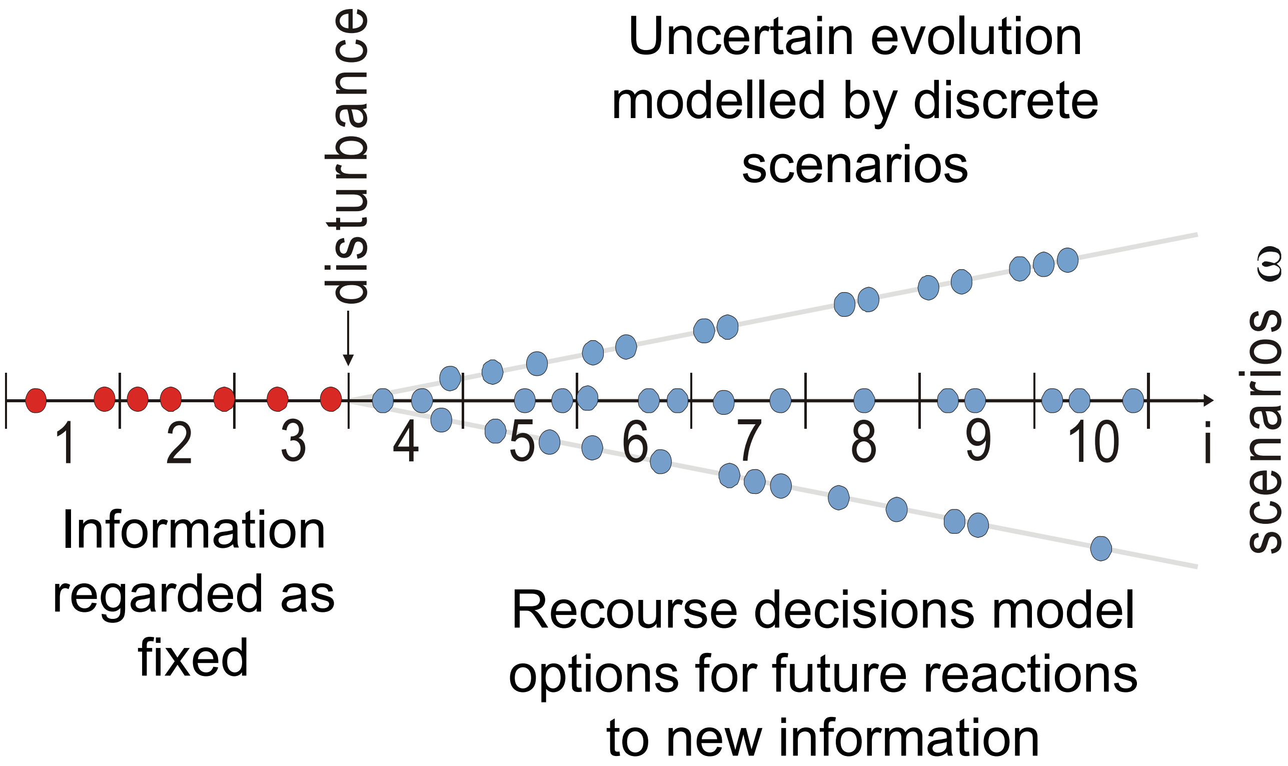
- Improve the quality of the model by parameter estimation
  - Numerical effort
  - Insufficient exitation during nominal operation
  - Structural plant-model mismatch

- Worst-case optimization for different models
  - Conservative approach, loss of performance
  - Does not reflect the existence of feedback

- **Two-stage optimization!**

# Two-stage decision problem

- Information and decision structure
  - First stage decisions **x** ≠ **f**(ω) (here and now)
  - Second stage decisions **y** = **f**(ω) (recourse)



# Two-stage formulation

$$\min_{\substack{u_k \cdots u_{k+N_p-1} \\ u_k^{*b} \cdots u_{k+N_p-1}^{*b}}} J_k = \min \left( \phi\left(y_{k+N_p|k}\right) + \sum_{j=0}^{N_p-1} \ell\left(y_{k+j|k}, u_{k+j|k}\right) \right)$$

$$\begin{aligned}
j = 1, \ldots, N_p \quad & b = 1, \ldots, B \\
y_{k+j} &\in \mathcal{Y} \\
u_{k+j-1} &\in \mathcal{U} \\
\Delta u_{k+j-1} &\in \Delta\mathcal{U} \\
0 &= y_{k+j} - f\left(\theta, y_{k+j-1}, \ldots, u_{k+j-1}, \ldots\right) \\
y_{k+j}^{*b} &\in \mathcal{Y} \\
u_{k+j-1}^{*b} &\in \mathcal{U} \\
\Delta u_{k+j-1}^{*b} &\in \Delta\mathcal{U} \\
0 &= y_{k+j}^{*b} - f\left(\theta^{*b}, y_{k+j-1}^{*b}, \ldots, u_{k+j-1}^{*b}, \ldots\right) \\
0 &= u_{k+i} - u_{k+i}^{*b} \qquad i = 0, \ldots, N_u' \\
y_{k+N_p} &\in W \ominus \mathcal{W}(\alpha)
\end{aligned}$$

# From control to optimal operations

- ✓ The gap between process control and process operations
- ✓ Control structure selection
- ✓ Real-time optimization
- ✓ En route from RTO to dynamic optimization
- ✓ Direct finite-horizon optimizing control
- ✓ Application example
- ✓ Plant-model mismatch
- **Summary, open issues, and future work**

# Summary

- The goal of process control is not set-point tracking but optimal performance!

  ⇨ direct finite horizon optimizing control
- **Main advantages:**
  - Performance
  - Clear, transparent and natural formulation of the problem, few tuning parameters, no interaction of different layers
- Feasible in real applications but requires engineering
- Numerically tractable due to advances in nonlinear dynamic optimization (Biegler et al., Bock et al.)
- Modelling and model accuracy are critical issues.
- Two-stage formulation leads to a uniform formulation of uncertainty-conscious online scheduling and control problems.

# Open issues

- **Modelling**
  - Dynamic models are expensive
  - Training simulators are often available, but models too complex
  - Grey box models, rigorous stationary nonlinear plus black-box linear dynamic models?
- **State estimation**
  - MHE formulations natural but computationally demanding
- **Stability**
  - Economic cost function may not be suitable to ensure stability

# More research topics

- Measurement-based optimization
- Constraint handling in case of infeasibility
- Integration of discrete degrees of freedom
- System archictecures – decentralization, coordination
- **Issues for real implementations:**
  - Operator interface
  - Plausibility checks, safety net
  - Reduction of complexity – à la NCO tracking?
- References


S. Engell, Feedback control for optimal process operation,*Journal of Process Control* 17 (2007), 203-219.

S. Engell, T. Scharf, and M. Völker: A Methodology for Control Structure Selection Based on Rigorous Process Models. 16th IFAC World Congress, Prague, 2005, Paper Code Tu-E14-TO/6

# The Team

- **Control Structure Selection:**

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- **SMB**:
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- **NMPC with multiple (NN) models:**
  Kai Dadhe

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- **... and to you for your kind attention!**